Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2025 – 01:33 pm GMT

PDB ID	:	9GYB
Title	:	Crystal structure of the recombinant CODH from Rhodopspirillum rubrum produced in Escherichia coli
Authors	:	Cavazza, C.; Contaldo, U.
Deposited on	:	2024-10-01
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

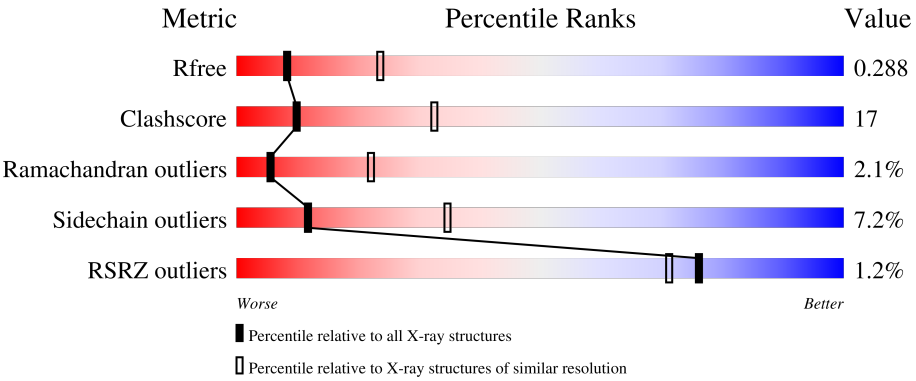
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	639	67% 27%
1	B	639	65% 30%
1	C	639	68% 27%
1	D	639	65% 30%
1	E	639	2% 51% 41%

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Mol	Chain	Length	Quality of chain
1	F	639	4% 47% 43% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	RQM	A	702	-	-	X	-
3	RQM	B	703	-	-	X	-
3	RQM	E	703	-	-	X	-
3	RQM	F	702	-	-	X	-

2 Entry composition (i)

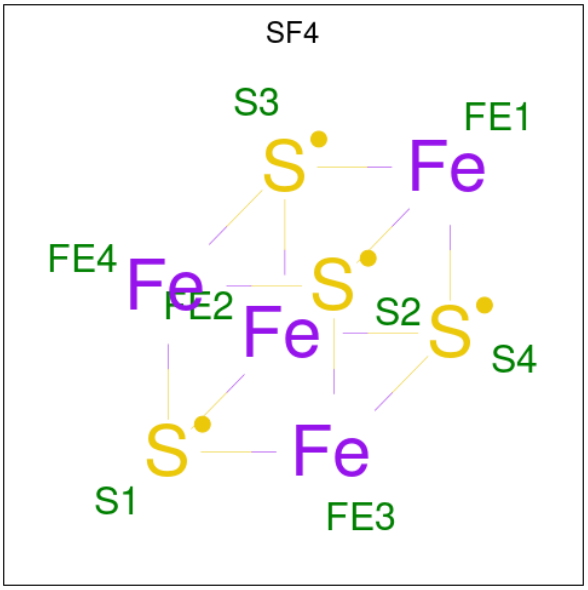
There are 4 unique types of molecules in this entry. The entry contains 27316 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Carbon monoxide dehydrogenase.

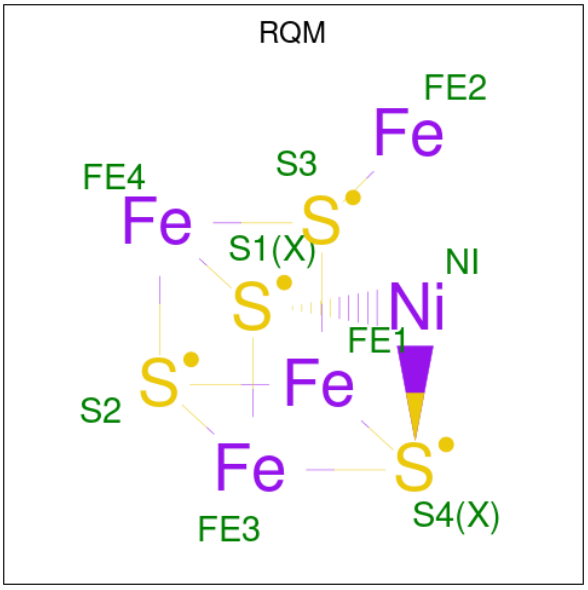
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	0	0
			4538	2845	804	855	34			
1	B	620	Total	C	N	O	S	0	0	0
			4538	2845	804	855	34			
1	C	620	Total	C	N	O	S	0	0	0
			4538	2845	804	855	34			
1	D	621	Total	C	N	O	S	0	0	0
			4547	2850	805	858	34			
1	E	617	Total	C	N	O	S	0	0	0
			4514	2830	800	851	33			
1	F	617	Total	C	N	O	S	0	0	0
			4514	2830	800	851	33			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0
2	E	1	Total Fe S 8 4 4	0	0
2	E	1	Total Fe S 8 4 4	0	0
2	F	1	Total Fe S 8 4 4	0	0

- Molecule 3 is Fe(3)-Ni(1)-S(4) cluster (three-letter code: RQM) (formula: Fe_4NiS_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe Ni S 9 4 1 4	0	0
3	B	1	Total Fe Ni S 9 4 1 4	0	0
3	C	1	Total Fe Ni S 9 4 1 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
3	E	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
3	F	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

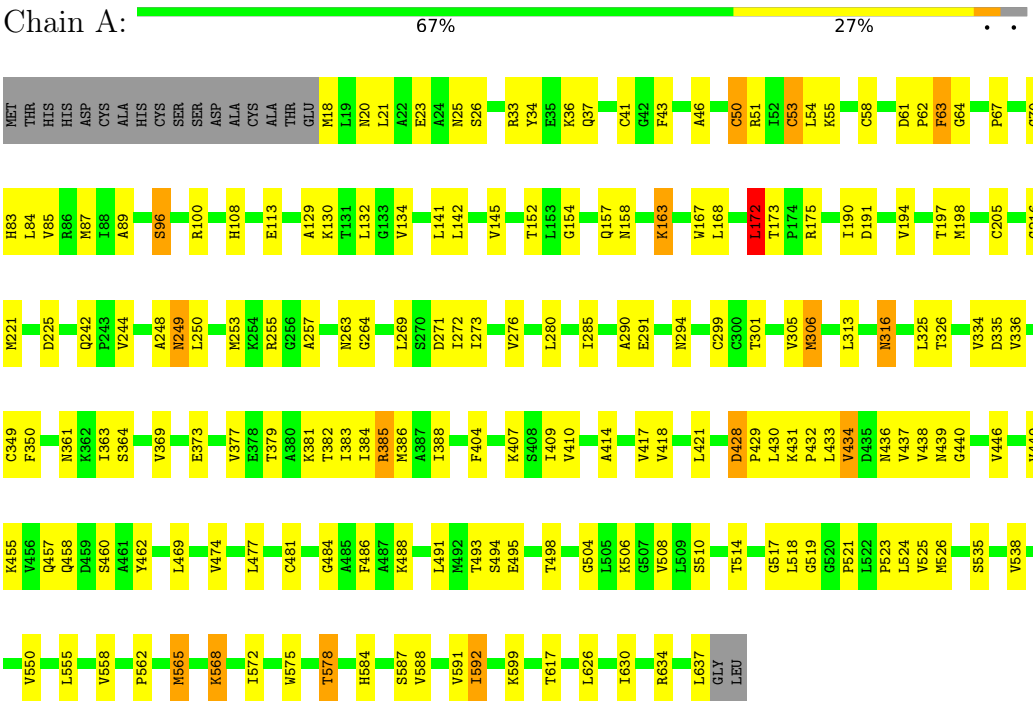
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Na	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

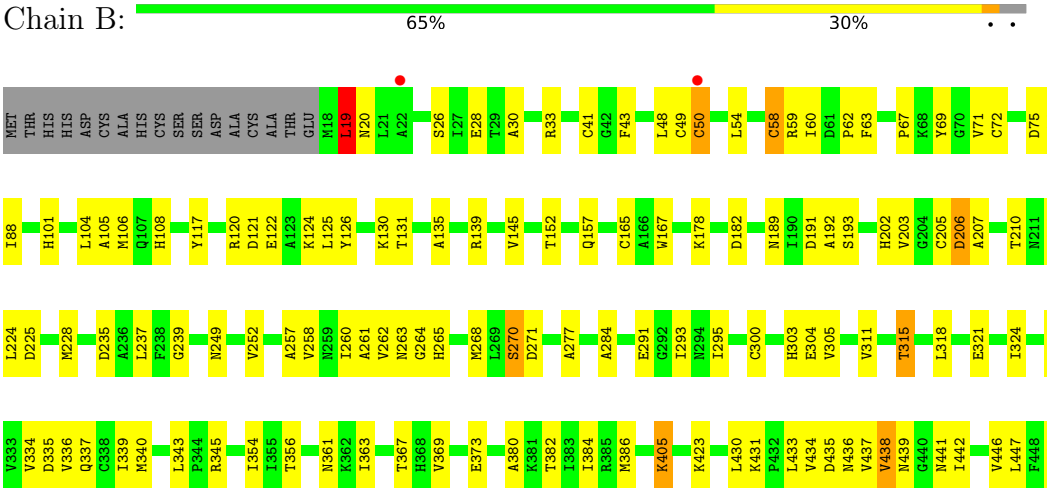
• Molecule 1: Carbon monoxide dehydrogenase

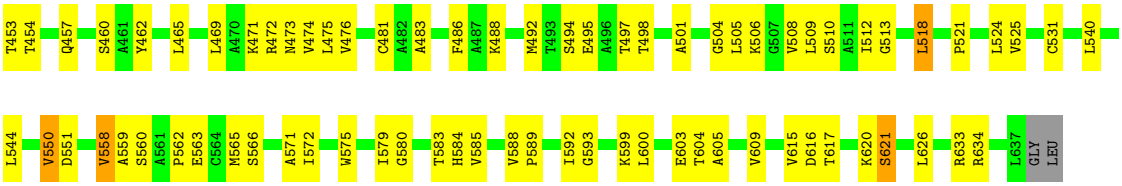
Chain A:



• Molecule 1: Carbon monoxide dehydrogenase

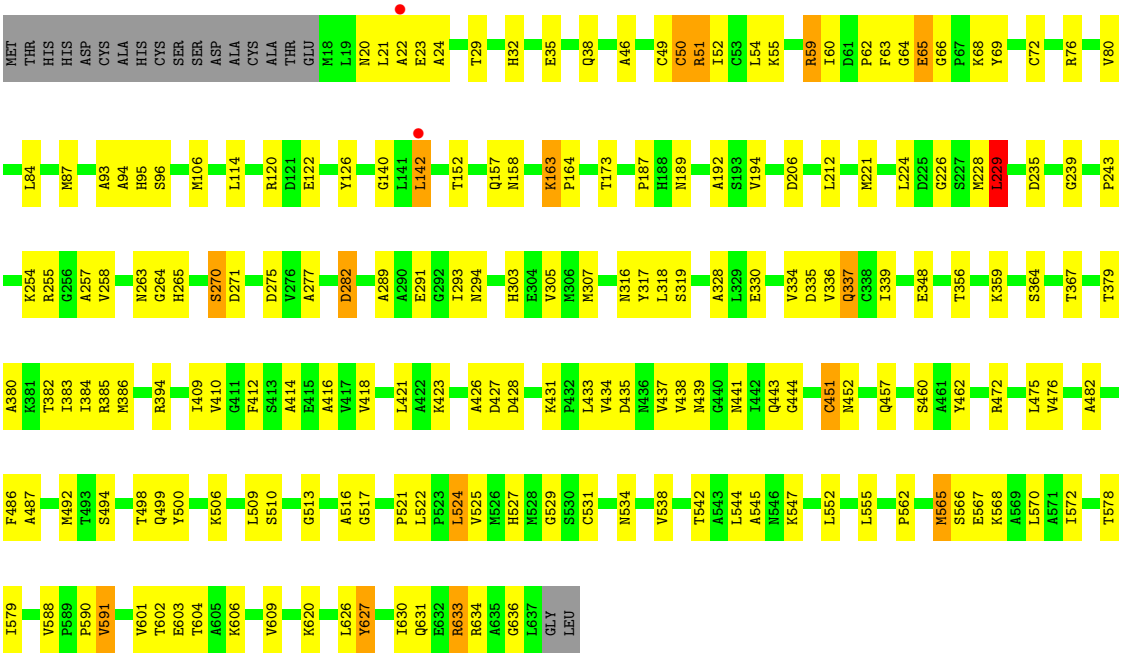
Chain B:





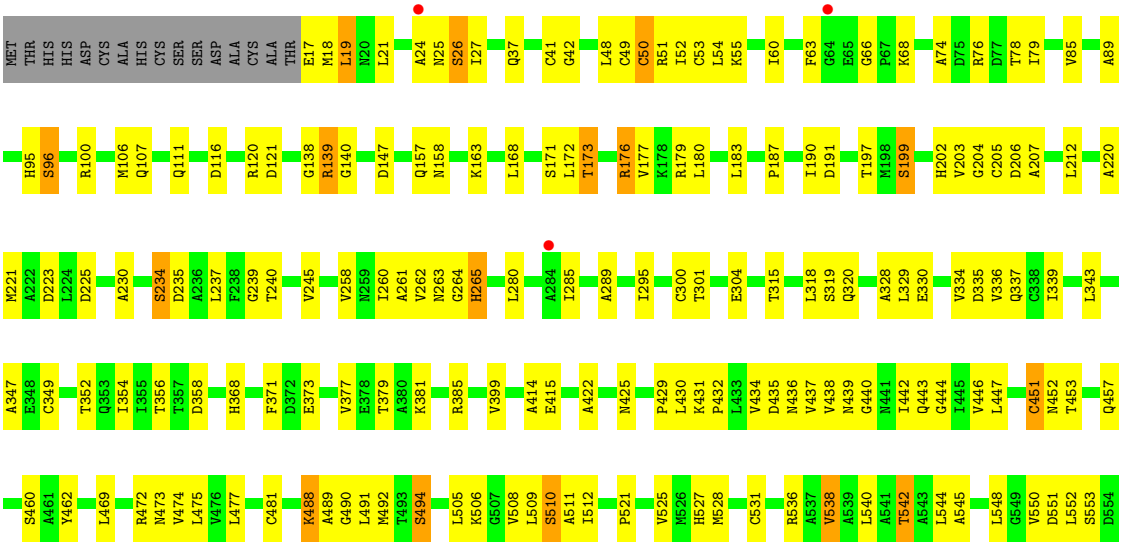
• Molecule 1: Carbon monoxide dehydrogenase

Chain C:



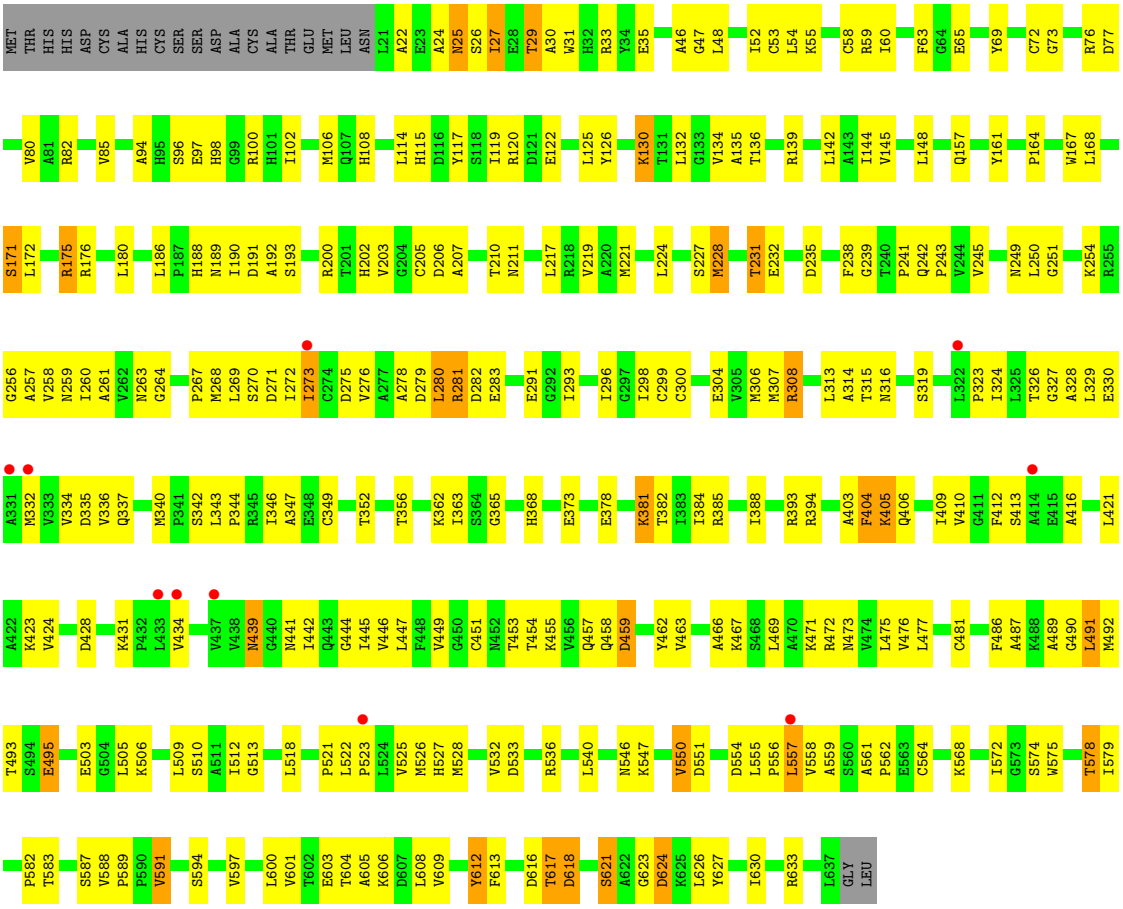
• Molecule 1: Carbon monoxide dehydrogenase

Chain D:



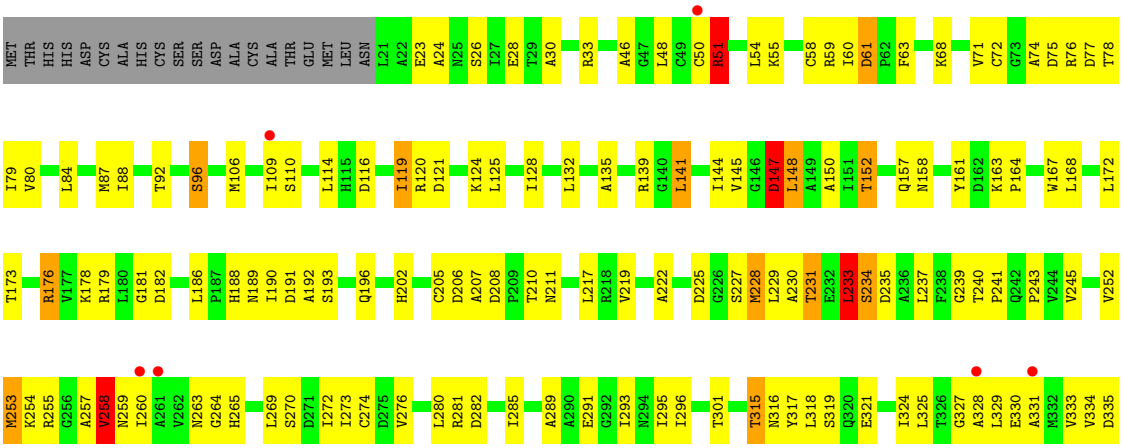
• Molecule 1: Carbon monoxide dehydrogenase

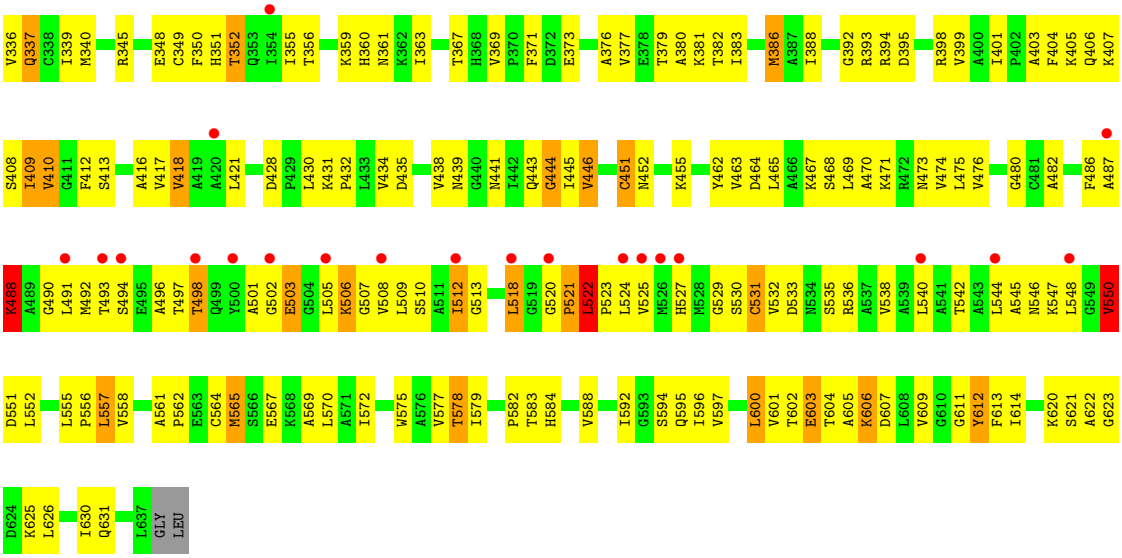
Chain E:



• Molecule 1: Carbon monoxide dehydrogenase

Chain F:




