Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 04:50 PM EDT

PDB ID	:	5ORF
Title	:	Structure of ovine serum albumin in P1 space group
Authors	:	Talaj, J.A.; Bujacz, A.; Bujacz, G.; Pietrzyk-Brzezinska, A.J.
Deposited on	:	2017-08-16
Resolution	:	2.54 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 (i) 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 (i)) were used in the production of this report:

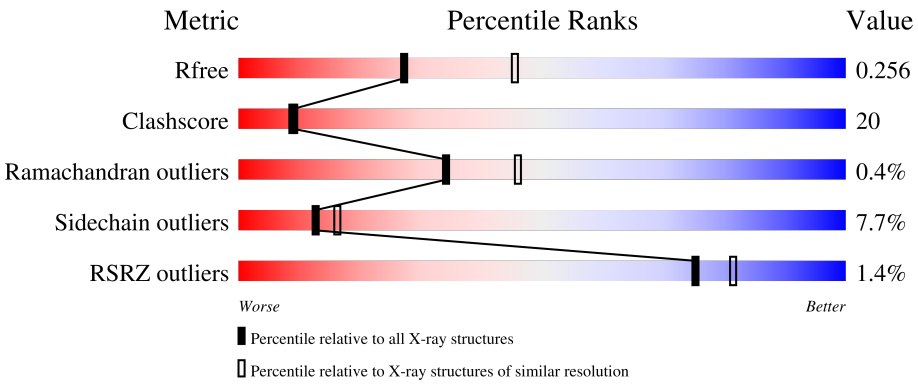
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.54 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	583	3% 57% 39% •
1	B	583	% 64% 33% •
1	C	583	% 63% 35% •
1	D	583	% 58% 38% •

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
2	PGE	C	602	-	-	X	-
4	PRO	C	605	-	-	X	-
4	PRO	D	603	-	-	X	-

2 Entry composition (i)

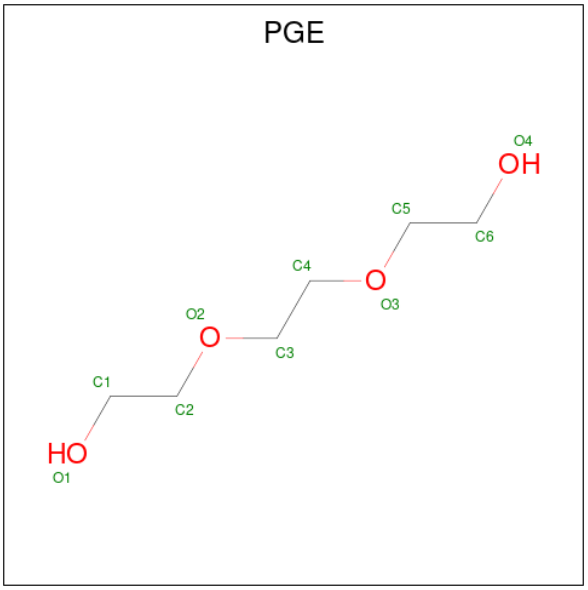
There are 5 unique types of molecules in this entry. The entry contains 19129 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	583	4645	2933	780	893	39	0	0	0
1	B	583	4645	2933	780	893	39	0	0	0
1	C	583	4645	2933	780	893	39	0	0	0
1	D	583	4645	2933	780	893	39	0	0	0

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	10	6	4	0	0
2	A	1	10	6	4	0	0

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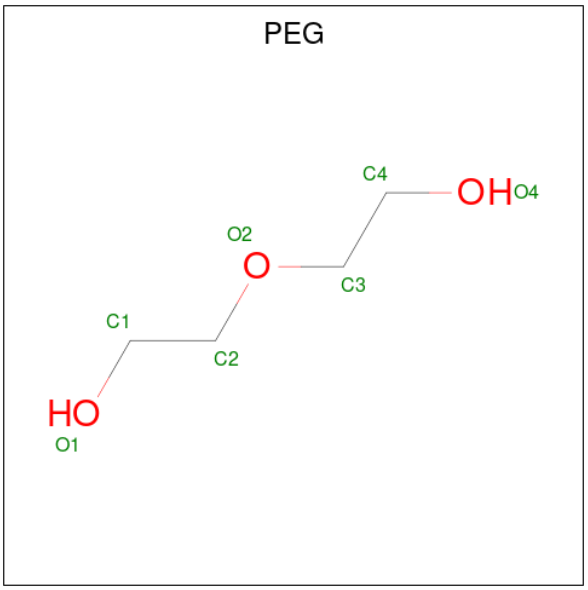
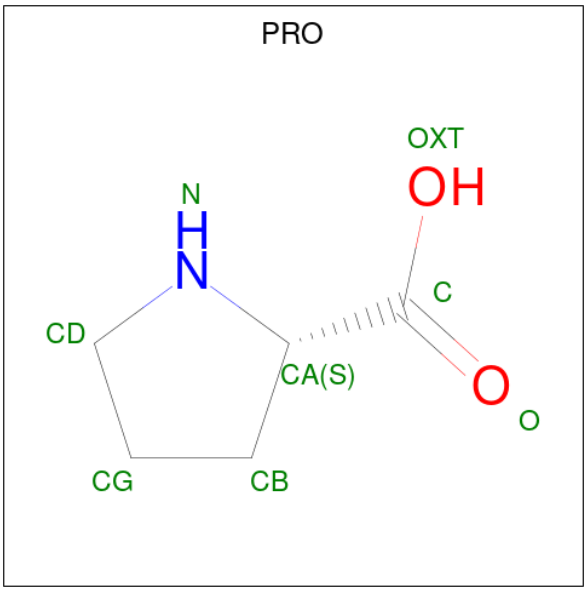
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	10	6	4	0	0
			Total	C	O		
2	C	1	10	6	4	0	0
			Total	C	O		
2	C	1	10	6	4	0	0
			Total	C	O		
2	D	1	10	6	4	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	7	4	3	0	0
			Total	C	O		
3	C	1	7	4	3	0	0

- Molecule 4 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	8	5	1	2	0	0
4	A	1	8	5	1	2	0	0
4	A	1	8	5	1	2	0	0
4	B	1	8	5	1	2	0	0
4	B	1	8	5	1	2	0	0
4	B	1	8	5	1	2	0	0
4	C	1	8	5	1	2	0	0
4	C	1	8	5	1	2	0	0
4	C	1	8	5	1	2	0	0
4	D	1	8	5	1	2	0	0
4	D	1	8	5	1	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	91	91	91	0	0

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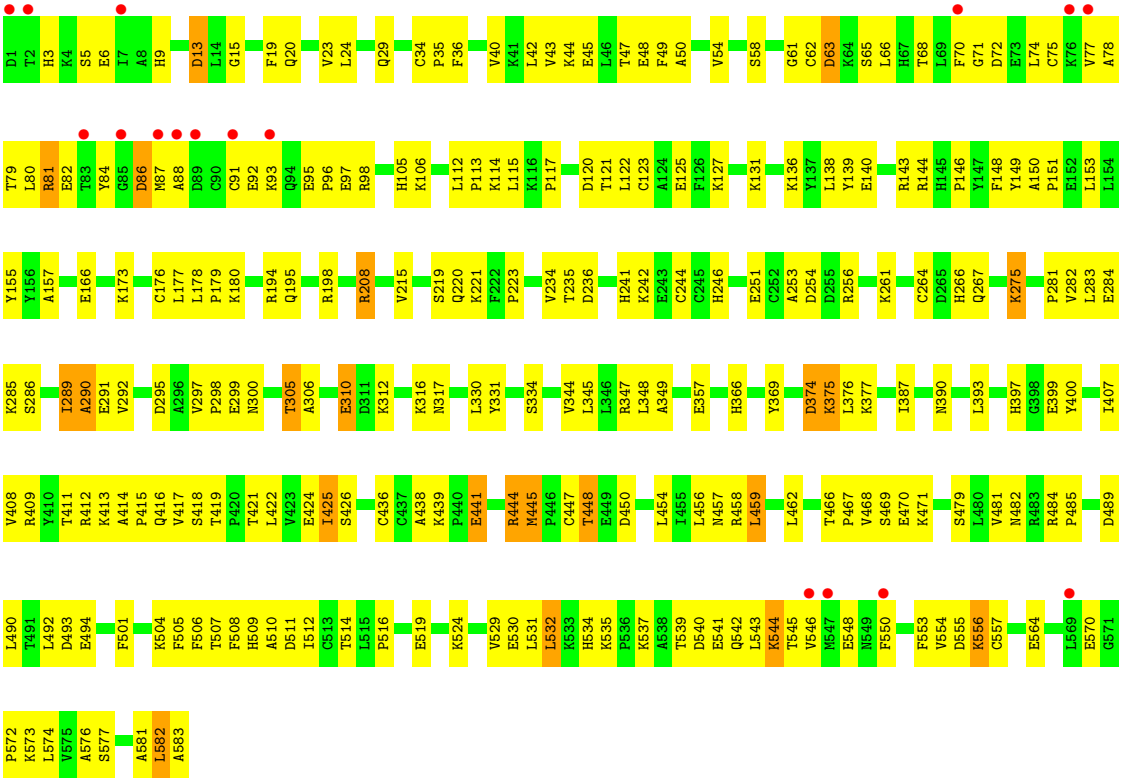
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	112	112	112	0	0
			Total	O		
5	C	87	87	87	0	0
			Total	O		
5	D	97	97	97	0	0

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.