V336 Q337 C338 I339 M340 R345 E348 C349 F350 H351 T352 Q353 I354 I355 T356 K359 H360 N361 K362 I363 T367 H368 V369 P370 F371 D372 E373 A376 V377 E378 T379 A380 K381 T382 I383 M386 A387 I388 G392 R393 R394 D395 R398 V399 A400 I401 P402 A403 F404 K405 Q406 K407
S408 I409 V410 G411 F412 S413 A416 V417 V418 A419 A420 L421 D428 P429 L430 K431 P432 L433 V434 D435 V438 N439 G440 N441 I442 Q443 G444 I445 V446 C451 N452 K455 Y462 V463 D464 L465 A466 K467 S468 L469 A470 K471 R472 N473 V474 L475 V476 G480 C481 A482 F486 A487
K488 A489 G490 L491 M492 T493 S494 E495 A496 T497 T498 Q499 Y500 A501 G502 E503 G504 L505 K506 G507 V508 L509 S510 A511 I512 G513 L518 G519 G520 P521 L522 P523 L524 V525 M526 H527 M528 G529 S530 C531 V532 D533 N534 S535 R536 A537 V538 A539 L540 A541 T542 A543 L544 A545 N546 K547 L548 G549 V550
D551 L552 L555 P556 L557 V558 A561 P562 E563 C564 M565 S566 E567 K568 A569 L570 A571 I572 W575 A576 V577 T578 I579 P582 T583 H584 V588 I592 G593 S594 Q595 I596 V597 L600 V601 T602 E603 T604 A605 K606 D607 L608 V609 G610 G611 Y612 F613 I614 K620 S621 A622 G623
D624 K625 L626 I630 Q631 L637 GLY LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.45Å 200.57Å 116.37Å 90.00° 111.21° 90.00°	Depositor
Resolution (Å)	47.71 – 2.90 47.71 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.71-2.90) 99.1 (47.71-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.227 , 0.288 0.227 , 0.288	Depositor DCC
R_{free} test set	1100 reflections (1.27%)	wwPDB-VP
Wilson B-factor (Å^2)	81.6	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 61.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	27316	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, NA, RQM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/4611	0.52	1/6265 (0.0%)
1	B	0.25	0/4611	0.51	0/6265
1	C	0.25	0/4611	0.51	1/6265 (0.0%)
1	D	0.26	0/4620	0.52	0/6277
1	E	0.28	0/4587	0.57	0/6233
1	F	0.29	0/4587	0.61	4/6233 (0.1%)
All	All	0.27	0/27627	0.54	6/37538 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	3
1	F	0	1
All	All	0	4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	522	LEU	CB-CG-CD1	-6.78	99.48	111.00
1	F	233	LEU	CB-CG-CD2	-6.74	99.55	111.00
1	F	233	LEU	CB-CG-CD1	6.60	122.22	111.00
1	A	172	LEU	CA-CB-CG	6.33	129.86	115.30
1	C	229	LEU	CA-CB-CG	5.71	128.44	115.30
1	F	61	ASP	CB-CG-OD2	5.67	123.41	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	25	ASN	Peptide
1	E	423	LYS	Peptide
1	E	616	ASP	Peptide
1	F	348	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4538	0	4609	125	0
1	B	4538	0	4608	135	0
1	C	4538	0	4609	127	0
1	D	4547	0	4614	138	0
1	E	4514	0	4582	224	1
1	F	4514	0	4582	269	1
2	A	8	0	0	1	0
2	B	16	0	0	0	0
2	C	16	0	0	0	0
2	D	8	0	0	0	0
2	E	16	0	0	1	0
2	F	8	0	0	0	0
3	A	9	0	0	2	0
3	B	9	0	0	3	0
3	C	9	0	0	1	0
3	D	9	0	0	0	0
3	E	9	0	0	2	0
3	F	9	0	0	2	0
4	D	1	0	0	0	0
All	All	27316	0	27604	947	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (947) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:503:GLU:HA	1:F:506:LYS:HD2	1.46	0.95
1:F:106:MET:HA	1:F:109:ILE:HG12	1.47	0.93
1:F:318:LEU:HD13	1:F:452:ASN:HB3	1.52	0.89
1:F:230:ALA:O	1:F:234:SER:OG	1.93	0.85
1:F:497:THR:OG1	1:F:522:LEU:O	1.94	0.85
1:F:512:ILE:HG13	1:F:522:LEU:HD11	1.58	0.85
1:E:447:LEU:HD23	1:E:477:LEU:HB2	1.58	0.85
1:D:472:ARG:HB3	1:D:627:TYR:HE1	1.42	0.84
1:A:50:CYS:SG	1:A:51:ARG:N	2.52	0.82
1:A:63:PHE:HD1	1:A:64:GLY:H	1.27	0.81
1:A:20:ASN:ND2	1:A:249:ASN:OD1	2.15	0.80
1:D:95:HIS:HD1	1:D:223:ASP:CG	1.85	0.80
1:F:263:ASN:HB3	1:F:334:VAL:HG12	1.65	0.78
1:E:73:GLY:O	1:F:345:ARG:NH2	2.17	0.78
1:F:510:SER:HA	1:F:521:PRO:HA	1.65	0.78
1:A:73:GLY:O	1:B:345:ARG:NH2	2.17	0.78
1:B:437:VAL:O	1:B:634:ARG:NH2	2.18	0.77
1:C:620:LYS:NZ	1:E:349:CYS:HA	1.99	0.76
1:D:176:ARG:NH2	1:D:609:VAL:O	2.18	0.75
1:C:487:ALA:HA	1:C:492:MET:HG3	1.69	0.75
1:E:327:GLY:O	1:E:394:ARG:NH1	2.19	0.75
1:B:262:VAL:HG11	1:B:270:SER:HB3	1.69	0.74
1:E:490:GLY:O	1:E:492:MET:N	2.21	0.74
1:D:230:ALA:O	1:D:234:SER:OG	2.06	0.74
1:F:280:LEU:HD21	1:F:381:LYS:HG2	1.69	0.74
1:F:473:ASN:HA	1:F:505:LEU:HB2	1.70	0.74
1:A:46:ALA:HB2	1:D:63:PHE:HB3	1.69	0.73
1:E:69:TYR:HB2	1:F:33:ARG:HD2	1.70	0.73
1:E:54:LEU:HB2	1:F:565:MET:HA	1.70	0.73
1:B:446:VAL:HG23	1:B:558:VAL:HG12	1.70	0.73
1:A:373:GLU:OE2	1:A:373:GLU:N	2.20	0.73
1:E:356:THR:OG1	1:E:368:HIS:ND1	2.20	0.72
1:F:152:THR:HG1	1:F:167:TRP:HE1	0.74	0.72
1:B:585:VAL:HG11	1:B:589:PRO:HD3	1.72	0.72
1:F:438:VAL:O	1:F:439:ASN:ND2	2.23	0.72
1:F:190:ILE:HD11	1:F:225:ASP:HB3	1.70	0.72
1:D:139:ARG:NH2	1:D:147:ASP:OD2	2.23	0.71
1:E:210:THR:HG22	1:E:600:LEU:HD11	1.72	0.71
1:E:52:ILE:HG22	1:E:203:VAL:HG13	1.73	0.71
1:C:494:SER:HB3	1:C:521:PRO:HD2	1.73	0.71
1:F:445:ILE:HB	1:F:557:LEU:HD23	1.71	0.71
1:C:620:LYS:HZ1	1:E:349:CYS:HA	1.53	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:269:LEU:HD11	1:F:333:VAL:HG11	1.71	0.70
1:A:377:VAL:HG12	1:A:381:LYS:HE3	1.74	0.70
1:B:258:VAL:HB	1:B:293:ILE:HG22	1.72	0.70
1:E:555:LEU:O	1:E:557:LEU:N	2.25	0.70
1:E:356:THR:HG1	1:E:368:HIS:HD1	1.38	0.70
1:F:410:VAL:HG11	1:F:527:HIS:HB3	1.73	0.70
1:D:335:ASP:OD1	1:D:336:VAL:N	2.22	0.69
1:D:603:GLU:O	1:D:605:ALA:N	2.24	0.69
1:A:71:VAL:O	1:B:33:ARG:NH1	2.25	0.69
1:F:259:ASN:ND2	1:F:328:ALA:O	2.22	0.69
1:B:33:ARG:NH2	1:B:321:GLU:OE2	2.26	0.69
1:E:330:GLU:OE2	1:E:394:ARG:NH2	2.22	0.69
1:F:87:MET:HG2	1:F:567:GLU:HG2	1.74	0.69
1:F:276:VAL:HG22	1:F:280:LEU:HD23	1.75	0.69
1:F:167:TRP:CZ2	1:F:233:LEU:HD21	2.26	0.69
1:A:334:VAL:HB	1:A:339:ILE:HD13	1.75	0.68
1:A:428:ASP:HB3	1:A:431:LYS:HB2	1.73	0.68
1:F:501:ALA:HA	1:F:524:LEU:HD22	1.75	0.68
1:F:173:THR:HG23	1:F:176:ARG:HB2	1.74	0.68
1:F:603:GLU:O	1:F:605:ALA:N	2.26	0.68
1:E:337:GLN:HE22	1:E:568:LYS:HD3	1.59	0.68
1:C:54:LEU:HB2	1:D:565:MET:HA	1.76	0.67
1:C:443:GLN:HE22	1:C:631:GLN:HE21	1.40	0.67
1:A:550:VAL:HG11	1:A:637:LEU:HD21	1.76	0.67
1:E:251:GLY:HA3	1:E:405:LYS:HG3	1.76	0.67
1:D:265:HIS:NE2	1:D:568:LYS:HE2	2.09	0.67
1:E:235:ASP:HA	1:E:308:ARG:HH12	1.60	0.67
1:E:623:GLY:HA2	1:E:626:LEU:HB2	1.76	0.67
1:E:346:ILE:HD12	1:E:347:ALA:H	1.60	0.67
1:F:74:ALA:HB1	1:F:78:THR:HB	1.75	0.67
1:E:114:LEU:HD11	1:E:373:GLU:HB3	1.76	0.66
1:F:462:TYR:HE2	1:F:562:PRO:HD2	1.58	0.66
1:C:317:TYR:HB3	1:C:452:ASN:HB2	1.78	0.66
1:F:119:ILE:HG21	1:F:141:LEU:HD12	1.77	0.66
1:E:249:ASN:OD1	1:E:250:LEU:N	2.26	0.66
1:C:35:GLU:HA	1:C:38:GLN:HG2	1.76	0.66
1:D:475:LEU:HD13	1:D:509:LEU:HD11	1.77	0.65
1:B:284:ALA:HB2	1:B:293:ILE:HG23	1.77	0.65
1:E:97:GLU:OE1	1:E:100:ARG:NH1	2.29	0.65
1:F:167:TRP:CH2	1:F:233:LEU:HD21	2.31	0.65
1:D:472:ARG:HB3	1:D:627:TYR:CE1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:THR:HG23	1:A:542:THR:HG22	1.79	0.65
1:D:318:LEU:HD23	1:D:452:ASN:CB	2.27	0.65
1:B:616:ASP:OD2	1:B:621:SER:OG	2.14	0.65
1:F:513:GLY:HA3	1:F:522:LEU:HG	1.77	0.65
1:A:306:MET:HE1	1:A:313:LEU:HB2	1.78	0.65
1:E:82:ARG:NH2	2:E:701:SF4:S1	2.70	0.65
1:F:80:VAL:HG21	1:F:594:SER:HB3	1.78	0.65
1:D:508:VAL:HG12	1:D:512:ILE:HD11	1.79	0.64
1:E:293:ILE:HD13	1:E:384:ILE:HG21	1.79	0.64
1:C:500:TYR:HB2	1:C:524:LEU:HD11	1.78	0.64
1:F:110:SER:HB3	1:F:145:VAL:HG12	1.77	0.64
1:E:273:ILE:HA	1:E:276:VAL:HG22	1.79	0.64
1:F:147:ASP:O	1:F:150:ALA:N	2.31	0.64
1:F:577:VAL:HG21	1:F:613:PHE:HD2	1.61	0.64
1:A:449:VAL:HG11	1:A:572:ILE:HG21	1.78	0.64
1:A:477:LEU:HD23	1:A:526:MET:HB2	1.80	0.64
1:C:258:VAL:HG13	1:C:330:GLU:HG3	1.80	0.64
1:F:315:THR:OG1	1:F:316:ASN:N	2.31	0.64
1:C:257:ALA:HB2	1:C:291:GLU:HB2	1.79	0.63
1:F:417:VAL:HG11	1:F:540:LEU:HD11	1.80	0.63
1:E:601:VAL:O	1:E:613:PHE:HB2	1.97	0.63
1:F:229:LEU:O	1:F:233:LEU:HB2	1.99	0.63
1:B:603:GLU:O	1:B:605:ALA:N	2.30	0.63
1:D:469:LEU:HD12	1:D:474:VAL:HG21	1.81	0.63
1:A:36:LYS:HE3	1:B:67:PRO:HA	1.80	0.63
1:C:527:HIS:HD2	1:C:529:GLY:H	1.45	0.63
1:F:491:LEU:HD23	1:F:524:LEU:HD23	1.80	0.63
1:E:446:VAL:HG12	1:E:558:VAL:HG22	1.80	0.63
1:A:510:SER:HA	1:A:521:PRO:HA	1.79	0.63
1:E:451:CYS:HB3	3:E:703:RQM:S2	2.38	0.63
1:F:409:ILE:HD11	1:F:523:PRO:HG3	1.80	0.63
1:A:584:HIS:HB2	1:A:626:LEU:HD21	1.81	0.62
1:F:512:ILE:CG1	1:F:522:LEU:HD11	2.29	0.62
1:E:454:THR:HG21	1:F:71:VAL:HG11	1.82	0.62
1:F:227:SER:O	1:F:231:THR:OG1	2.17	0.62
1:F:328:ALA:HB2	1:F:399:VAL:HG13	1.80	0.62
1:A:62:PRO:HG3	1:D:63:PHE:HE1	1.62	0.62
1:A:498:THR:HG23	1:A:521:PRO:HG3	1.81	0.62
1:C:437:VAL:O	1:C:634:ARG:NH2	2.28	0.62
1:D:318:LEU:HD23	1:D:452:ASN:HB3	1.81	0.62
1:D:627:TYR:HE2	1:D:631:GLN:HE21	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:544:LEU:HD22	1:F:555:LEU:HD21	1.80	0.62
1:F:612:TYR:CE1	1:F:614:ILE:HD11	2.35	0.62
1:F:612:TYR:HE1	1:F:614:ILE:HD11	1.65	0.61
1:B:495:GLU:N	1:B:495:GLU:OE1	2.32	0.61
1:C:63:PHE:HB3	1:F:46:ALA:HB2	1.82	0.61
1:E:335:ASP:OD1	1:E:336:VAL:N	2.31	0.61
1:E:130:LYS:O	1:E:132:LEU:N	2.33	0.61
1:E:572:ILE:HA	1:E:575:TRP:NE1	2.16	0.61
1:F:125:LEU:HD23	1:F:141:LEU:HD13	1.81	0.61
1:F:546:ASN:O	1:F:548:LEU:N	2.33	0.61
1:E:164:PRO:HB3	1:E:186:LEU:HD23	1.81	0.61
1:B:481:CYS:HB2	3:B:703:RQM:S1	2.40	0.61
1:D:173:THR:HG23	1:D:176:ARG:HB2	1.82	0.61
1:D:280:LEU:HD21	1:D:385:ARG:HE	1.65	0.61
1:E:315:THR:OG1	1:E:319:SER:OG	2.16	0.61
1:E:603:GLU:O	1:E:605:ALA:N	2.26	0.61
1:A:157:GLN:HB2	1:B:157:GLN:HB2	1.82	0.60
1:D:66:GLY:O	1:D:68:LYS:NZ	2.34	0.60
1:E:492:MET:HG3	1:E:525:VAL:HG13	1.83	0.60
1:E:337:GLN:NE2	1:E:568:LYS:HD3	2.16	0.60
1:D:95:HIS:ND1	1:D:223:ASP:OD2	2.35	0.60
1:A:205:CYS:HA	1:B:361:ASN:HD21	1.67	0.60
1:D:437:VAL:O	1:D:634:ARG:NH2	2.33	0.60
1:F:410:VAL:HG22	1:F:412:PHE:CE1	2.35	0.60
1:F:509:LEU:O	1:F:522:LEU:HD12	2.02	0.60
1:A:409:ILE:HG23	1:A:523:PRO:HG3	1.84	0.60
1:E:442:ILE:HG22	1:E:505:LEU:HD12	1.84	0.60
1:E:449:VAL:HG23	1:E:561:ALA:HB2	1.83	0.60
1:B:105:ALA:O	1:B:108:HIS:N	2.35	0.60
1:F:48:LEU:HB3	1:F:60:ILE:HB	1.84	0.60
1:F:410:VAL:HG11	1:F:527:HIS:CD2	2.37	0.59
1:B:252:VAL:HG12	1:B:405:LYS:HG3	1.85	0.59
1:F:418:VAL:HA	1:F:421:LEU:HB2	1.85	0.59
1:C:226:GLY:HA2	1:C:229:LEU:HD22	1.83	0.59
1:C:426:ALA:O	1:C:427:ASP:HB2	2.01	0.59
1:E:98:HIS:HD1	1:E:532:VAL:HG21	1.67	0.59
1:E:135:ALA:HB3	1:E:139:ARG:HD2	1.84	0.59
1:E:239:GLY:O	1:E:308:ARG:NH1	2.33	0.59
1:E:119:ILE:HD13	1:E:125:LEU:HD13	1.83	0.59
1:E:559:ALA:HB3	1:E:583:THR:HG23	1.84	0.59
1:E:27:ILE:HG21	1:E:346:ILE:HD13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:LEU:HA	1:E:145:VAL:HG12	1.84	0.59
1:F:181:GLY:HA2	1:F:186:LEU:HD13	1.84	0.59
1:F:410:VAL:HG22	1:F:412:PHE:HE1	1.68	0.59
1:D:492:MET:HG2	1:D:525:VAL:HG22	1.85	0.59
1:E:462:TYR:CE1	1:E:562:PRO:HD2	2.38	0.59
1:A:336:VAL:HA	1:A:361:ASN:HD22	1.68	0.59
1:E:431:LYS:HA	1:E:434:VAL:HG12	1.85	0.59
1:E:475:LEU:HD22	1:E:476:VAL:H	1.66	0.59
1:A:347:ALA:O	1:A:349:CYS:N	2.36	0.58
1:E:336:VAL:HG12	1:E:337:GLN:HG3	1.85	0.58
1:E:329:LEU:O	1:E:352:THR:OG1	2.19	0.58
1:E:558:VAL:HG21	1:E:626:LEU:HD22	1.84	0.58
1:F:259:ASN:HB2	1:F:296:ILE:HD11	1.84	0.58
1:A:572:ILE:HA	1:A:575:TRP:NE1	2.17	0.58
1:D:17:GLU:N	1:D:457:GLN:HG3	2.18	0.58
1:F:444:GLY:HA3	1:F:630:ILE:HD12	1.84	0.58
1:C:49:CYS:O	1:D:51:ARG:NH1	2.35	0.58
1:D:48:LEU:HD21	1:D:593:GLY:HA3	1.86	0.58
1:A:491:LEU:HD23	1:A:524:LEU:HD23	1.83	0.58
1:B:300:CYS:HA	1:B:303:HIS:HD2	1.69	0.58
1:B:451:CYS:SG	1:B:565:MET:HG3	2.44	0.58
1:C:264:GLY:HA3	1:C:335:ASP:OD1	2.02	0.58
1:E:231:THR:HG21	1:E:533:ASP:HA	1.86	0.58
1:F:577:VAL:HG21	1:F:613:PHE:CD2	2.39	0.58
1:A:46:ALA:HA	1:A:592:ILE:HG13	1.86	0.58
1:A:257:ALA:HB2	1:A:291:GLU:HB2	1.85	0.58
1:B:50:CYS:SG	1:B:58:CYS:SG	3.00	0.58
1:B:125:LEU:HD11	1:B:145:VAL:HG22	1.86	0.58
1:E:202:HIS:HB3	1:E:205:CYS:SG	2.44	0.58
1:E:279:ASP:O	1:E:281:ARG:NH1	2.36	0.58
1:F:245:VAL:HG13	1:F:409:ILE:HG22	1.83	0.58
1:B:339:ILE:HD12	1:B:363:ILE:HD11	1.86	0.58
1:E:328:ALA:HA	1:E:394:ARG:NH1	2.18	0.58
1:E:445:ILE:HG22	1:E:475:LEU:HB3	1.83	0.58
1:B:335:ASP:OD1	1:B:336:VAL:N	2.33	0.58
1:F:28:GLU:H	1:F:28:GLU:CD	2.07	0.58
1:B:20:ASN:ND2	1:B:249:ASN:OD1	2.37	0.58
1:E:281:ARG:H	1:E:281:ARG:HD3	1.69	0.58
1:F:463:VAL:HG13	1:F:491:LEU:HD11	1.85	0.57
1:C:120:ARG:NH2	1:C:275:ASP:OD2	2.36	0.57
1:E:587:SER:O	1:F:54:LEU:HD11	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:CYS:HA	1:D:481:CYS:HB2	1.87	0.57
1:F:241:PRO:HG2	1:F:413:SER:HB3	1.85	0.57
1:F:336:VAL:HA	1:F:361:ASN:ND2	2.19	0.57
1:C:439:ASN:ND2	1:C:441:ASN:OD1	2.37	0.57
1:D:260:ILE:HB	1:D:295:ILE:HD13	1.86	0.57
1:E:340:MET:O	1:E:343:LEU:HG	2.04	0.57
1:F:421:LEU:HD22	1:F:432:PRO:HG2	1.87	0.57
1:F:606:LYS:NZ	1:F:607:ASP:OD2	2.35	0.57
1:A:498:THR:HA	1:A:506:LYS:HD3	1.86	0.57
1:F:339:ILE:HD11	1:F:363:ILE:HD11	1.87	0.57
1:C:60:ILE:HG21	1:C:76:ARG:HB3	1.87	0.57
1:E:259:ASN:N	1:E:330:GLU:OE1	2.38	0.57
1:F:124:LYS:NZ	1:F:240:THR:OG1	2.27	0.57
1:F:230:ALA:HB3	1:F:532:VAL:HG11	1.86	0.57
1:A:108:HIS:HB3	1:A:113:GLU:HB2	1.86	0.57
1:D:560:SER:HB2	1:D:626:LEU:HD11	1.87	0.56
1:A:285:ILE:HG22	1:A:290:ALA:HA	1.87	0.56
1:B:224:LEU:O	1:B:228:MET:HG3	2.05	0.56
1:B:497:THR:HA	1:B:524:LEU:HD13	1.86	0.56
1:E:621:SER:HA	1:E:624:ASP:HB2	1.86	0.56
1:F:121:ASP:HB2	1:F:239:GLY:HA2	1.86	0.56
1:F:501:ALA:CA	1:F:524:LEU:HD22	2.34	0.56
1:C:95:HIS:HE1	1:C:572:ILE:HD11	1.71	0.56
1:C:423:LYS:NZ	1:C:516:ALA:HA	2.20	0.56
1:E:55:LYS:HA	1:F:455:LYS:HE3	1.87	0.56
1:E:227:SER:O	1:E:231:THR:OG1	2.24	0.56
1:F:233:LEU:O	1:F:237:LEU:HD12	2.06	0.56
1:E:96:SER:HB2	1:E:190:ILE:HG21	1.87	0.56
1:F:28:GLU:N	1:F:28:GLU:OE1	2.37	0.56
1:F:79:ILE:HD12	1:F:79:ILE:H	1.71	0.56
1:B:124:LYS:NZ	1:B:235:ASP:OD2	2.36	0.56
1:B:473:ASN:HA	1:B:505:LEU:HB2	1.88	0.56
1:C:255:ARG:O	1:C:394:ARG:NH2	2.38	0.56
1:E:189:ASN:HB3	1:E:192:ALA:HB3	1.88	0.56
1:D:443:GLN:OE1	1:D:631:GLN:NE2	2.37	0.56
1:F:408:SER:HB3	1:F:492:MET:HG2	1.87	0.56
1:E:241:PRO:HD2	1:E:413:SER:HB3	1.86	0.56
1:C:22:ALA:O	1:C:24:ALA:N	2.39	0.56
1:F:333:VAL:HG22	1:F:355:ILE:HD11	1.88	0.56
1:F:428:ASP:HB3	1:F:431:LYS:HB2	1.88	0.56
1:B:261:ALA:HB3	1:B:332:MET:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASN:HB3	1:A:334:VAL:HG12	1.87	0.56
1:D:414:ALA:HA	1:D:540:LEU:HD11	1.88	0.56
1:E:463:VAL:HG23	1:E:491:LEU:HD11	1.87	0.56
1:D:168:LEU:HG	1:D:225:ASP:HB2	1.87	0.55
1:D:442:ILE:HD11	1:D:475:LEU:H	1.71	0.55
1:F:54:LEU:HD13	1:F:54:LEU:O	2.06	0.55
1:F:476:VAL:HG12	1:F:525:VAL:HG13	1.87	0.55
1:C:472:ARG:HD2	1:C:627:TYR:CD2	2.42	0.55
1:E:202:HIS:CE1	1:F:567:GLU:HB2	2.42	0.55
1:C:443:GLN:HE22	1:C:631:GLN:NE2	2.04	0.55
1:F:401:ILE:HD12	1:F:401:ILE:H	1.71	0.55
1:B:580:GLY:O	1:B:633:ARG:NH2	2.37	0.55
1:E:481:CYS:N	3:E:703:RQM:S1	2.65	0.55
1:F:469:LEU:HD22	1:F:474:VAL:HG21	1.88	0.55
1:C:498:THR:HA	1:C:506:LYS:HD3	1.87	0.55
1:D:96:SER:HB2	1:D:190:ILE:HG21	1.89	0.55
1:B:441:ASN:HD22	1:B:504:GLY:HA2	1.72	0.55
1:B:501:ALA:HB1	1:B:505:LEU:HD12	1.87	0.55
1:C:330:GLU:OE2	1:C:394:ARG:NH1	2.38	0.55
1:D:265:HIS:CD2	1:D:568:LYS:HZ3	2.25	0.55
1:D:572:ILE:HA	1:D:575:TRP:NE1	2.22	0.55