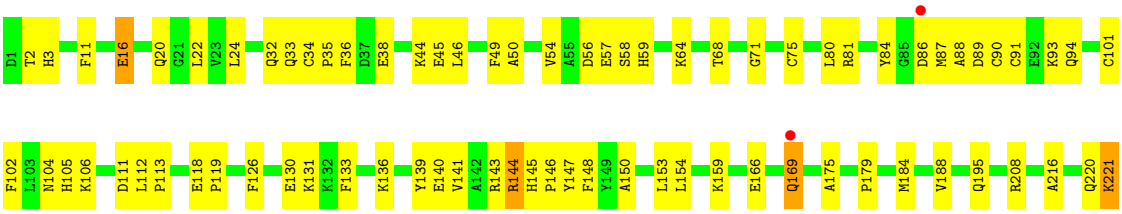
• Molecule 1: Serum albumin

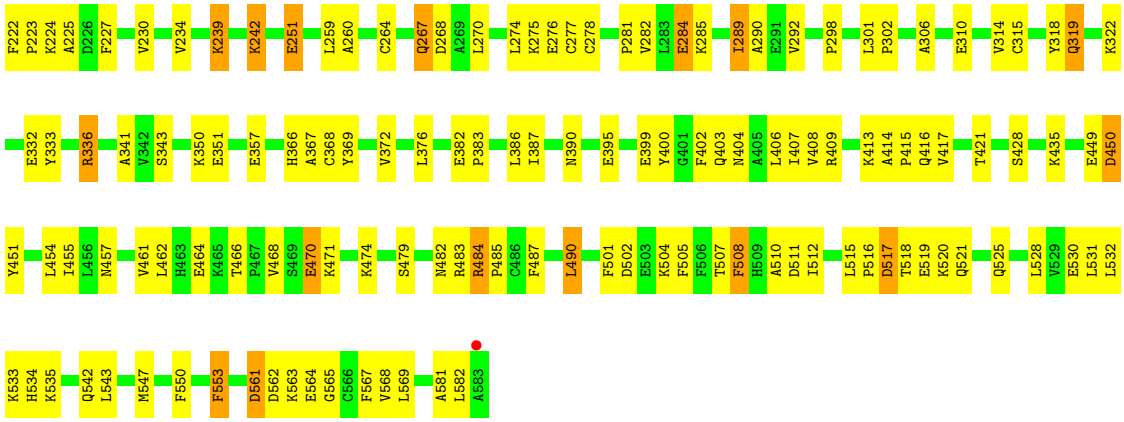
Chain A: 3% 57% 39%



• Molecule 1: Serum albumin

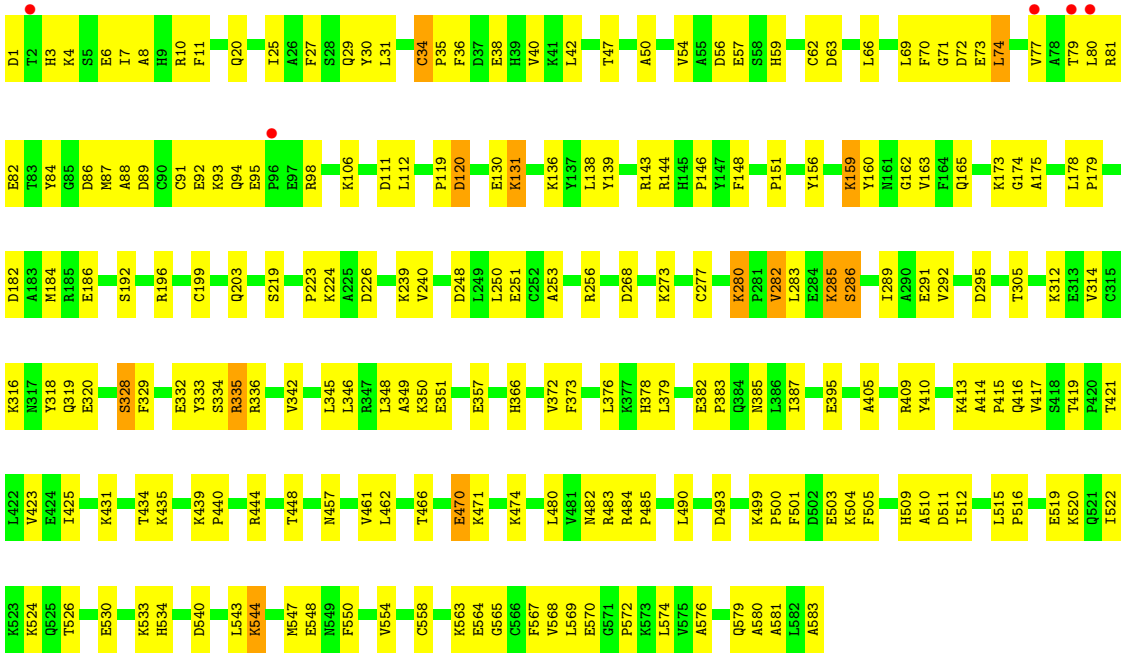
Chain B: % 64% 33%





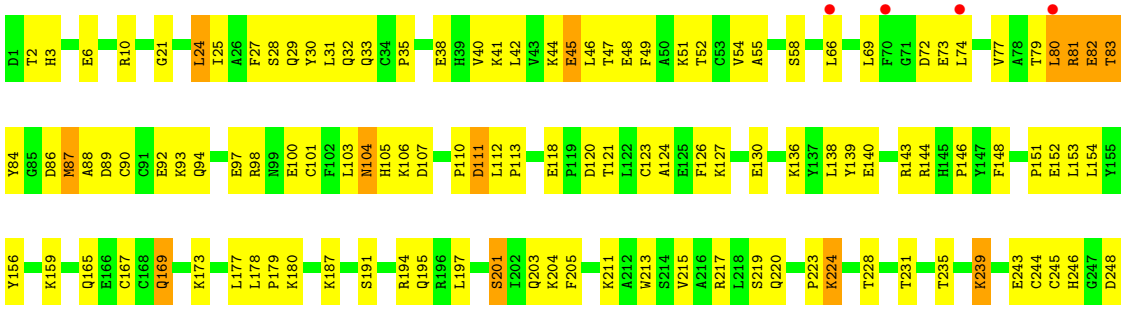
• Molecule 1: Serum albumin

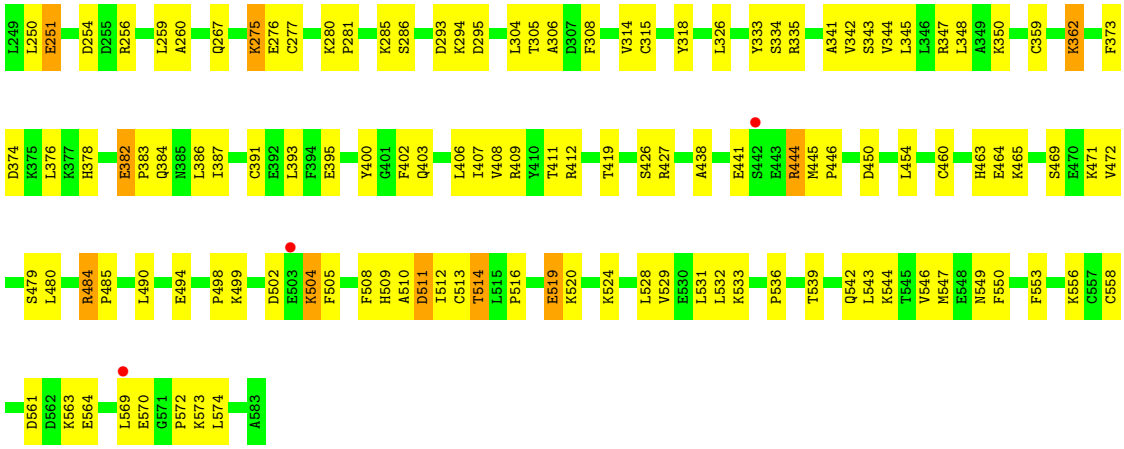
Chain C:



• Molecule 1: Serum albumin

Chain D:




L249 L250 E251 D254 D255 R256 L259 A260 Q267 K275 E276 C277 K280 P281 K285 S286 D293 K294 D295 L304 T305 A306 D307 F308 V314 C315 Y318 L326 Y333 S334 R335 A341 V342 S343 V344 L345 L346 R347 L348 A349 K350 C359 K362 F373
D374 K375 L376 K377 H378 E382 P383 Q384 N385 L386 I387 C391 E392 L393 F394 E395 Y400 G401 F402 Q403 L406 I407 V408 R409 Y410 T411 R412 T419 S426 R427 A438 E441 S442 E443 R444 M445 P446 D450 L454 C460 H463 E464 K465 S469 E470 K471 V472
S479 L480 R484 P485 L490 E494 P498 K499 D502 E503 K504 F505 F508 H509 A510 D511 I512 C513 T514 L515 P516 E519 K520 K524 L528 V529 E530 L531 L532 K533 P536 T539 Q542 L543 K544 T545 V546 M547 E548 N549 F550 F553 K556 C557 C558
D561 D562 K563 E564 L569 E570 G571 P572 K573 L574 A583

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	77.82Å 78.05Å 109.71Å 89.81° 74.54° 73.15°	Depositor
Resolution (Å)	49.00 – 2.54 49.50 – 2.54	Depositor EDS
% Data completeness (in resolution range)	90.2 (49.00-2.54) 90.2 (49.50-2.54)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.196 , 0.258 0.194 , 0.256	Depositor DCC
R_{free} test set	1414 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19129	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.15% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, PEG

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	0.95	0/4742	1.00	0/6402
1	B	0.96	0/4742	1.01	0/6402
1	C	0.98	0/4742	1.01	0/6402
1	D	0.99	0/4742	1.04	0/6402
All	All	0.97	0/18968	1.01	0/25608

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4645	0	4548	199	0
1	B	4645	0	4548	165	0
1	C	4645	0	4548	173	0
1	D	4645	0	4552	213	0
2	A	20	0	28	1	0
2	B	10	0	14	3	0
2	C	20	0	28	10	0
2	D	10	0	14	3	0
3	A	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	7	0	10	0	0
4	A	24	0	21	4	0
4	B	24	0	21	1	0
4	C	24	0	21	9	0
4	D	16	0	14	6	0
5	A	91	0	0	8	0
5	B	112	0	0	14	0
5	C	87	0	0	5	0
5	D	97	0	0	4	0
All	All	19129	0	18377	743	0

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 20.