1:F:124:LYS:HE3	1:F:235:ASP:HB3	1.89	0.55
1:F:555:LEU:O	1:F:557:LEU:N	2.40	0.55
1:F:561:ALA:HB1	1:F:564:CYS:HB3	1.89	0.55
1:E:243:PRO:HD3	1:E:416:ALA:HB1	1.89	0.55
1:B:462:TYR:CE1	1:B:562:PRO:HD2	2.41	0.55
1:F:409:ILE:H	1:F:493:THR:HA	1.72	0.55
1:A:62:PRO:HG3	1:D:63:PHE:CE1	2.41	0.54
1:F:583:THR:O	1:F:613:PHE:HB2	2.07	0.54
1:E:421:LEU:HA	1:E:512:ILE:HD11	1.90	0.54
1:F:258:VAL:HG11	1:F:388:ILE:HG22	1.88	0.54
1:B:501:ALA:HB3	1:B:506:LYS:HB2	1.88	0.54
1:C:570:LEU:HD21	1:D:54:LEU:HD11	1.89	0.54
1:E:167:TRP:O	1:E:171:SER:OG	2.25	0.54
1:B:433:LEU:HD23	1:B:544:LEU:HD13	1.90	0.54
1:D:138:GLY:O	1:D:140:GLY:N	2.41	0.54
1:F:225:ASP:O	1:F:229:LEU:HD23	2.07	0.54
1:F:235:ASP:OD2	1:F:536:ARG:NH1	2.30	0.54
1:C:62:PRO:HG3	1:F:63:PHE:HE2	1.73	0.54
1:F:270:SER:HA	1:F:273:ILE:HG13	1.90	0.54
1:B:62:PRO:HA	1:B:76:ARG:HH21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ALA:HB2	1:C:194:VAL:HG21	1.89	0.54
1:D:300:CYS:O	1:D:304:GLU:HG2	2.08	0.54
1:F:487:ALA:O	1:F:488:LYS:HB3	2.08	0.54
1:F:75:ASP:O	1:F:78:THR:N	2.41	0.54
1:F:330:GLU:OE2	1:F:394:ARG:NH2	2.33	0.54
1:A:89:ALA:HB2	1:A:197:THR:HG21	1.90	0.54
1:A:301:THR:O	1:A:305:VAL:HG22	2.07	0.54
1:F:264:GLY:HA3	1:F:335:ASP:OD1	2.08	0.54
1:A:363:ILE:HA	1:B:207:ALA:HB3	1.89	0.53
1:D:202:HIS:HB3	1:D:205:CYS:SG	2.47	0.53
1:D:561:ALA:HB1	1:D:564:CYS:HB3	1.89	0.53
1:E:224:LEU:HD22	1:E:579:ILE:HD11	1.90	0.53
1:A:439:ASN:OD1	1:A:440:GLY:N	2.42	0.53
1:A:565:MET:HA	1:B:54:LEU:HB2	1.89	0.53
1:B:206:ASP:HB3	1:B:212:LEU:HD21	1.91	0.53
1:B:324:ILE:HD11	1:B:354:ILE:HD11	1.89	0.53
1:E:492:MET:SD	1:E:527:HIS:HB2	2.48	0.53
1:E:627:TYR:HA	1:E:630:ILE:HG22	1.91	0.53
1:F:334:VAL:HG22	1:F:355:ILE:O	2.08	0.53
1:B:210:THR:HA	1:B:600:LEU:HD11	1.89	0.53
1:F:148:LEU:O	1:F:152:THR:HB	2.09	0.53
1:A:462:TYR:CE1	1:A:562:PRO:HD2	2.44	0.53
1:A:336:VAL:HA	1:A:361:ASN:ND2	2.23	0.53
1:E:114:LEU:HD12	1:E:117:TYR:CD1	2.43	0.53
1:B:121:ASP:HB2	1:B:239:GLY:HA2	1.91	0.53
1:B:117:TYR:OH	1:B:268:MET:O	2.25	0.53
1:B:270:SER:HB2	1:B:305:VAL:HG11	1.90	0.53
1:B:451:CYS:HA	3:B:703:RQM:S1	2.49	0.53
1:B:584:HIS:HB2	1:B:626:LEU:HD21	1.90	0.53
1:C:80:VAL:O	1:C:84:LEU:HD23	2.09	0.53
1:D:315:THR:HG21	1:D:320:GLN:HA	1.91	0.53
1:D:462:TYR:CE1	1:D:562:PRO:HD2	2.43	0.53
1:D:473:ASN:HA	1:D:505:LEU:HB2	1.91	0.53
1:E:473:ASN:HA	1:E:505:LEU:HB2	1.90	0.53
1:E:513:GLY:O	1:E:518:LEU:HB2	2.09	0.53
1:F:451:CYS:HB2	3:F:702:RQM:S2	2.36	0.53
1:A:141:LEU:O	1:A:145:VAL:HG12	2.08	0.53
1:B:566:SER:OG	3:B:703:RQM:S4	2.61	0.53
1:B:189:ASN:HB3	1:B:192:ALA:HB3	1.90	0.53
1:E:362:LYS:HD2	1:E:363:ILE:N	2.24	0.53
1:A:248:ALA:HB1	1:A:488:LYS:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:439:ASN:OD1	1:D:440:GLY:N	2.42	0.52
1:F:176:ARG:NH2	1:F:609:VAL:O	2.41	0.52
1:B:202:HIS:HB3	1:B:205:CYS:SG	2.49	0.52
1:C:157:GLN:HB2	1:D:157:GLN:HB2	1.92	0.52
1:D:50:CYS:HB2	1:D:79:ILE:HG23	1.91	0.52
1:A:64:GLY:HA3	1:D:42:GLY:HA2	1.91	0.52
1:B:508:VAL:O	1:B:512:ILE:HD12	2.10	0.52
1:C:69:TYR:O	1:D:37:GLN:NE2	2.43	0.52
1:C:544:LEU:HD23	1:C:555:LEU:HD13	1.90	0.52
1:D:446:VAL:HG23	1:D:558:VAL:HG23	1.91	0.52
1:E:256:GLY:C	1:E:291:GLU:HG3	2.30	0.52
1:D:53:CYS:HB3	1:D:203:VAL:CG2	2.39	0.52
1:F:116:ASP:OD2	1:F:376:ALA:N	2.40	0.52
1:F:260:ILE:HD13	1:F:331:ALA:HB3	1.91	0.52
1:E:477:LEU:HA	1:E:525:VAL:O	2.09	0.52
1:F:75:ASP:O	1:F:77:ASP:N	2.43	0.52
1:F:584:HIS:HB2	1:F:626:LEU:HD21	1.92	0.52
1:B:48:LEU:HB3	1:B:60:ILE:HB	1.92	0.52
1:B:572:ILE:HA	1:B:575:TRP:NE1	2.25	0.52
1:E:250:LEU:HB2	1:E:404:PHE:HD2	1.74	0.52
1:F:258:VAL:HG21	1:F:293:ILE:HD13	1.92	0.52
1:A:96:SER:HB2	1:A:190:ILE:HG21	1.92	0.51
1:E:503:GLU:HA	1:E:506:LYS:HG2	1.93	0.51
1:C:527:HIS:CD2	1:C:529:GLY:H	2.26	0.51
1:D:180:LEU:HD21	1:D:609:VAL:HG23	1.92	0.51
1:E:406:GLN:HE21	1:E:490:GLY:HA2	1.76	0.51
1:F:572:ILE:HA	1:F:575:TRP:NE1	2.25	0.51
1:B:382:THR:O	1:B:386:MET:HG3	2.10	0.51
1:E:257:ALA:HB2	1:E:291:GLU:HB2	1.92	0.51
1:F:190:ILE:HG12	1:F:222:ALA:HB1	1.91	0.51
1:F:243:PRO:HD3	1:F:416:ALA:HB1	1.92	0.51
1:F:272:ILE:O	1:F:276:VAL:HG12	2.11	0.51
1:B:263:ASN:O	1:B:334:VAL:HA	2.10	0.51
1:B:300:CYS:O	1:B:304:GLU:HG2	2.10	0.51
1:D:494:SER:HB3	1:D:521:PRO:HD2	1.92	0.51
1:E:76:ARG:HH11	1:E:594:SER:HA	1.75	0.51
1:E:324:ILE:HG21	1:E:347:ALA:HB2	1.91	0.51
1:B:260:ILE:HB	1:B:295:ILE:HG22	1.92	0.51
1:E:476:VAL:HG13	1:E:525:VAL:HA	1.93	0.51
1:A:54:LEU:HD11	1:B:589:PRO:HA	1.93	0.51
1:B:513:GLY:O	1:B:518:LEU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:260:ILE:HG23	1:F:295:ILE:HD13	1.92	0.51
1:F:403:ALA:O	1:F:405:LYS:N	2.44	0.51
1:F:505:LEU:HA	1:F:508:VAL:HG22	1.92	0.51
1:F:597:VAL:O	1:F:601:VAL:HG22	2.10	0.51
1:A:41:CYS:SG	1:A:43:PHE:HB2	2.51	0.51
1:A:382:THR:O	1:A:386:MET:HG3	2.11	0.51
1:B:277:ALA:HA	1:B:293:ILE:HD11	1.93	0.51
1:D:447:LEU:HD23	1:D:477:LEU:HB2	1.92	0.51
1:E:33:ARG:NH2	1:F:71:VAL:O	2.34	0.51
1:F:335:ASP:OD1	1:F:336:VAL:N	2.41	0.51
1:A:37:GLN:NE2	1:B:69:TYR:O	2.44	0.51
1:E:617:THR:OG1	1:E:618:ASP:N	2.42	0.51
1:F:258:VAL:CG2	1:F:293:ILE:HD13	2.41	0.51
1:A:630:ILE:O	1:A:634:ARG:HG3	2.10	0.50
1:C:603:GLU:OE1	1:C:606:LYS:NZ	2.43	0.50
1:B:336:VAL:HA	1:B:361:ASN:ND2	2.27	0.50
1:E:206:ASP:OD1	1:E:211:ASN:ND2	2.43	0.50
1:F:158:ASN:HD21	1:F:163:LYS:HB3	1.77	0.50
1:B:152:THR:OG1	1:B:167:TRP:NE1	2.40	0.50
1:D:381:LYS:O	1:D:385:ARG:HG2	2.10	0.50
1:D:506:LYS:O	1:D:510:SER:OG	2.20	0.50
1:F:269:LEU:HD23	1:F:371:PHE:CD2	2.47	0.50
1:C:235:ASP:O	1:C:239:GLY:N	2.38	0.50
1:E:180:LEU:HD12	1:E:180:LEU:H	1.76	0.50
1:F:355:ILE:HA	1:F:367:THR:O	2.12	0.50
1:A:335:ASP:OD1	1:A:336:VAL:N	2.34	0.50
1:B:498:THR:HA	1:B:506:LYS:HE2	1.94	0.50
1:C:51:ARG:NH1	1:D:49:CYS:O	2.43	0.50
1:D:50:CYS:SG	1:D:52:ILE:HD12	2.52	0.50
1:E:136:THR:HA	1:E:144:ILE:HG12	1.93	0.50
1:B:261:ALA:HB2	1:B:329:LEU:HD11	1.94	0.50
1:C:303:HIS:O	1:C:307:MET:HG2	2.12	0.50
1:D:235:ASP:O	1:D:239:GLY:N	2.39	0.50
1:F:409:ILE:O	1:F:410:VAL:HB	2.11	0.50
1:A:152:THR:OG1	1:A:167:TRP:NE1	2.39	0.50
1:F:78:THR:HG23	1:F:207:ALA:HA	1.93	0.50
1:F:443:GLN:O	1:F:474:VAL:HA	2.11	0.50
1:A:436:ASN:HA	1:A:439:ASN:ND2	2.26	0.50
1:B:41:CYS:SG	1:B:43:PHE:HB2	2.52	0.50
1:E:55:LYS:NZ	1:F:317:TYR:HE2	2.10	0.50
1:F:577:VAL:HG13	1:F:612:TYR:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:SER:HB3	1:B:219:VAL:HG23	1.93	0.50
1:B:592:ILE:HD12	1:E:63:PHE:HA	1.93	0.50
1:D:328:ALA:HB2	1:D:399:VAL:HG13	1.93	0.50
1:F:281:ARG:O	1:F:285:ILE:HD12	2.11	0.50
1:E:47:GLY:HA2	1:F:51:ARG:NH2	2.27	0.49
1:E:200:ARG:HH21	1:F:360:HIS:HA	1.76	0.49
1:E:254:LYS:N	1:E:259:ASN:HD21	2.10	0.49
1:F:327:GLY:HA3	1:F:398:ARG:O	2.11	0.49
1:E:202:HIS:ND1	1:F:567:GLU:OE1	2.41	0.49
1:F:507:GLY:O	1:F:510:SER:OG	2.26	0.49
1:B:380:ALA:O	1:B:384:ILE:HD12	2.13	0.49
1:C:94:ALA:HA	1:D:199:SER:HB2	1.94	0.49
1:B:453:THR:HG22	1:B:563:GLU:HB3	1.93	0.49
1:B:152:THR:HG1	1:B:167:TRP:HE1	1.57	0.49
1:F:493:THR:H	1:F:496:ALA:HB2	1.77	0.49
1:A:157:GLN:HB2	1:B:157:GLN:CB	2.43	0.49
1:B:75:ASP:OD1	1:B:75:ASP:N	2.39	0.49
1:C:475:LEU:HD12	1:C:476:VAL:H	1.77	0.49
1:D:431:LYS:HE3	1:D:435:ASP:OD1	2.13	0.49
1:C:431:LYS:NZ	1:C:435:ASP:OD2	2.39	0.49
1:A:306:MET:CE	1:A:313:LEU:HB2	2.41	0.49
1:C:339:ILE:H	1:D:204:GLY:HA3	1.78	0.49
1:A:545:ALA:HB2	1:A:555:LEU:HD11	1.95	0.49
1:B:120:ARG:NH2	1:B:271:ASP:OD1	2.37	0.49
1:B:475:LEU:HD13	1:B:509:LEU:HD21	1.94	0.49
1:C:542:THR:HA	1:C:552:LEU:HD21	1.94	0.49
1:E:29:THR:HG23	1:E:31:TRP:H	1.77	0.49
1:E:486:PHE:HB3	1:E:525:VAL:HG11	1.94	0.49
1:A:272:ILE:O	1:A:276:VAL:HG23	2.13	0.49
1:E:509:LEU:HG	1:E:522:LEU:HB2	1.95	0.49
1:F:152:THR:HG23	1:F:229:LEU:HD13	1.94	0.49
1:F:494:SER:O	1:F:521:PRO:HG2	2.13	0.49
1:F:596:ILE:HD12	1:F:596:ILE:H	1.78	0.49
1:A:190:ILE:HD11	1:A:225:ASP:OD2	2.13	0.48
1:C:451:CYS:HB2	3:C:703:RQM:S2	2.52	0.48
1:C:513:GLY:HA3	1:C:521:PRO:HA	1.94	0.48
1:E:486:PHE:CD2	1:E:525:VAL:HG21	2.47	0.48
1:F:84:LEU:O	1:F:88:ILE:HG13	2.13	0.48
1:F:434:VAL:O	1:F:438:VAL:HG23	2.13	0.48
1:F:451:CYS:HB2	1:F:452:ASN:H	1.50	0.48
1:A:249:ASN:HB3	1:A:404:PHE:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:PRO:HD3	1:C:416:ALA:HB1	1.95	0.48
1:D:492:MET:SD	1:D:527:HIS:HB2	2.53	0.48
1:E:157:GLN:HB2	1:F:157:GLN:HB3	1.94	0.48
1:E:202:HIS:HE1	1:F:567:GLU:HB2	1.77	0.48
1:B:550:VAL:HG22	1:B:551:ASP:H	1.78	0.48
1:E:403:ALA:O	1:E:405:LYS:N	2.45	0.48
1:E:589:PRO:O	1:E:591:VAL:N	2.40	0.48
1:A:34:TYR:HA	1:B:71:VAL:HG22	1.94	0.48
1:B:508:VAL:HG22	1:B:512:ILE:HD11	1.94	0.48
1:C:318:LEU:HG	1:C:452:ASN:HB3	1.94	0.48
1:D:551:ASP:OD1	1:D:552:LEU:N	2.46	0.48
1:F:193:SER:HB3	1:F:219:VAL:HG23	1.95	0.48
1:F:253:MET:HB3	1:F:259:ASN:HD22	1.79	0.48
1:F:273:ILE:HA	1:F:276:VAL:HG12	1.94	0.48
1:A:421:LEU:HD23	1:A:432:PRO:HB2	1.95	0.48
1:E:323:PRO:O	1:E:326:THR:OG1	2.30	0.48
1:E:550:VAL:HG12	1:E:551:ASP:H	1.78	0.48
1:F:462:TYR:CE1	1:F:482:ALA:HA	2.48	0.48
1:C:509:LEU:HG	1:C:522:LEU:HB2	1.94	0.48
1:F:462:TYR:CE2	1:F:562:PRO:HD2	2.45	0.48
1:C:63:PHE:HA	1:F:592:ILE:HD12	1.95	0.48
1:D:462:TYR:HE1	1:D:562:PRO:HD2	1.77	0.48
1:D:627:TYR:HE2	1:D:631:GLN:NE2	2.09	0.48
1:E:168:LEU:HD13	1:E:172:LEU:HD21	1.95	0.48
1:E:442:ILE:HG13	1:E:442:ILE:O	2.14	0.48
1:F:561:ALA:N	1:F:584:HIS:O	2.27	0.48
1:B:560:SER:HB2	1:B:626:LEU:HD11	1.94	0.48
1:D:100:ARG:NH2	1:D:191:ASP:OD1	2.47	0.48
1:D:202:HIS:CG	1:D:203:VAL:H	2.32	0.48
1:F:206:ASP:OD2	1:F:211:ASN:ND2	2.44	0.48
1:E:447:LEU:HD13	1:E:449:VAL:HG13	1.96	0.48
1:F:351:HIS:O	1:F:352:THR:OG1	2.27	0.48
1:E:29:THR:HG23	1:E:30:ALA:N	2.29	0.48
1:C:337:GLN:HG3	1:D:205:CYS:SG	2.54	0.47
1:E:384:ILE:O	1:E:388:ILE:HG12	2.14	0.47
1:F:410:VAL:HG11	1:F:527:HIS:HD2	1.77	0.47
1:B:436:ASN:HA	1:B:439:ASN:HD21	1.79	0.47
1:C:380:ALA:O	1:C:384:ILE:HG13	2.13	0.47
1:C:486:PHE:HB3	1:C:525:VAL:HG21	1.96	0.47
1:C:566:SER:HB2	1:D:202:HIS:CE1	2.50	0.47
1:F:276:VAL:HG11	1:F:380:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ARG:NH1	1:C:271:ASP:OD1	2.47	0.47
1:C:189:ASN:HB3	1:C:192:ALA:HB3	1.97	0.47
1:E:108:HIS:HB3	1:E:114:LEU:HD23	1.95	0.47
1:E:439:ASN:HD22	1:E:441:ASN:H	1.62	0.47
1:E:306:MET:HG2	1:E:410:VAL:HG21	1.96	0.47
1:E:597:VAL:O	1:E:601:VAL:HG22	2.15	0.47
1:A:517:GLY:O	1:A:519:GLY:N	2.47	0.47
1:E:509:LEU:HD21	1:E:523:PRO:O	2.13	0.47
1:A:517:GLY:C	1:A:519:GLY:H	2.18	0.47
1:C:66:GLY:H	1:C:68:LYS:HE2	1.79	0.47
1:C:435:ASP:O	1:C:438:VAL:HG12	2.15	0.47
1:E:221:MET:SD	1:E:578:THR:OG1	2.73	0.47
1:E:575:TRP:HA	1:E:578:THR:HG23	1.97	0.47
1:F:125:LEU:HD22	1:F:145:VAL:HG23	1.96	0.47
1:F:257:ALA:HA	1:F:289:ALA:HB1	1.97	0.47
1:A:33:ARG:NH1	1:B:71:VAL:O	2.48	0.47
1:A:205:CYS:HA	1:B:361:ASN:ND2	2.30	0.47
1:C:334:VAL:HG23	1:C:356:THR:HA	1.96	0.47
1:D:158:ASN:HD21	1:D:163:LYS:HB3	1.78	0.47
1:E:102:ILE:HG13	1:E:268:MET:SD	2.54	0.47
1:E:205:CYS:SG	1:F:337:GLN:HA	2.55	0.47
1:F:68:LYS:O	1:F:68:LYS:HG3	2.14	0.47
1:F:564:CYS:HB2	1:F:569:ALA:HB1	1.96	0.47
1:C:462:TYR:HE1	1:C:562:PRO:HD2	1.80	0.47
1:D:89:ALA:HB2	1:D:197:THR:HG21	1.97	0.47
1:D:436:ASN:HA	1:D:439:ASN:ND2	2.30	0.47
1:E:122:GLU:O	1:E:126:TYR:HD2	1.97	0.47
1:E:238:PHE:HB2	1:E:308:ARG:HD2	1.96	0.47
1:E:272:ILE:O	1:E:275:ASP:HB3	2.15	0.47
1:E:458:GLN:O	1:E:458:GLN:HG2	2.15	0.47
1:F:77:ASP:OD1	1:F:596:ILE:HD13	2.15	0.47
1:F:545:ALA:HB1	1:F:550:VAL:O	2.14	0.47
1:B:451:CYS:HA	1:B:481:CYS:HB2	1.96	0.47
1:E:77:ASP:OD1	1:E:594:SER:OG	2.33	0.47
1:E:409:ILE:HG12	1:E:492:MET:O	2.15	0.47
1:A:54:LEU:HB3	1:B:565:MET:HA	1.97	0.46
1:B:305:VAL:HG23	1:B:311:VAL:HB	1.97	0.46
1:C:317:TYR:HE2	1:D:55:LYS:HZ3	1.62	0.46
1:E:378:GLU:OE1	1:E:378:GLU:N	2.37	0.46
1:F:497:THR:O	1:F:506:LYS:HE3	2.15	0.46
1:A:385:ARG:HA	1:A:388:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:VAL:HB	1:C:339:ILE:HD13	1.96	0.46
1:C:379:THR:O	1:C:383:ILE:HG12	2.15	0.46
1:F:463:VAL:HG12	1:F:467:LYS:HE2	1.98	0.46
1:C:282:ASP:OD1	1:C:282:ASP:N	2.43	0.46
1:E:47:GLY:O	1:E:80:VAL:HG12	2.15	0.46
1:F:409:ILE:HD11	1:F:523:PRO:CG	2.46	0.46
1:A:264:GLY:HA3	1:A:335:ASP:OD1	2.15	0.46
1:B:49:CYS:SG	1:B:50:CYS:N	2.88	0.46
1:C:50:CYS:SG	1:C:52:ILE:HG13	2.55	0.46
1:C:254:LYS:HB2	1:C:257:ALA:HB3	1.96	0.46
1:D:261:ALA:HB2	1:D:329:LEU:HD11	1.96	0.46
1:D:371:PHE:HA	1:D:379:THR:HG21	1.98	0.46
1:E:94:ALA:HB1	1:E:337:GLN:NE2	2.31	0.46
1:E:624:ASP:HA	1:E:627:TYR:CZ	2.50	0.46
1:C:476:VAL:HG11	1:C:525:VAL:HG12	1.97	0.46
1:E:120:ARG:NH1	1:E:271:ASP:OD1	2.47	0.46
1:F:161:TYR:HA	1:F:188:HIS:CG	2.51	0.46
1:F:317:TYR:HB2	3:F:702:RQM:S2	2.56	0.46
1:F:430:LEU:O	1:F:434:VAL:HG12	2.16	0.46
1:A:194:VAL:O	1:A:198:MET:HG2	2.15	0.46
1:A:484:GLY:O	1:A:488:LYS:HG3	2.16	0.46
1:B:19:LEU:HG	1:B:20:ASN:H	1.81	0.46
1:C:457:GLN:HB2	1:C:460:SER:OG	2.16	0.46
1:F:379:THR:O	1:F:383:ILE:HG12	2.16	0.46
1:F:486:PHE:CD1	1:F:525:VAL:HG11	2.50	0.46
1:E:428:ASP:HB3	1:E:431:LYS:HB2	1.97	0.46
1:F:446:VAL:HG12	1:F:476:VAL:HA	1.96	0.46
1:A:446:VAL:HG23	1:A:558:VAL:HG12	1.97	0.46
1:B:167:TRP:HB3	1:B:228:MET:HE3	1.98	0.46
1:E:207:ALA:HB3	1:F:363:ILE:HG23	1.97	0.46
1:F:327:GLY:HA2	1:F:350:PHE:CD1	2.50	0.46
1:F:602:THR:O	1:F:612:TYR:HB2	2.15	0.46
1:A:142:LEU:HA	1:A:145:VAL:CG1	2.46	0.46
1:A:154:GLY:HA2	1:A:157:GLN:HG2	1.97	0.46
1:D:85:VAL:HG12	1:D:197:THR:HG23	1.97	0.46
1:E:454:THR:HG22	1:F:55:LYS:HG2	1.98	0.46
1:E:555:LEU:O	1:E:633:ARG:HD3	2.16	0.46
1:A:53:CYS:SG	1:B:565:MET:HE2	2.56	0.45
1:B:579:ILE:HD13	1:B:579:ILE:HA	1.81	0.45
1:F:124:LYS:HE2	1:F:124:LYS:HB2	1.49	0.45
1:A:158:ASN:HD21	1:A:163:LYS:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:SER:HA	1:A:538:VAL:HG22	1.98	0.45
1:D:472:ARG:HD2	1:D:627:TYR:CD1	2.52	0.45
1:E:263:ASN:O	1:E:334:VAL:HA	2.16	0.45
1:F:132:LEU:HD23	1:F:132:LEU:HA	1.81	0.45
1:F:392:GLY:C	1:F:393:ARG:HD2	2.37	0.45
1:F:443:GLN:O	1:F:474:VAL:HG12	2.16	0.45
1:A:129:ALA:HB1	1:A:134:VAL:HB	1.98	0.45
1:A:481:CYS:CB	3:A:702:RQM:S1	3.04	0.45
1:F:471:LYS:HA	1:F:502:GLY:HA3	1.99	0.45
1:A:430:LEU:O	1:A:434:VAL:HG12	2.17	0.45
1:B:19:LEU:HG	1:B:20:ASN:N	2.31	0.45
1:C:114:LEU:HD23	1:C:114:LEU:HA	1.85	0.45
1:D:356:THR:OG1	1:D:368:HIS:ND1	2.38	0.45
1:D:508:VAL:O	1:D:512:ILE:HD12	2.15	0.45
1:F:30:ALA:HB2	1:F:340:MET:HE1	1.99	0.45
1:B:264:GLY:HA3	1:B:335:ASP:OD1	2.16	0.45
1:C:54:LEU:HD21	1:D:590:PRO:HD3	1.98	0.45
1:C:552:LEU:HD12	1:C:579:ILE:CG2	2.47	0.45
1:E:180:LEU:HB2	1:E:186:LEU:CD1	2.45	0.45
1:E:555:LEU:C	1:E:633:ARG:HD3	2.36	0.45
1:F:202:HIS:HB3	1:F:205:CYS:SG	2.56	0.45
1:A:494:SER:HB3	1:A:521:PRO:HD2	1.99	0.45
1:C:601:VAL:HG23	1:C:602:THR:HG23	1.97	0.45
1:E:193:SER:HB3	1:E:219:VAL:HG23	1.98	0.45
1:F:324:ILE:HG23	1:F:325:LEU:HD23	1.98	0.45
1:A:433:LEU:O	1:A:437:VAL:HG23	2.16	0.45
1:A:544:LEU:HD23	1:A:555:LEU:HD13	1.99	0.45
1:B:434:VAL:O	1:B:438:VAL:HG22	2.16	0.45
1:E:217:LEU:HD13	1:E:578:THR:HG22	1.98	0.45
1:F:273:ILE:HA	1:F:276:VAL:CG1	2.46	0.45
1:F:601:VAL:HB	1:F:613:PHE:CE2	2.51	0.45
1:A:306:MET:HG2	1:A:410:VAL:HG21	1.99	0.45
1:C:270:SER:HB2	1:C:305:VAL:HG11	1.99	0.45
1:D:538:VAL:O	1:D:542:THR:OG1	2.27	0.45