All (743) 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:D:33:GLN:N	1:D:84:TYR:OH	1.66	1.25
1:C:174:GLY:H	4:C:605:PRO:HB3	1.12	1.12
1:C:409:ARG:HH21	2:C:601:PGE:H22	1.11	1.10
1:D:79:THR:HB	1:D:83:THR:CG2	1.82	1.10
1:D:79:THR:HB	1:D:83:THR:HG23	1.17	1.08
1:D:248:ASP:HB3	1:D:251:GLU:HG2	1.42	0.99
1:D:46:LEU:HD21	1:D:73:GLU:HG3	1.43	0.99
1:D:86:ASP:HB2	1:D:105:HIS:CD2	1.98	0.99
1:C:174:GLY:N	4:C:605:PRO:HB3	1.79	0.96
1:C:1:ASP:HB3	1:C:3:HIS:HE1	1.31	0.96
1:C:409:ARG:NH2	2:C:601:PGE:H22	1.80	0.95
1:D:86:ASP:HB2	1:D:105:HIS:HD2	1.31	0.93
1:A:577:SER:O	1:A:581:ALA:HB3	1.67	0.92
1:C:383:PRO:O	1:C:387:ILE:HG12	1.70	0.92
1:D:409:ARG:HB2	4:D:603:PRO:HG3	1.53	0.90
1:B:383:PRO:O	1:B:387:ILE:HG13	1.72	0.90
1:D:79:THR:CB	1:D:83:THR:HG23	2.03	0.87
1:A:387:ILE:HG12	1:A:448:THR:HG21	1.57	0.87
1:D:77:VAL:O	1:D:79:THR:HG23	1.74	0.87
1:C:289:ILE:O	1:C:292:VAL:HG12	1.75	0.85
1:C:20:GLN:HE21	1:C:47:THR:HG21	1.41	0.85
1:C:35:PRO:HG2	1:C:38:GLU:HG2	1.58	0.85
1:D:100:GLU:HG3	1:D:101:CYS:N	1.91	0.85
1:B:93:LYS:HG2	1:B:94:GLN:H	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ILE:O	1:A:292:VAL:HG12	1.77	0.85
1:D:33:GLN:H	1:D:84:TYR:HH	0.89	0.85
1:C:86:ASP:O	1:C:89:ASP:HB2	1.76	0.84
1:C:564:GLU:O	1:C:568:VAL:HG23	1.76	0.84
1:C:29:GLN:HG2	1:C:146:PRO:HA	1.60	0.84
1:D:197:LEU:O	1:D:201:SER:OG	1.96	0.83
1:D:508:PHE:HE2	1:D:550:PHE:HE2	1.22	0.83
1:A:544:LYS:O	1:A:548:GLU:HG3	1.79	0.82
1:A:421:THR:HG23	1:A:462:LEU:HD13	1.62	0.82
1:A:208:ARG:HG3	1:D:130:GLU:OE2	1.80	0.82
1:C:50:ALA:O	1:C:54:VAL:HG23	1.80	0.81
1:D:508:PHE:HE2	1:D:550:PHE:CE2	1.98	0.81
1:D:508:PHE:CE2	1:D:550:PHE:CE2	2.69	0.81
1:A:484:ARG:HB3	1:A:485:PRO:HD3	1.62	0.81
1:D:86:ASP:CB	1:D:105:HIS:CD2	2.64	0.81
1:C:550:PHE:HD1	1:C:574:LEU:HD11	1.47	0.80
1:D:74:LEU:O	1:D:77:VAL:HG12	1.81	0.80
1:A:494:GLU:OE2	1:A:537:LYS:NZ	2.13	0.80
1:C:1:ASP:HB3	1:C:3:HIS:CE1	2.17	0.79
1:C:409:ARG:HG3	2:C:602:PGE:H1	1.65	0.79
1:A:267:GLN:OE1	1:A:275:LYS:HD3	1.83	0.79
1:D:275:LYS:HG2	1:D:276:GLU:H	1.47	0.79
1:D:86:ASP:CB	1:D:105:HIS:HD2	1.96	0.78
1:A:74:LEU:C	1:A:74:LEU:HD23	2.04	0.78
1:A:306:ALA:HB2	4:A:606:PRO:HD3	1.64	0.77
1:D:275:LYS:HD3	1:D:275:LYS:H	1.49	0.77
1:B:386:LEU:HD11	5:B:785:HOH:O	1.84	0.76
1:C:174:GLY:H	4:C:605:PRO:CB	1.95	0.76
1:B:140:GLU:OE1	1:B:143:ARG:HD3	1.85	0.76
1:A:411:THR:HG21	1:A:532:LEU:HB3	1.68	0.75
1:C:470:GLU:CD	1:C:470:GLU:H	1.90	0.75
1:D:31:LEU:HA	1:D:84:TYR:HE2	1.52	0.74
1:B:315:CYS:O	1:B:319:GLN:HB2	1.87	0.74
1:D:77:VAL:HG13	1:D:79:THR:CG2	2.17	0.74
1:B:276:GLU:HG3	1:B:277:CYS:H	1.51	0.74
1:D:386:LEU:HD21	2:D:601:PGE:H42	1.69	0.74
1:B:471:LYS:O	1:B:474:LYS:HB3	1.87	0.73
1:D:504:LYS:HE2	1:D:505:PHE:CE1	2.21	0.73
1:B:126:PHE:CE1	1:B:130:GLU:HG3	2.24	0.73
1:D:30:TYR:HE1	1:D:103:LEU:HD23	1.54	0.73
1:C:547:MET:CE	2:C:602:PGE:O4	2.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:LEU:HB3	1:C:519:GLU:HB2	1.71	0.72
1:D:40:VAL:O	1:D:44:LYS:HG3	1.89	0.72
1:B:289:ILE:HG22	1:B:290:ALA:N	2.02	0.72
1:A:74:LEU:HD23	1:A:74:LEU:O	1.90	0.72
1:B:101:CYS:SG	1:B:105:HIS:HE1	2.12	0.72
1:A:72:ASP:HA	5:A:738:HOH:O	1.89	0.72
1:B:90:CYS:HB2	1:B:102:PHE:CE1	2.25	0.72
1:B:251:GLU:CD	1:B:251:GLU:H	1.93	0.72
1:D:80:LEU:C	1:D:82:GLU:H	1.90	0.72
1:C:93:LYS:HG2	1:C:94:GLN:H	1.54	0.71
1:D:41:LYS:O	1:D:45:GLU:HG2	1.90	0.71
1:A:330:LEU:HD13	1:A:349:ALA:HB2	1.71	0.71
1:B:267:GLN:OE1	1:B:275:LYS:HG3	1.90	0.71
1:C:84:TYR:HB3	1:C:87:MET:HE2	1.72	0.71
1:A:48:GLU:OE1	1:A:48:GLU:HA	1.91	0.70
1:B:90:CYS:SG	1:B:105:HIS:HE1	2.15	0.70
1:B:93:LYS:CG	1:B:94:GLN:H	2.03	0.70
1:B:57:GLU:HG2	5:B:783:HOH:O	1.90	0.70
1:B:16:GLU:O	1:B:20:GLN:HG3	1.91	0.70
1:B:148:PHE:CD1	1:B:153:LEU:HB2	2.26	0.70
1:A:550:PHE:CD1	1:A:574:LEU:HD21	2.26	0.70
1:D:248:ASP:HB3	1:D:251:GLU:CG	2.18	0.70
1:B:484:ARG:HB3	1:B:485:PRO:HD3	1.72	0.69
1:D:33:GLN:HG3	1:D:84:TYR:HE1	1.56	0.69
1:D:343:SER:OG	1:D:450:ASP:OD1	2.07	0.69
1:A:357:GLU:OE1	1:A:357:GLU:HA	1.93	0.69
1:B:267:GLN:OE1	1:B:275:LYS:HE3	1.92	0.69
1:B:415:PRO:HD2	1:B:416:GLN:NE2	2.08	0.69
1:A:576:ALA:HA	4:A:604:PRO:O	1.91	0.69
1:C:66:LEU:HD13	1:C:250:LEU:HD12	1.74	0.69
1:B:86:ASP:O	1:B:87:MET:HG2	1.93	0.68
1:D:84:TYR:HB3	1:D:105:HIS:CE1	2.29	0.68
1:C:405:ALA:HA	2:C:602:PGE:H32	1.74	0.68
1:C:471:LYS:HE3	1:C:490:LEU:HD22	1.76	0.68
1:C:550:PHE:CD1	1:C:574:LEU:HD11	2.29	0.68
1:B:64:LYS:HD2	1:B:68:THR:HG21	1.75	0.67
1:B:90:CYS:SG	1:B:105:HIS:CE1	2.88	0.67
1:A:577:SER:O	1:A:581:ALA:CB	2.42	0.67
1:B:302:PRO:HA	4:B:604:PRO:OXT	1.94	0.67
1:C:439:LYS:O	1:C:444:ARG:NH2	2.26	0.67
1:B:519:GLU:OE2	1:B:519:GLU:HA	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:LEU:HB3	1:C:570:GLU:OE1	1.95	0.66
1:A:42:LEU:HA	1:A:45:GLU:OE1	1.95	0.66
1:A:531:LEU:HD21	1:A:546:VAL:HG11	1.76	0.66
1:D:275:LYS:HG2	1:D:276:GLU:N	2.11	0.66
1:D:411:THR:HG21	1:D:532:LEU:HB2	1.78	0.66
1:D:471:LYS:HE2	1:D:490:LEU:HD22	1.76	0.66
1:C:520:LYS:O	1:C:524:LYS:HG3	1.96	0.65
1:D:409:ARG:CB	4:D:603:PRO:HG3	2.25	0.65
1:A:413:LYS:HD3	1:A:490:LEU:HB2	1.78	0.65
1:A:509:HIS:HB2	1:A:511:ASP:OD1	1.96	0.65
1:C:174:GLY:CA	4:C:605:PRO:HB3	2.25	0.65
1:A:484:ARG:HB3	1:A:485:PRO:CD	2.26	0.65
1:B:318:TYR:OH	1:B:322:LYS:HE3	1.96	0.65
1:C:282:VAL:HG12	5:C:739:HOH:O	1.96	0.64
1:D:508:PHE:CE2	1:D:550:PHE:HE2	2.07	0.64
1:C:84:TYR:CB	1:C:87:MET:CE	2.75	0.64
1:C:119:PRO:HB2	4:C:605:PRO:HD3	1.80	0.64
1:C:30:TYR:CD2	1:C:74:LEU:HD11	2.32	0.64
1:B:543:LEU:O	1:B:547:MET:HG3	1.97	0.64
1:A:441:GLU:HA	1:A:444:ARG:HB2	1.78	0.64
1:B:140:GLU:OE1	1:B:144:ARG:NH2	2.31	0.64
1:D:33:GLN:N	1:D:84:TYR:HH	1.72	0.64
1:B:36:PHE:HB2	1:B:139:TYR:CE2	2.33	0.64
1:A:282:VAL:O	1:A:285:LYS:HB3	1.98	0.63
1:C:71:GLY:HA3	1:C:98:ARG:CZ	2.28	0.63
1:C:516:PRO:HG2	1:C:519:GLU:HG2	1.80	0.63
1:A:149:TYR:OH	1:A:256:ARG:HD2	1.98	0.63
1:A:148:PHE:CD1	1:A:153:LEU:HB2	2.34	0.63
1:C:328:SER:O	1:C:332:GLU:HG2	1.99	0.63
1:D:93:LYS:O	1:D:98:ARG:HD3	1.99	0.63
1:D:77:VAL:HG13	1:D:79:THR:HG23	1.80	0.62
1:D:203:GLN:HA	1:D:203:GLN:OE1	1.99	0.62
1:A:5:SER:CB	1:A:62:CYS:O	2.47	0.62
1:D:251:GLU:H	1:D:251:GLU:CD	2.02	0.62
1:A:81:ARG:O	1:A:84:TYR:HD2	1.82	0.62
1:A:223:PRO:HD2	1:A:295:ASP:HB3	1.82	0.62
1:C:416:GLN:OE1	1:C:416:GLN:N	2.27	0.62
1:C:151:PRO:HG3	1:C:253:ALA:HA	1.81	0.62
1:C:120:ASP:OD1	4:C:605:PRO:N	2.33	0.62
1:A:530:GLU:HA	1:A:530:GLU:OE1	1.99	0.62
1:D:24:LEU:HD12	1:D:28:SER:OG	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:GLN:HE21	1:A:47:THR:HG21	1.64	0.61
1:C:382:GLU:OE1	1:C:383:PRO:HD3	2.00	0.61
1:A:15:GLY:O	1:A:19:PHE:HB2	1.99	0.61
1:A:264:CYS:O	1:A:267:GLN:HG2	2.00	0.61
1:C:415:PRO:O	1:C:533:LYS:HE3	2.00	0.61
1:D:277:CYS:O	1:D:285:LYS:HG3	2.00	0.61
1:A:504:LYS:HE3	1:A:505:PHE:CE2	2.35	0.61
1:C:414:ALA:O	1:C:417:VAL:HG23	2.00	0.61
1:A:374:ASP:N	1:A:374:ASP:OD1	2.33	0.61
1:A:281:PRO:HG2	1:A:284:GLU:HG3	1.82	0.61
1:C:38:GLU:OE1	1:C:38:GLU:HA	2.01	0.61
1:B:332:GLU:OE1	1:B:336:ARG:NH2	2.34	0.61
1:C:421:THR:O	1:C:425:ILE:HG12	2.01	0.60
1:D:33:GLN:CA	1:D:84:TYR:OH	2.49	0.60
1:D:79:THR:CB	1:D:83:THR:CG2	2.71	0.60
1:D:246:HIS:O	1:D:246:HIS:ND1	2.35	0.60
1:A:471:LYS:HD2	1:A:493:ASP:OD2	2.01	0.60
1:B:507:THR:C	1:B:508:PHE:CD2	2.74	0.60
1:B:516:PRO:HB2	5:B:718:HOH:O	2.01	0.60
1:D:409:ARG:HD3	2:D:601:PGE:H6	1.84	0.60
1:B:351:GLU:HB3	1:B:376:LEU:HD22	1.83	0.60