1:F:260:ILE:HD11	1:F:333:VAL:HG23	1.98	0.45
1:F:498:THR:HA	1:F:506:LYS:HE2	1.98	0.45
1:F:577:VAL:O	1:F:611:GLY:HA3	2.16	0.45
1:A:421:LEU:HB3	1:A:429:PRO:O	2.17	0.45
1:D:53:CYS:HB3	1:D:203:VAL:HG22	1.98	0.45
1:D:53:CYS:SG	1:D:55:LYS:HB2	2.56	0.45
1:E:269:LEU:O	1:E:273:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:THR:HG21	1:E:319:SER:O	2.16	0.45
1:E:606:LYS:HB3	1:E:612:TYR:CD2	2.52	0.45
1:C:87:MET:O	1:C:567:GLU:HB3	2.17	0.45
1:C:382:THR:O	1:C:386:MET:HG3	2.17	0.45
1:D:508:VAL:O	1:D:511:ALA:N	2.50	0.45
1:E:175:ARG:NH2	1:E:546:ASN:OD1	2.50	0.45
1:F:46:ALA:HA	1:F:592:ILE:HG13	1.98	0.45
1:F:274:CYS:SG	1:F:295:ILE:HG21	2.57	0.45
1:B:483:ALA:HB1	1:B:492:MET:HE1	1.98	0.44
1:C:443:GLN:HA	1:C:634:ARG:HH21	1.82	0.44
1:D:422:ALA:HA	1:D:425:ASN:O	2.17	0.44
1:D:545:ALA:HB2	1:D:555:LEU:HD11	1.99	0.44
1:E:55:LYS:HZ3	1:F:317:TYR:HE2	1.61	0.44
1:E:424:VAL:HG21	1:E:512:ILE:HD12	1.99	0.44
1:F:96:SER:HB2	1:F:190:ILE:HG21	1.99	0.44
1:F:273:ILE:HD12	1:F:274:CYS:N	2.32	0.44
1:F:582:PRO:HA	1:F:612:TYR:O	2.18	0.44
1:A:481:CYS:HB2	3:A:702:RQM:S1	2.56	0.44
1:E:167:TRP:HZ3	1:E:232:GLU:HG3	1.82	0.44
1:E:235:ASP:HA	1:E:308:ARG:NH1	2.29	0.44
1:E:332:MET:SD	1:E:343:LEU:HD13	2.58	0.44
1:A:384:ILE:O	1:A:388:ILE:HG23	2.17	0.44
1:A:469:LEU:O	1:A:474:VAL:HG22	2.18	0.44
1:B:257:ALA:HB2	1:B:291:GLU:HB2	1.99	0.44
1:C:492:MET:HE3	1:C:527:HIS:HB2	2.00	0.44
1:C:510:SER:HA	1:C:521:PRO:HB3	1.99	0.44
1:C:620:LYS:HZ3	1:E:349:CYS:HA	1.81	0.44
1:D:116:ASP:CG	1:D:377:VAL:HG23	2.37	0.44
1:F:409:ILE:HG13	1:F:492:MET:O	2.18	0.44
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.71	0.44
1:D:187:PRO:HD3	1:D:221:MET:HB2	1.98	0.44
1:E:413:SER:HA	1:E:536:ARG:HD3	1.99	0.44
1:B:88:ILE:HG23	1:B:571:ALA:HA	1.98	0.44
1:C:410:VAL:HG12	1:C:492:MET:HE3	1.98	0.44
1:F:497:THR:HG23	1:F:506:LYS:HA	1.99	0.44
1:A:221:MET:SD	1:A:578:THR:HB	2.58	0.44
1:A:379:THR:O	1:A:383:ILE:HG12	2.17	0.44
1:B:63:PHE:CG	1:E:46:ALA:HB2	2.52	0.44
1:B:315:THR:HG22	1:B:488:LYS:NZ	2.33	0.44
1:B:559:ALA:HB3	1:B:583:THR:HG23	2.00	0.44
1:C:55:LYS:HG2	1:D:453:THR:OG1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:ARG:C	1:C:636:GLY:H	2.20	0.44
1:E:53:CYS:HB3	1:E:55:LYS:HG2	1.99	0.44
1:F:269:LEU:HD23	1:F:371:PHE:HD2	1.81	0.44
1:B:30:ALA:HA	1:B:33:ARG:NH1	2.32	0.44
1:E:76:ARG:O	1:E:80:VAL:HG13	2.18	0.44
1:E:472:ARG:HD2	1:E:627:TYR:CD2	2.53	0.44
1:E:495:GLU:H	1:E:495:GLU:HG2	1.46	0.44
1:F:106:MET:HA	1:F:109:ILE:CG1	2.33	0.44
1:F:124:LYS:CE	1:F:235:ASP:HB3	2.47	0.44
1:A:242:GLN:O	1:A:244:VAL:HG23	2.18	0.44
1:B:130:LYS:HE3	1:B:130:LYS:HB3	1.85	0.44
1:B:135:ALA:O	1:B:139:ARG:HD3	2.17	0.44
1:C:152:THR:HG23	1:C:229:LEU:HD12	1.98	0.44
1:C:258:VAL:O	1:C:294:ASN:N	2.49	0.44
1:E:547:LYS:O	1:E:547:LYS:HD3	2.18	0.44
1:F:443:GLN:OE1	1:F:631:GLN:NE2	2.51	0.44
1:A:70:GLY:HA3	2:A:701:SF4:S2	2.58	0.44
1:A:457:GLN:O	1:A:460:SER:OG	2.27	0.44
1:C:84:LEU:HD21	1:C:590:PRO:O	2.16	0.44
1:C:421:LEU:HD21	1:C:433:LEU:HD22	1.99	0.44
1:F:164:PRO:HB3	1:F:186:LEU:HB3	2.00	0.44
1:F:189:ASN:HB3	1:F:192:ALA:HB3	2.00	0.44
1:A:493:THR:OG1	1:A:495:GLU:OE1	2.32	0.43
1:B:318:LEU:HD12	1:B:318:LEU:HA	1.87	0.43
1:B:334:VAL:HG23	1:B:356:THR:HA	1.99	0.43
1:C:433:LEU:O	1:C:437:VAL:HG23	2.18	0.43
1:C:443:GLN:HA	1:C:634:ARG:HE	1.82	0.43
1:C:578:THR:HA	1:C:609:VAL:HG11	2.00	0.43
1:D:600:LEU:HD23	1:D:600:LEU:HA	1.84	0.43
1:F:339:ILE:CD1	1:F:363:ILE:HD11	2.48	0.43
1:A:269:LEU:O	1:A:273:ILE:HG12	2.18	0.43
1:A:451:CYS:HB2	1:A:452:ASN:H	1.58	0.43
1:B:435:ASP:O	1:B:439:ASN:ND2	2.51	0.43
1:C:173:THR:HG23	1:C:542:THR:HG22	2.00	0.43
1:D:18:MET:O	1:D:19:LEU:HB2	2.18	0.43
1:D:21:LEU:HD21	1:D:488:LYS:NZ	2.33	0.43
1:D:95:HIS:ND1	1:D:223:ASP:OD1	2.49	0.43
1:E:148:LEU:HD23	1:E:148:LEU:HA	1.89	0.43
1:E:463:VAL:CG2	1:E:467:LYS:HE3	2.49	0.43
1:A:85:VAL:HG22	1:A:216:GLY:HA3	2.00	0.43
1:C:545:ALA:HB2	1:C:555:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:LEU:HD11	1:D:381:LYS:HG2	2.00	0.43
1:E:161:TYR:HA	1:E:188:HIS:CG	2.53	0.43
1:E:264:GLY:HA3	1:E:335:ASP:OD1	2.18	0.43
1:E:300:CYS:O	1:E:304:GLU:HG2	2.17	0.43
1:F:486:PHE:CD2	1:F:491:LEU:HD13	2.53	0.43
1:A:253:MET:HA	1:A:294:ASN:ND2	2.33	0.43
1:B:457:GLN:HG2	1:B:460:SER:HB3	2.00	0.43
1:C:140:GLY:O	1:C:142:LEU:N	2.44	0.43
1:E:597:VAL:HA	1:E:600:LEU:HB2	2.01	0.43
1:F:324:ILE:HD11	1:F:352:THR:OG1	2.19	0.43
1:F:408:SER:HB3	1:F:492:MET:CG	2.48	0.43
1:F:567:GLU:HA	1:F:570:LEU:HD23	2.00	0.43
1:A:455:LYS:HE2	1:B:54:LEU:O	2.18	0.43
1:B:600:LEU:HD23	1:B:600:LEU:HA	1.86	0.43
1:C:444:GLY:HA3	1:C:630:ILE:HD13	2.00	0.43
1:C:565:MET:HA	1:D:54:LEU:HB2	1.99	0.43
1:D:78:THR:OG1	1:D:207:ALA:O	2.32	0.43
1:D:489:ALA:O	1:D:491:LEU:N	2.51	0.43
1:E:444:GLY:HA3	1:E:630:ILE:HD11	2.00	0.43
1:E:24:ALA:C	1:E:26:SER:H	2.22	0.43
1:F:178:LYS:NZ	1:F:182:ASP:OD2	2.45	0.43
1:A:306:MET:HE1	1:A:313:LEU:CB	2.47	0.43
1:A:462:TYR:HE1	1:A:562:PRO:HD2	1.84	0.43
1:A:486:PHE:CD2	1:A:525:VAL:HG11	2.54	0.43
1:E:260:ILE:CD1	1:E:384:ILE:HG23	2.49	0.43
1:F:119:ILE:HG23	1:F:119:ILE:O	2.18	0.43
1:F:225:ASP:HA	1:F:228:MET:HG3	2.00	0.43
1:F:329:LEU:O	1:F:351:HIS:NE2	2.52	0.43
1:F:349:CYS:O	1:F:350:PHE:HB2	2.18	0.43
1:F:392:GLY:O	1:F:393:ARG:NH1	2.41	0.43
1:C:46:ALA:HB2	1:F:63:PHE:HB3	2.00	0.43
1:C:472:ARG:HD2	1:C:627:TYR:HD2	1.84	0.43
1:D:434:VAL:O	1:D:437:VAL:HG22	2.18	0.43
1:D:469:LEU:HB3	1:D:474:VAL:CG2	2.49	0.43
1:D:528:MET:O	1:D:536:ARG:HD2	2.19	0.43
1:E:82:ARG:HA	1:E:85:VAL:HG22	1.99	0.43
1:F:217:LEU:HB3	1:F:578:THR:HG21	1.99	0.43
1:F:579:ILE:HD13	1:F:579:ILE:HA	1.86	0.43
1:C:63:PHE:O	1:C:65:GLU:N	2.39	0.43
1:C:95:HIS:CE1	1:C:572:ILE:HD11	2.52	0.43
1:D:120:ARG:HB2	1:D:237:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:LYS:HD3	1:E:130:LYS:HA	1.69	0.43
1:E:280:LEU:HD13	1:E:282:ASP:OD1	2.19	0.43
1:E:550:VAL:HG12	1:E:551:ASP:N	2.33	0.43
1:F:538:VAL:O	1:F:542:THR:HG23	2.19	0.43
1:F:620:LYS:HD2	1:F:620:LYS:HA	1.84	0.43
1:A:142:LEU:HA	1:A:145:VAL:HG12	2.00	0.42
1:B:469:LEU:O	1:B:474:VAL:HG22	2.19	0.42
1:B:476:VAL:HG11	1:B:525:VAL:HG12	2.01	0.42
1:C:335:ASP:CG	1:C:336:VAL:H	2.23	0.42
1:C:431:LYS:HE3	1:C:431:LYS:HB3	1.91	0.42
1:D:422:ALA:HB2	1:D:429:PRO:HG3	2.01	0.42
1:E:462:TYR:HB3	1:E:486:PHE:CE1	2.53	0.42
1:F:334:VAL:HG23	1:F:356:THR:HA	2.01	0.42
1:F:336:VAL:HA	1:F:361:ASN:HD22	1.84	0.42
1:F:558:VAL:HG11	1:F:626:LEU:HD22	2.00	0.42
1:F:578:THR:HG23	1:F:609:VAL:HG21	2.00	0.42
1:A:250:LEU:HD12	1:A:326:THR:HG21	2.00	0.42
1:B:63:PHE:HB3	1:E:46:ALA:HB2	2.01	0.42
1:C:122:GLU:O	1:C:126:TYR:HD1	2.02	0.42
1:D:553:SER:O	1:D:633:ARG:NE	2.52	0.42
1:E:224:LEU:HG	1:E:228:MET:SD	2.59	0.42
1:A:18:MET:HG2	1:A:458:GLN:O	2.19	0.42
1:A:55:LYS:HE3	1:A:71:VAL:CG1	2.49	0.42
1:B:462:TYR:HB3	1:B:486:PHE:CE1	2.54	0.42
1:C:29:THR:H	1:C:32:HIS:HB2	1.84	0.42
1:D:18:MET:HB2	1:D:460:SER:HB3	2.02	0.42
1:D:27:ILE:HD12	1:D:27:ILE:HA	1.92	0.42
1:E:231:THR:CG2	1:E:533:ASP:HA	2.49	0.42
1:E:261:ALA:HA	1:E:296:ILE:O	2.19	0.42
1:E:263:ASN:OD1	1:E:298:ILE:HB	2.18	0.42
1:F:321:GLU:O	1:F:324:ILE:HG22	2.20	0.42
1:C:434:VAL:HG21	1:C:547:LYS:HG2	2.02	0.42
1:D:429:PRO:O	1:D:432:PRO:HD2	2.19	0.42
1:E:409:ILE:HG13	1:E:523:PRO:HG3	2.02	0.42
1:E:463:VAL:HG22	1:E:467:LYS:HE3	2.01	0.42
1:E:510:SER:HA	1:E:521:PRO:HA	2.02	0.42
1:A:168:LEU:O	1:A:172:LEU:HD22	2.20	0.42
1:C:263:ASN:HB3	1:C:334:VAL:HG12	2.02	0.42
1:D:318:LEU:HD23	1:D:452:ASN:HB2	2.01	0.42
1:D:415:GLU:OE1	1:D:415:GLU:N	2.51	0.42
1:E:267:PRO:HA	1:E:270:SER:OG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:GLY:O	1:A:508:VAL:HG23	2.20	0.42
1:B:510:SER:HA	1:B:521:PRO:HA	2.01	0.42
1:D:451:CYS:HB2	1:D:452:ASN:H	1.76	0.42
1:E:296:ILE:HD12	1:E:314:ALA:HB2	2.02	0.42
1:E:378:GLU:O	1:E:381:LYS:HG3	2.19	0.42
1:F:252:VAL:HA	1:F:405:LYS:HE2	2.00	0.42
1:F:258:VAL:HG23	1:F:293:ILE:HA	2.02	0.42
1:F:510:SER:HA	1:F:521:PRO:CA	2.44	0.42
1:F:596:ILE:O	1:F:600:LEU:HD23	2.19	0.42
1:B:165:CYS:HB3	1:B:225:ASP:OD2	2.19	0.42
1:C:206:ASP:HB3	1:C:212:LEU:HD21	2.02	0.42
1:C:486:PHE:CB	1:C:525:VAL:HG21	2.50	0.42
1:D:53:CYS:HB3	1:D:203:VAL:HG21	2.02	0.42
1:D:262:VAL:HG23	1:D:301:THR:HG23	2.01	0.42
1:D:285:ILE:HA	1:D:289:ALA:O	2.19	0.42
1:E:453:THR:HG23	1:E:455:LYS:H	1.83	0.42
1:F:167:TRP:CH2	1:F:233:LEU:CD2	3.01	0.42
1:F:520:GLY:HA3	1:F:521:PRO:HD3	1.83	0.42
1:F:527:HIS:HE1	1:F:529:GLY:O	2.01	0.42
1:A:53:CYS:O	1:B:565:MET:HB2	2.19	0.42
1:B:465:LEU:HD12	1:B:562:PRO:HG3	2.01	0.42
1:B:486:PHE:CB	1:B:525:VAL:HG21	2.49	0.42
1:C:163:LYS:HE2	1:C:164:PRO:O	2.20	0.42
1:C:277:ALA:O	1:C:293:ILE:HD12	2.20	0.42
1:E:445:ILE:HA	1:E:475:LEU:O	2.20	0.42
1:F:92:THR:O	1:F:96:SER:HB3	2.19	0.42
1:F:114:LEU:HD12	1:F:114:LEU:HA	1.87	0.42
1:B:442:ILE:HD11	1:B:508:VAL:HG11	2.02	0.42
1:C:158:ASN:HD21	1:C:163:LYS:HB3	1.85	0.42
1:C:187:PRO:HD3	1:C:221:MET:HB2	2.01	0.42
1:C:224:LEU:O	1:C:228:MET:HG3	2.19	0.42
1:C:414:ALA:O	1:C:418:VAL:HG23	2.20	0.42
1:D:263:ASN:HB3	1:D:334:VAL:HG12	2.01	0.42
1:F:609:VAL:C	1:F:611:GLY:H	2.22	0.42
1:A:217:LEU:O	1:A:221:MET:HG2	2.20	0.42
1:D:430:LEU:HD13	1:D:430:LEU:HA	1.89	0.42
1:E:299:CYS:HB3	1:E:300:CYS:H	1.76	0.42
1:E:381:LYS:HD2	1:E:382:THR:N	2.34	0.42
1:E:574:SER:O	1:E:578:THR:HG23	2.20	0.42
1:F:276:VAL:O	1:F:280:LEU:HD23	2.20	0.42
1:F:406:GLN:OE1	1:F:406:GLN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:621:SER:O	1:F:625:LYS:HG3	2.20	0.42
1:A:100:ARG:NH2	1:A:191:ASP:OD1	2.53	0.41
1:A:216:GLY:HA2	1:A:219:VAL:HG12	2.02	0.41
1:A:250:LEU:O	1:A:253:MET:HG3	2.20	0.41
1:A:316:ASN:OD1	1:A:458:GLN:NE2	2.53	0.41
1:B:76:ARG:HD3	1:B:593:GLY:O	2.20	0.41
1:B:340:MET:O	1:B:343:LEU:HD12	2.20	0.41
1:B:430:LEU:O	1:B:434:VAL:HG23	2.20	0.41
1:D:107:GLN:O	1:D:111:GLN:HG3	2.20	0.41
1:D:172:LEU:HB2	1:D:177:VAL:HG23	2.01	0.41
1:D:179:ARG:O	1:D:183:LEU:HG	2.20	0.41
1:E:100:ARG:NH1	1:F:196:GLN:HE21	2.17	0.41
1:E:280:LEU:HD12	1:E:283:GLU:CG	2.50	0.41
1:E:344:PRO:HB3	1:E:365:GLY:C	2.40	0.41
1:A:263:ASN:OD1	1:A:299:CYS:HB2	2.20	0.41
1:B:258:VAL:HG13	1:B:330:GLU:HG2	2.01	0.41
1:B:447:LEU:HG	1:B:449:VAL:HG13	2.02	0.41
1:B:620:LYS:HA	1:B:620:LYS:HD3	1.80	0.41
1:D:264:GLY:C	1:D:301:THR:HB	2.40	0.41
1:E:445:ILE:HD11	1:E:557:LEU:HD12	2.03	0.41
1:E:550:VAL:CG1	1:E:554:ASP:HB2	2.50	0.41
1:F:335:ASP:CG	1:F:336:VAL:H	2.22	0.41
1:F:480:GLY:N	1:F:529:GLY:O	2.46	0.41
1:F:535:SER:HA	1:F:538:VAL:HG22	2.02	0.41
1:A:172:LEU:HA	1:A:542:THR:HG21	2.03	0.41
1:E:342:SER:O	1:E:346:ILE:HG22	2.19	0.41
1:E:412:PHE:O	1:E:528:MET:HG2	2.20	0.41
1:F:518:LEU:HD12	1:F:518:LEU:HA	1.90	0.41
1:F:623:GLY:HA2	1:F:626:LEU:HB2	2.01	0.41
1:A:568:LYS:HG3	1:B:202:HIS:CE1	2.55	0.41
1:B:122:GLU:O	1:B:126:TYR:HD1	2.04	0.41
1:B:373:GLU:CD	1:B:373:GLU:H	2.24	0.41
1:C:328:ALA:HA	1:C:394:ARG:HD2	2.01	0.41
1:D:258:VAL:HG13	1:D:330:GLU:HG2	2.01	0.41
1:D:343:LEU:HB3	1:D:354:ILE:HD13	2.02	0.41
1:F:61:ASP:OD2	1:F:63:PHE:N	2.47	0.41
1:F:135:ALA:O	1:F:139:ARG:NH1	2.53	0.41
1:F:359:LYS:HG3	1:F:360:HIS:CD2	2.56	0.41
1:F:470:ALA:CB	1:F:524:LEU:HD11	2.50	0.41
1:B:104:LEU:HD23	1:B:104:LEU:HA	1.89	0.41
1:B:592:ILE:H	1:B:592:ILE:HG12	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ARG:HH21	1:D:41:CYS:HB2	1.86	0.41
1:E:72:CYS:SG	1:E:73:GLY:N	2.93	0.41
1:E:254:LYS:H	1:E:259:ASN:HD21	1.68	0.41
1:E:444:GLY:CA	1:E:630:ILE:HD11	2.50	0.41
1:E:558:VAL:HB	1:E:582:PRO:O	2.20	0.41
1:F:139:ARG:HB2	1:F:144:ILE:HD11	2.02	0.41
1:F:408:SER:HA	1:F:493:THR:HG22	2.03	0.41
1:A:25:ASN:O	1:A:26:SER:OG	2.35	0.41
1:A:83:HIS:O	1:A:87:MET:HG3	2.20	0.41
1:B:339:ILE:CD1	1:B:363:ILE:HD11	2.50	0.41
1:D:347:ALA:C	1:D:349:CYS:H	2.24	0.41
1:E:100:ARG:NH2	1:E:191:ASP:OD2	2.54	0.41
1:E:471:LYS:HB3	1:E:471:LYS:HE3	1.69	0.41
1:F:172:LEU:HG	1:F:176:ARG:HB3	2.03	0.41
1:F:324:ILE:CD1	1:F:352:THR:HG21	2.51	0.41
1:F:410:VAL:CG1	1:F:527:HIS:HD2	2.34	0.41
1:A:325:LEU:HA	1:A:350:PHE:CZ	2.55	0.41
1:A:417:VAL:O	1:A:421:LEU:HD12	2.21	0.41
1:C:409:ILE:HG22	1:C:412:PHE:CE1	2.56	0.41
1:C:487:ALA:CA	1:C:492:MET:HG3	2.46	0.41
1:E:191:ASP:HB3	1:F:191:ASP:HB3	2.03	0.41
1:E:307:MET:HE3	1:E:307:MET:HB3	1.98	0.41
1:E:575:TRP:O	1:E:579:ILE:HG13	2.21	0.41
1:F:269:LEU:HD11	1:F:333:VAL:CG1	2.47	0.41
1:F:382:THR:O	1:F:386:MET:HE3	2.21	0.41
1:B:178:LYS:HE3	1:B:182:ASP:OD2	2.21	0.41
1:C:84:LEU:HD11	1:C:591:VAL:HG13	2.03	0.41
1:C:265:HIS:CE1	1:C:568:LYS:HZ1	2.39	0.41
1:C:626:LEU:HD23	1:C:626:LEU:HA	1.91	0.41
1:D:121:ASP:HB2	1:D:239:GLY:HA2	2.03	0.41
1:D:206:ASP:HB3	1:D:212:LEU:HD21	2.03	0.41
1:D:334:VAL:HB	1:D:339:ILE:HD13	2.02	0.41
1:E:462:TYR:HB3	1:E:486:PHE:CZ	2.56	0.41
1:A:191:ASP:HB3	1:B:191:ASP:HB3	2.03	0.41
1:A:414:ALA:O	1:A:418:VAL:HG23	2.21	0.41
1:A:592:ILE:H	1:A:592:ILE:HG12	1.57	0.41
1:B:462:TYR:HE1	1:B:562:PRO:HD2	1.85	0.41
1:C:534:ASN:O	1:C:538:VAL:HG23	2.21	0.41
1:C:633:ARG:HD3	1:C:633:ARG:HA	1.83	0.41
1:D:220:ALA:O	1:D:223:ASP:HB3	2.20	0.41
1:E:48:LEU:HB3	1:E:60:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:PRO:CB	1:E:186:LEU:HD23	2.50	0.41
1:E:258:VAL:HG13	1:E:293:ILE:HA	2.03	0.41
1:E:454:THR:H	1:F:55:LYS:HG2	1.85	0.41
1:E:459:ASP:OD1	1:E:459:ASP:N	2.54	0.41
1:F:542:THR:HA	1:F:552:LEU:HD11	2.01	0.41
1:B:334:VAL:HB	1:B:339:ILE:HD13	2.03	0.40
1:D:596:ILE:HD12	1:D:596:ILE:H	1.85	0.40
1:E:242:GLN:HG3	1:E:243:PRO:HD2	2.03	0.40
1:F:282:ASP:OD1	1:F:282:ASP:N	2.53	0.40
1:A:61:ASP:HB2	1:A:67:PRO:HD2	2.04	0.40
1:C:21:LEU:HD12	1:C:21:LEU:HA	1.92	0.40
1:D:434:VAL:HG22	1:D:548:LEU:HD21	2.03	0.40
1:D:442:ILE:HD11	1:D:444:GLY:O	2.22	0.40
1:D:510:SER:HA	1:D:521:PRO:HB3	2.03	0.40
1:E:278:ALA:O	1:E:281:ARG:HD3	2.21	0.40
1:F:231:THR:HG21	1:F:533:ASP:HA	2.04	0.40
1:F:265:HIS:N	1:F:301:THR:OG1	2.54	0.40
1:F:409:ILE:HD11	1:F:523:PRO:HD3	2.03	0.40
1:F:475:LEU:HD23	1:F:476:VAL:N	2.37	0.40
1:C:157:GLN:CB	1:D:157:GLN:HB2	2.50	0.40
1:C:462:TYR:CE2	1:C:482:ALA:HA	2.56	0.40
1:C:579:ILE:HD13	1:C:579:ILE:HA	1.82	0.40
1:E:245:VAL:HG22	1:E:409:ILE:HG22	2.03	0.40
1:E:316:ASN:OD1	1:E:316:ASN:N	2.54	0.40
1:F:144:ILE:H	1:F:144:ILE:HD12	1.86	0.40
1:F:230:ALA:CB	1:F:532:VAL:HG11	2.52	0.40
1:F:371:PHE:CE1	1:F:373:GLU:HA	2.57	0.40
1:F:465:LEU:HD21	1:F:622:ALA:HB3	2.04	0.40
1:F:490:GLY:O	1:F:493:THR:HG23	2.21	0.40
1:F:551:ASP:OD1	1:F:552:LEU:N	2.51	0.40
1:D:60:ILE:HG21	1:D:76:ARG:HB3	2.04	0.40
1:D:329:LEU:O	1:D:352:THR:OG1	2.26	0.40
1:E:362:LYS:HG3	1:F:208:ASP:HB2	2.03	0.40
1:E:404:PHE:HD1	1:E:404:PHE:HA	1.74	0.40
1:F:355:ILE:O	1:F:355:ILE:HD12	2.21	0.40
1:B:106:MET:HE3	1:B:106:MET:HB3	1.98	0.40
1:D:422:ALA:HA	1:D:425:ASN:C	2.41	0.40
1:E:176:ARG:HG2	1:E:551:ASP:OD1	2.22	0.40
1:E:466:ALA:HB2	1:E:486:PHE:CE1	2.57	0.40
1:E:487:ALA:O	1:E:489:ALA:N	2.45	0.40
1:E:490:GLY:O	1:E:493:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:626:LEU:HD23	1:E:626:LEU:HA	1.91	0.40
1:F:124:LYS:O	1:F:128:ILE:HG23	2.22	0.40
1:F:139:ARG:HE	1:F:139:ARG:HB3	1.72	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:LYS:NZ	1:F:291:GLU:OE2[1_655]	2.15	0.05