1:B:289:ILE:O	1:B:292:VAL:HG12	2.02	0.60
1:B:56:ASP:HB3	5:B:790:HOH:O	2.00	0.59
1:A:194:ARG:HA	1:A:454:LEU:HD22	1.84	0.59
1:B:225:ALA:HB2	1:B:270:LEU:HD23	1.85	0.59
1:D:382:GLU:OE1	1:D:383:PRO:HD3	2.01	0.59
1:D:547:MET:HG2	5:D:780:HOH:O	2.01	0.59
1:D:550:PHE:CE2	1:D:574:LEU:HD21	2.38	0.59
1:A:140:GLU:HA	1:A:143:ARG:HD3	1.84	0.59
1:B:507:THR:C	1:B:508:PHE:HD2	2.06	0.59
1:B:276:GLU:HG3	1:B:277:CYS:N	2.17	0.59
1:B:298:PRO:HB2	1:B:301:LEU:HD21	1.84	0.59
1:B:421:THR:HG23	1:B:462:LEU:HD12	1.84	0.59
1:C:84:TYR:CG	1:C:87:MET:CE	2.85	0.59
1:C:395:GLU:OE1	1:C:395:GLU:HA	2.02	0.59
1:D:148:PHE:CD1	1:D:153:LEU:HB2	2.37	0.59
1:D:30:TYR:C	1:D:31:LEU:HD23	2.23	0.59
1:C:71:GLY:C	1:C:98:ARG:NH2	2.55	0.59
1:C:581:ALA:O	1:C:583:ALA:O	2.21	0.59
1:A:289:ILE:HG22	1:A:290:ALA:N	2.18	0.58
1:C:20:GLN:NE2	1:C:47:THR:HG21	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:ASP:O	1:C:92:GLU:N	2.32	0.58
1:D:304:LEU:O	1:D:306:ALA:N	2.37	0.58
1:B:450:ASP:O	1:B:454:LEU:HG	2.03	0.58
1:D:391:CYS:O	1:D:395:GLU:HG2	2.02	0.58
1:B:90:CYS:CB	1:B:102:PHE:CE1	2.86	0.58
1:C:173:LYS:HB2	4:C:605:PRO:HA	1.86	0.58
1:C:580:ALA:O	1:C:583:ALA:HB3	2.03	0.58
1:B:46:LEU:O	1:B:50:ALA:N	2.34	0.58
1:B:112:LEU:HB3	1:B:113:PRO:HD2	1.86	0.58
1:C:501:PHE:CD2	1:C:579:GLN:NE2	2.72	0.58
1:B:90:CYS:HB2	1:B:102:PHE:HE1	1.66	0.58
1:A:86:ASP:OD2	1:A:86:ASP:N	2.36	0.58
1:C:329:PHE:CE2	1:C:349:ALA:HA	2.39	0.58
1:C:544:LYS:HA	1:C:547:MET:HE3	1.85	0.58
1:D:33:GLN:HG3	1:D:84:TYR:CE1	2.38	0.58
1:D:33:GLN:CG	1:D:84:TYR:HE1	2.16	0.58
1:D:69:LEU:O	1:D:73:GLU:HG2	2.04	0.58
1:A:539:THR:HG22	1:A:541:GLU:H	1.68	0.57
1:C:547:MET:HE1	2:C:602:PGE:O4	2.03	0.57
1:C:316:LYS:O	1:C:320:GLU:HG2	2.04	0.57
1:C:219:SER:HB2	1:C:334:SER:HB2	1.87	0.57
1:D:38:GLU:O	1:D:42:LEU:HG	2.05	0.57
1:D:173:LYS:O	1:D:177:LEU:HD13	2.02	0.57
1:A:471:LYS:HE2	1:A:490:LEU:HD22	1.84	0.57
1:D:419:THR:HG23	1:D:529:VAL:HG11	1.85	0.57
1:B:44:LYS:HG3	1:B:45:GLU:HG3	1.86	0.57
1:C:273:LYS:HD2	1:C:295:ASP:HA	1.85	0.57
1:B:508:PHE:CD2	1:B:508:PHE:N	2.71	0.57
1:C:84:TYR:CG	1:C:87:MET:HE1	2.40	0.57
1:D:259:LEU:HD12	1:D:259:LEU:O	2.05	0.56
1:D:33:GLN:CG	1:D:84:TYR:CE1	2.88	0.56
1:D:167:CYS:HB3	1:D:177:LEU:HD12	1.87	0.56
1:A:138:LEU:HD21	1:A:157:ALA:HB2	1.87	0.56
1:B:81:ARG:HA	1:B:88:ALA:HB2	1.88	0.56
1:C:31:LEU:HD22	1:C:80:LEU:HD22	1.86	0.56
1:D:25:ILE:HD11	1:D:138:LEU:HD22	1.87	0.56
1:D:450:ASP:O	1:D:454:LEU:HG	2.05	0.56
1:D:228:THR:O	1:D:231:THR:HB	2.05	0.56
1:D:86:ASP:O	1:D:89:ASP:OD2	2.22	0.56
1:C:466:THR:O	1:C:466:THR:HG23	2.05	0.56
1:D:531:LEU:HD11	1:D:546:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:ARG:HB3	1:C:485:PRO:HD3	1.86	0.56
1:A:82:GLU:HA	1:A:88:ALA:HB2	1.88	0.56
1:B:415:PRO:O	1:B:533:LYS:HE2	2.06	0.56
1:C:554:VAL:O	1:C:558:CYS:HB2	2.06	0.56
1:D:77:VAL:O	1:D:77:VAL:HG13	2.06	0.55
1:A:79:THR:HG23	1:A:91:CYS:SG	2.46	0.55
1:A:375:LYS:HD3	1:A:375:LYS:C	2.27	0.55
1:D:445:MET:O	1:D:446:PRO:C	2.40	0.55
1:A:407:ILE:HG12	1:A:426:SER:HB3	1.88	0.55
1:D:293:ASP:OD1	1:D:294:LYS:N	2.39	0.55
1:A:139:TYR:O	1:A:143:ARG:HG2	2.05	0.55
1:B:366:HIS:HA	1:B:369:TYR:CZ	2.41	0.55
1:C:4:LYS:HZ3	1:C:57:GLU:HB3	1.72	0.55
1:B:106:LYS:HG2	1:B:146:PRO:HB2	1.87	0.55
1:A:299:GLU:OE1	1:A:299:GLU:HA	2.05	0.55
1:A:400:TYR:OH	1:A:524:LYS:NZ	2.35	0.55
1:D:239:LYS:O	1:D:243:GLU:HG3	2.06	0.55
1:C:434:THR:O	1:D:561:ASP:HB2	2.06	0.55
1:D:97:GLU:O	1:D:100:GLU:HG2	2.07	0.55
1:B:531:LEU:HD11	1:B:582:LEU:HD11	1.87	0.54
1:C:80:LEU:HB2	1:C:88:ALA:HB2	1.89	0.54
1:D:47:THR:O	1:D:51:LYS:HG3	2.06	0.54
1:A:84:TYR:CD1	1:A:87:MET:HG3	2.42	0.54
1:B:139:TYR:O	1:B:143:ARG:HG2	2.06	0.54
1:B:216:ALA:O	1:B:220:GLN:HG3	2.07	0.54