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	618/639 (97%)	558 (90%)	53 (9%)	7 (1%)	12 37
1	B	618/639 (97%)	553 (90%)	58 (9%)	7 (1%)	12 37
1	C	618/639 (97%)	561 (91%)	49 (8%)	8 (1%)	10 33
1	D	619/639 (97%)	556 (90%)	51 (8%)	12 (2%)	6 24
1	E	615/639 (96%)	527 (86%)	73 (12%)	15 (2%)	5 19
1	F	615/639 (96%)	523 (85%)	64 (10%)	28 (5%)	2 8
All	All	3703/3834 (97%)	3278 (88%)	348 (9%)	77 (2%)	5 22

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	26	SER
1	C	65	GLU
1	D	265	HIS
1	D	490	GLY
1	E	27	ILE

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Mol	Chain	Res	Type
1	E	405	LYS
1	E	457	GLN
1	E	491	LEU
1	E	617	THR
1	F	352	THR
1	F	404	PHE
1	F	410	VAL
1	F	444	GLY
1	F	488	LYS
1	F	521	PRO
1	F	604	THR
1	F	612	TYR
1	A	23	GLU
1	C	23	GLU
1	C	517	GLY
1	D	24	ALA
1	E	65	GLU
1	E	404	PHE
1	E	556	PRO
1	F	23	GLU
1	F	26	SER
1	F	51	ARG
1	F	76	ARG
1	F	531	CYS
1	A	21	LEU
1	A	347	ALA
1	A	518	LEU
1	B	588	VAL
1	C	142	LEU
1	D	74	ALA
1	D	139	ARG
1	D	604	THR
1	E	25	ASN
1	F	147	ASP
1	F	254	LYS
1	F	588	VAL
1	F	603	GLU
1	B	19	LEU
1	B	405	LYS
1	C	289	ALA
1	C	588	VAL
1	D	19	LEU

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Mol	Chain	Res	Type
1	D	26	SER
1	D	565	MET
1	D	588	VAL
1	E	526	MET
1	E	588	VAL
1	F	148	LEU
1	F	337	GLN
1	F	556	PRO
1	A	130	LYS
1	B	337	GLN
1	C	337	GLN
1	D	25	ASN
1	E	604	THR
1	F	24	ALA
1	F	395	ASP
1	F	530	SER
1	F	547	LYS
1	A	348	GLU
1	A	588	VAL
1	B	604	THR
1	D	337	GLN
1	E	22	ALA
1	E	618	ASP
1	F	518	LEU
1	E	550	VAL
1	F	409	ILE
1	C	64	GLY
1	F	258	VAL
1	F	550	VAL
1	B	550	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	475/490 (97%)	443 (93%)	32 (7%)	13 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	475/490 (97%)	441 (93%)	34 (7%)	12 35
1	C	475/490 (97%)	447 (94%)	28 (6%)	16 45
1	D	476/490 (97%)	447 (94%)	29 (6%)	15 43
1	E	472/490 (96%)	438 (93%)	34 (7%)	12 35
1	F	472/490 (96%)	423 (90%)	49 (10%)	5 18
All	All	2845/2940 (97%)	2639 (93%)	206 (7%)	12 35