1:B:251:GLU:CD	1:B:251:GLU:N	2.60	0.54
1:C:256:ARG:CZ	1:C:286:SER:HB2	2.38	0.54
1:D:350:LYS:NZ	1:D:479:SER:OG	2.40	0.54
1:B:59:HIS:HB2	5:B:790:HOH:O	2.06	0.54
1:A:261:LYS:O	1:A:264:CYS:N	2.40	0.54
1:A:177:LEU:O	1:A:180:LYS:N	2.41	0.54
1:B:184:MET:O	1:B:188:VAL:HG23	2.08	0.54
1:D:386:LEU:HG	2:D:601:PGE:H3	1.88	0.54
1:D:406:LEU:HD23	1:D:409:ARG:HD2	1.90	0.54
1:A:24:LEU:HB2	1:A:43:VAL:HG21	1.89	0.54
1:B:112:LEU:CD1	1:B:143:ARG:HE	2.21	0.54
1:B:415:PRO:HD2	1:B:416:GLN:HE22	1.72	0.54
1:D:223:PRO:HD2	1:D:295:ASP:HB3	1.89	0.54
1:B:84:TYR:O	1:B:86:ASP:N	2.39	0.53
1:B:508:PHE:HD2	1:B:508:PHE:N	2.07	0.53
1:D:412:ARG:NH1	4:D:603:PRO:OXT	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:VAL:HG12	5:B:772:HOH:O	2.09	0.53
1:B:501:PHE:HB2	1:B:534:HIS:CE1	2.44	0.53
1:C:130:GLU:OE1	1:C:165:GLN:NE2	2.41	0.53
1:C:348:LEU:HD23	1:C:379:LEU:HD12	1.91	0.53
1:A:253:ALA:O	1:A:254:ASP:C	2.45	0.53
1:B:542:GLN:NE2	1:B:581:ALA:O	2.41	0.53
1:A:424:GLU:HG2	1:A:425:ILE:HD13	1.88	0.53
1:A:582:LEU:N	1:A:582:LEU:HD12	2.24	0.53
1:B:112:LEU:HD13	1:B:143:ARG:NH2	2.23	0.53
1:B:414:ALA:O	1:B:417:VAL:HG23	2.08	0.53
1:C:378:HIS:CE1	1:C:379:LEU:HG	2.43	0.53
1:D:54:VAL:HG12	1:D:54:VAL:O	2.09	0.53
1:A:471:LYS:HE2	1:A:490:LEU:CD2	2.38	0.53
1:B:400:TYR:CE1	1:B:521:GLN:HG2	2.43	0.53
1:B:428:SER:HB3	1:B:455:ILE:HG12	1.90	0.53
1:C:419:THR:O	1:C:423:VAL:HG23	2.09	0.53
1:D:112:LEU:HB3	1:D:113:PRO:HD2	1.91	0.53
1:A:61:GLY:C	1:A:63:ASP:H	2.10	0.53
1:B:260:ALA:HB1	1:B:285:LYS:HD2	1.91	0.53
1:D:572:PRO:O	1:D:573:LYS:C	2.46	0.53
1:A:86:ASP:HB3	1:A:105:HIS:CD2	2.44	0.53
1:B:281:PRO:HG2	1:B:284:GLU:HB2	1.90	0.53
1:C:94:GLN:O	1:C:98:ARG:N	2.40	0.53
1:D:156:TYR:HE1	1:D:187:LYS:HD2	1.74	0.53
1:A:45:GLU:O	1:A:48:GLU:HB2	2.09	0.53
1:A:256:ARG:NH1	5:A:709:HOH:O	2.39	0.53
1:C:148:PHE:CE2	1:C:192:SER:HB2	2.44	0.53
1:D:106:LYS:HG2	1:D:146:PRO:HB2	1.91	0.53
1:C:409:ARG:O	1:C:413:LYS:HG3	2.10	0.52
1:D:24:LEU:HD11	1:D:139:TYR:HB2	1.90	0.52
1:D:194:ARG:HA	1:D:454:LEU:HD22	1.90	0.52
1:C:256:ARG:NH2	5:C:705:HOH:O	2.41	0.52
1:A:5:SER:HB3	1:A:62:CYS:O	2.08	0.52
1:C:174:GLY:HA3	4:C:605:PRO:HB3	1.91	0.52
1:D:438:ALA:HB3	5:D:732:HOH:O	2.10	0.52
1:A:377:LYS:HE2	5:A:780:HOH:O	2.08	0.52
1:B:470:GLU:CD	1:B:470:GLU:H	2.12	0.52
1:C:329:PHE:HE2	1:C:349:ALA:HA	1.75	0.52
1:A:3:HIS:ND1	1:A:6:GLU:OE2	2.43	0.52
1:C:511:ASP:O	1:C:515:LEU:HG	2.10	0.52
1:C:576:ALA:HA	5:C:716:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:LEU:O	1:C:379:LEU:HB2	2.09	0.52
1:A:112:LEU:HB3	1:A:113:PRO:HD2	1.92	0.52
1:B:402:PHE:CZ	2:B:601:PGE:H6	2.45	0.52
1:D:213:TRP:CE2	1:D:342:VAL:HG11	2.45	0.52
1:D:528:LEU:O	1:D:532:LEU:CD2	2.57	0.52
1:A:412:ARG:O	1:A:492:LEU:HA	2.10	0.52
1:B:501:PHE:CG	1:B:502:ASP:N	2.78	0.52
1:D:318:TYR:HE1	1:D:326:LEU:HD11	1.74	0.52
1:A:282:VAL:HG13	1:A:283:LEU:N	2.24	0.51
1:A:106:LYS:HG2	1:A:146:PRO:HB2	1.91	0.51
1:A:555:ASP:O	1:A:557:CYS:N	2.43	0.51
1:B:221:LYS:NZ	1:B:290:ALA:O	2.44	0.51
1:B:484:ARG:HB3	1:B:485:PRO:CD	2.41	0.51
1:C:174:GLY:O	1:C:178:LEU:HB2	2.11	0.51
1:A:50:ALA:O	1:A:54:VAL:HG23	2.10	0.51
1:C:251:GLU:OE1	1:C:251:GLU:N	2.35	0.51
1:A:539:THR:HG22	1:A:541:GLU:N	2.26	0.51
1:D:359:CYS:HA	1:D:362:LYS:HG3	1.93	0.51
1:A:219:SER:HB2	1:A:334:SER:HB2	1.93	0.51
1:B:71:GLY:O	1:B:75:CYS:N	2.41	0.51
1:B:220:GLN:O	1:B:223:PRO:HD3	2.10	0.51
1:A:150:ALA:O	1:A:151:PRO:C	2.47	0.51
1:A:438:ALA:HB3	5:B:768:HOH:O	2.09	0.51
1:C:224:LYS:NZ	1:C:268:ASP:O	2.33	0.51
1:C:277:CYS:HA	1:C:280:LYS:HD2	1.92	0.51
1:A:540:ASP:HA	1:A:543:LEU:HD12	1.93	0.51
1:D:304:LEU:O	1:D:305:THR:C	2.49	0.51
1:D:148:PHE:CE1	1:D:153:LEU:HB2	2.46	0.50