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	CYS
1	A	53	CYS
1	A	58	CYS
1	A	63	PHE
1	A	84	LEU
1	A	96	SER
1	A	132	LEU
1	A	163	LYS
1	A	172	LEU
1	A	175	ARG
1	A	249	ASN
1	A	255	ARG
1	A	271	ASP
1	A	306	MET
1	A	316	ASN
1	A	364	SER
1	A	369	VAL
1	A	385	ARG
1	A	407	LYS
1	A	428	ASP
1	A	434	VAL
1	A	438	VAL
1	A	451	CYS
1	A	514	THR
1	A	565	MET
1	A	568	LYS
1	A	578	THR
1	A	587	SER
1	A	591	VAL
1	A	592	ILE

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Mol	Chain	Res	Type
1	A	599	LYS
1	A	617	THR
1	B	19	LEU
1	B	28	GLU
1	B	50	CYS
1	B	58	CYS
1	B	59	ARG
1	B	72	CYS
1	B	84	LEU
1	B	101	HIS
1	B	131	THR
1	B	203	VAL
1	B	206	ASP
1	B	237	LEU
1	B	265	HIS
1	B	270	SER
1	B	315	THR
1	B	367	THR
1	B	369	VAL
1	B	423	LYS
1	B	431	LYS
1	B	438	VAL
1	B	451	CYS
1	B	454	THR
1	B	471	LYS
1	B	472	ARG
1	B	494	SER
1	B	518	LEU
1	B	531	CYS
1	B	540	LEU
1	B	558	VAL
1	B	599	LYS
1	B	609	VAL
1	B	615	VAL
1	B	617	THR
1	B	621	SER
1	C	20	ASN
1	C	50	CYS
1	C	51	ARG
1	C	59	ARG
1	C	72	CYS
1	C	96	SER

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Mol	Chain	Res	Type
1	C	106	MET
1	C	163	LYS
1	C	229	LEU
1	C	270	SER
1	C	282	ASP
1	C	316	ASN
1	C	319	SER
1	C	348	GLU
1	C	359	LYS
1	C	364	SER
1	C	367	THR
1	C	385	ARG
1	C	428	ASP
1	C	451	CYS
1	C	499	GLN
1	C	524	LEU
1	C	531	CYS
1	C	565	MET
1	C	591	VAL
1	C	604	THR
1	C	627	TYR
1	C	633	ARG
1	D	26	SER
1	D	50	CYS
1	D	96	SER
1	D	106	MET
1	D	171	SER
1	D	173	THR
1	D	176	ARG
1	D	199	SER
1	D	234	SER
1	D	240	THR
1	D	245	VAL
1	D	319	SER
1	D	358	ASP
1	D	373	GLU
1	D	438	VAL
1	D	451	CYS
1	D	488	LYS
1	D	494	SER
1	D	510	SER
1	D	531	CYS

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Mol	Chain	Res	Type
1	D	538	VAL
1	D	542	THR
1	D	544	LEU
1	D	550	VAL
1	D	565	MET
1	D	578	THR
1	D	585	VAL
1	D	621	SER
1	D	627	TYR
1	E	29	THR
1	E	35	GLU
1	E	58	CYS
1	E	59	ARG
1	E	106	MET
1	E	115	HIS
1	E	130	LYS
1	E	134	VAL
1	E	171	SER
1	E	175	ARG
1	E	228	MET
1	E	231	THR
1	E	273	ILE
1	E	280	LEU
1	E	281	ARG
1	E	308	ARG
1	E	313	LEU
1	E	381	LYS
1	E	385	ARG
1	E	393	ARG
1	E	439	ASN
1	E	459	ASP
1	E	469	LEU
1	E	495	GLU
1	E	540	LEU
1	E	557	LEU
1	E	564	CYS
1	E	578	THR
1	E	591	VAL
1	E	608	LEU
1	E	609	VAL
1	E	612	TYR
1	E	621	SER

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Mol	Chain	Res	Type
1	E	624	ASP
1	F	50	CYS
1	F	51	ARG
1	F	58	CYS
1	F	59	ARG
1	F	72	CYS
1	F	96	SER
1	F	119	ILE
1	F	120	ARG
1	F	141	LEU
1	F	147	ASP
1	F	152	THR
1	F	168	LEU
1	F	176	ARG
1	F	179	ARG
1	F	210	THR
1	F	228	MET
1	F	231	THR
1	F	233	LEU
1	F	234	SER
1	F	253	MET
1	F	255	ARG
1	F	258	VAL
1	F	315	THR
1	F	319	SER
1	F	369	VAL
1	F	377	VAL
1	F	386	MET
1	F	407	LYS
1	F	418	VAL
1	F	435	ASP
1	F	441	ASN
1	F	446	VAL
1	F	451	CYS
1	F	464	ASP
1	F	468	SER
1	F	488	LYS
1	F	498	THR
1	F	503	GLU
1	F	506	LYS
1	F	512	ILE
1	F	522	LEU

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Mol	Chain	Res	Type
1	F	531	CYS
1	F	550	VAL
1	F	557	LEU
1	F	565	MET
1	F	578	THR
1	F	595	GLN
1	F	600	LEU
1	F	606	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	98	HIS
1	A	361	ASN
1	A	452	ASN
1	B	20	ASN
1	B	337	GLN
1	B	361	ASN
1	B	441	ASN
1	C	98	HIS
1	C	107	GLN
1	C	303	HIS
1	C	443	GLN
1	C	457	GLN
1	C	527	HIS
1	D	98	HIS
1	D	337	GLN
1	D	441	ASN
1	E	38	GLN
1	E	196	GLN
1	E	320	GLN
1	E	337	GLN
1	E	351	HIS
1	E	439	ASN
1	F	196	GLN
1	F	361	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	RQM	C	703	1	0,12,12	-	-	-		
3	RQM	F	702	1	0,12,12	-	-	-		
2	SF4	C	701	1	0,12,12	-	-	-		
2	SF4	A	701	1	0,12,12	-	-	-		
3	RQM	D	702	1	0,12,12	-	-	-		
3	RQM	E	703	1	0,12,12	-	-	-		
2	SF4	C	702	1	0,12,12	-	-	-		
2	SF4	B	701	1	0,12,12	-	-	-		
2	SF4	E	702	1	0,12,12	-	-	-		
2	SF4	F	701	1	0,12,12	-	-	-		
2	SF4	B	702	1	0,12,12	-	-	-		
2	SF4	D	701	1	0,12,12	-	-	-		
2	SF4	E	701	1	0,12,12	-	-	-		
3	RQM	A	702	1	0,12,12	-	-	-		
3	RQM	B	703	1	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	RQM	C	703	1	-	-	0/4/4/4
3	RQM	F	702	1	-	-	0/4/4/4
2	SF4	C	701	1	-	-	0/6/5/5
2	SF4	A	701	1	-	-	0/6/5/5
3	RQM	D	702	1	-	-	0/4/4/4
3	RQM	E	703	1	-	-	0/4/4/4
2	SF4	C	702	1	-	-	0/6/5/5
2	SF4	B	701	1	-	-	0/6/5/5
2	SF4	E	702	1	-	-	0/6/5/5
2	SF4	F	701	1	-	-	0/6/5/5
2	SF4	B	702	1	-	-	0/6/5/5
2	SF4	D	701	1	-	-	0/6/5/5
2	SF4	E	701	1	-	-	0/6/5/5
3	RQM	A	702	1	-	-	0/4/4/4
3	RQM	B	703	1	-	-	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	703	RQM	1	0
3	F	702	RQM	2	0
2	A	701	SF4	1	0
3	E	703	RQM	2	0
2	E	701	SF4	1	0
3	A	702	RQM	2	0
3	B	703	RQM	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	620/639 (97%)	-0.25	0 100 100	43, 69, 90, 110	0
1	B	620/639 (97%)	-0.34	2 (0%) 90 88	44, 67, 87, 107	0
1	C	620/639 (97%)	-0.33	2 (0%) 90 88	47, 68, 90, 116	0
1	D	621/639 (97%)	-0.37	3 (0%) 87 84	43, 67, 88, 108	0
1	E	617/639 (96%)	0.16	10 (1%) 70 64	72, 103, 129, 146	0
1	F	617/639 (96%)	0.34	27 (4%) 39 33	76, 109, 135, 149	0
All	All	3715/3834 (96%)	-0.13	44 (1%) 76 71	43, 75, 123, 149	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	50	CYS	4.5
1	F	520	GLY	4.1
1	F	512	ILE	3.9
1	F	544	LEU	3.8
1	E	414	ALA	3.6
1	F	487	ALA	3.6
1	F	540	LEU	3.2
1	E	332	MET	3.1
1	D	64	GLY	3.0
1	F	328	ALA	3.0
1	F	420	ALA	3.0
1	F	525	VAL	3.0
1	E	273	ILE	2.8
1	E	437	VAL	2.8
1	F	498	THR	2.8
1	F	354	ILE	2.8
1	E	557	LEU	2.7
1	D	24	ALA	2.7
1	F	505	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	433	LEU	2.6
1	F	526	MET	2.6
1	C	22	ALA	2.6
1	F	518	LEU	2.6
1	F	331	ALA	2.6
1	E	331	ALA	2.5
1	F	500	TYR	2.5
1	F	502	GLY	2.5
1	F	508	VAL	2.4
1	B	22	ALA	2.3
1	F	493	THR	2.3
1	F	524	LEU	2.3
1	F	527	HIS	2.3
1	C	142	LEU	2.3
1	F	491	LEU	2.3
1	F	109	ILE	2.2
1	E	523	PRO	2.2
1	B	50	CYS	2.2
1	D	284	ALA	2.1
1	F	260	ILE	2.1
1	E	434	VAL	2.1
1	F	261	ALA	2.1
1	F	494	SER	2.1
1	E	322	LEU	2.0
1	F	548	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	RQM	A	702	9/9	0.82	0.13	72,80,95,97	9
3	RQM	F	702	9/9	0.85	0.09	92,104,115,118	9
3	RQM	D	702	9/9	0.87	0.09	61,79,94,107	9
3	RQM	C	703	9/9	0.91	0.09	71,88,98,108	9
2	SF4	C	701	8/8	0.91	0.16	89,110,130,132	0
3	RQM	B	703	9/9	0.91	0.08	62,74,84,97	9
3	RQM	E	703	9/9	0.93	0.07	84,105,115,125	9
2	SF4	F	701	8/8	0.93	0.12	93,116,127,132	0
2	SF4	A	701	8/8	0.95	0.11	64,87,94,96	0
2	SF4	B	701	8/8	0.96	0.10	79,93,111,115	0
2	SF4	C	702	8/8	0.96	0.10	73,91,107,109	0
2	SF4	D	701	8/8	0.96	0.11	62,86,95,101	0
2	SF4	E	701	8/8	0.96	0.10	76,83,90,102	8
2	SF4	E	702	8/8	0.96	0.10	75,114,125,129	0
2	SF4	B	702	8/8	0.96	0.10	64,84,97,98	0
4	NA	D	703	1/1	0.96	0.13	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.