1:B:33:GLN:OE1	1:B:112:LEU:HD21	2.11	0.50
1:C:4:LYS:NZ	1:C:57:GLU:HB3	2.27	0.50
1:C:38:GLU:OE1	1:C:38:GLU:CA	2.59	0.50
1:D:528:LEU:O	1:D:532:LEU:HD22	2.11	0.50
1:A:507:THR:CG2	1:A:509:HIS:CE1	2.95	0.50
1:D:556:LYS:NZ	1:D:570:GLU:HG3	2.26	0.50
1:B:314:VAL:HG12	1:B:315:CYS:N	2.25	0.50
1:D:42:LEU:HA	1:D:45:GLU:CG	2.42	0.50
1:D:469:SER:OG	1:D:472:VAL:HG23	2.11	0.50
1:A:444:ARG:O	1:A:447:CYS:HB3	2.12	0.50
1:B:451:TYR:O	1:B:455:ILE:HD12	2.11	0.50
1:C:63:ASP:OD2	1:C:63:ASP:N	2.36	0.49
1:C:156:TYR:O	1:C:184:MET:HE3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:CZ	1:A:286:SER:HB3	2.41	0.49
1:B:470:GLU:CD	1:B:470:GLU:N	2.65	0.49
1:C:199:CYS:O	1:C:203:GLN:HB2	2.12	0.49
1:A:140:GLU:O	1:A:144:ARG:NH1	2.44	0.49
1:A:306:ALA:HA	1:A:310:GLU:CD	2.33	0.49
1:B:147:TYR:O	1:B:148:PHE:C	2.48	0.49
1:B:166:GLU:O	1:B:169:GLN:HG3	2.12	0.49
1:B:413:LYS:HB3	1:B:490:LEU:HB3	1.95	0.49
1:D:69:LEU:O	1:D:73:GLU:CG	2.60	0.49
1:D:72:ASP:OD1	1:D:73:GLU:HG2	2.13	0.49
1:A:195:GLN:O	1:A:195:GLN:HG3	2.10	0.49
1:A:545:THR:CG2	1:A:582:LEU:HD21	2.42	0.49
1:B:195:GLN:O	1:B:195:GLN:HG3	2.12	0.49
1:B:535:LYS:HD2	5:B:801:HOH:O	2.12	0.49
1:B:562:ASP:OD2	1:B:565:GLY:HA3	2.13	0.49
1:C:70:PHE:O	1:C:74:LEU:HG	2.13	0.49
1:D:27:PHE:HE1	1:D:42:LEU:HB3	1.78	0.49
1:D:539:THR:OG1	1:D:542:GLN:HG3	2.12	0.49
1:B:22:LEU:HG	1:B:154:LEU:HD11	1.94	0.49
1:B:24:LEU:HD21	1:B:36:PHE:HE1	1.77	0.49
1:C:36:PHE:HB2	1:C:139:TYR:CE2	2.47	0.49
1:C:160:TYR:O	1:C:163:VAL:HB	2.11	0.49
1:C:544:LYS:HA	1:C:547:MET:CE	2.41	0.49
1:B:93:LYS:CG	1:B:94:GLN:N	2.74	0.49
1:A:84:TYR:CG	1:A:87:MET:HG3	2.47	0.49
1:A:95:GLU:HA	1:A:96:PRO:HA	1.59	0.49
1:A:390:ASN:OD1	1:A:409:ARG:NH1	2.44	0.49
1:A:138:LEU:CD2	1:A:157:ALA:HB2	2.43	0.49
1:D:100:GLU:HG3	1:D:101:CYS:H	1.69	0.49
1:B:230:VAL:O	1:B:234:VAL:HG23	2.12	0.49
1:C:56:ASP:HB3	5:C:776:HOH:O	2.13	0.49
1:C:540:ASP:O	1:C:543:LEU:HB2	2.12	0.49
1:D:126:PHE:HZ	1:D:165:GLN:HG3	1.77	0.49
1:A:20:GLN:NE2	1:A:47:THR:HG21	2.27	0.49
1:A:77:VAL:HG13	1:A:78:ALA:H	1.78	0.49
1:B:101:CYS:SG	1:B:105:HIS:CE1	3.01	0.49
1:B:141:VAL:O	1:B:145:HIS:HD2	1.95	0.49
1:C:162:GLY:O	1:C:165:GLN:HB2	2.13	0.48
1:A:345:LEU:HA	1:A:348:LEU:HD12	1.95	0.48
1:C:34:CYS:H	1:C:84:TYR:HH	1.60	0.48
1:A:82:GLU:CA	1:A:88:ALA:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:PHE:CD1	1:C:54:VAL:HG21	2.48	0.48
1:D:304:LEU:C	1:D:306:ALA:N	2.64	0.48
1:D:403:GLN:HG2	1:D:427:ARG:HA	1.95	0.48
1:A:419:THR:HG23	1:A:529:VAL:HG11	1.96	0.48
1:A:516:PRO:HG2	1:A:519:GLU:CG	2.44	0.48
1:A:235:THR:HG22	1:A:236:ASP:OD1	2.13	0.48
1:A:501:PHE:HD2	1:A:534:HIS:CD2	2.31	0.48
1:A:550:PHE:O	1:A:554:VAL:HG23	2.13	0.48
4:A:606:PRO:HD2	5:A:747:HOH:O	2.13	0.48
1:B:553:PHE:CZ	1:B:567:PHE:CD1	3.01	0.48
1:D:3:HIS:N	1:D:6:GLU:OE2	2.46	0.48
1:D:156:TYR:CE1	1:D:187:LYS:HD2	2.47	0.48
1:A:347:ARG:HG2	1:A:481:VAL:CG1	2.44	0.48
1:C:66:LEU:CD1	1:C:250:LEU:HD12	2.42	0.48
1:C:182:ASP:O	1:C:186:GLU:HG2	2.14	0.48
1:D:81:ARG:HB3	1:D:81:ARG:CZ	2.43	0.48
1:D:204:LYS:NZ	1:D:464:GLU:HG3	2.28	0.48
1:A:347:ARG:HG2	1:A:481:VAL:HG12	1.95	0.48
1:C:510:ALA:HA	1:C:567:PHE:CE2	2.48	0.48
1:D:498:PRO:HG3	1:D:536:PRO:HG2	1.94	0.48
1:A:507:THR:HG22	1:A:509:HIS:CE1	2.49	0.48
1:A:510:ALA:HB3	1:B:179:PRO:HB3	1.96	0.48
1:B:561:ASP:OD1	1:B:561:ASP:N	2.45	0.48
1:C:71:GLY:C	1:C:98:ARG:HH22	2.17	0.48
1:D:80:LEU:C	1:D:82:GLU:N	2.62	0.48
1:D:387:ILE:HD11	1:D:445:MET:HG3	1.95	0.48
1:C:289:ILE:O	1:C:292:VAL:CG1	2.55	0.48
1:A:393:LEU:HD12	1:A:397:HIS:ND1	2.29	0.47
1:C:6:GLU:OE2	1:C:10:ARG:NE	2.47	0.47
1:D:100:GLU:CG	1:D:101:CYS:N	2.71	0.47
1:D:348:LEU:CD2	1:D:376:LEU:HB3	2.44	0.47
1:A:127:LYS:HD2	1:A:127:LYS:O	2.14	0.47
1:B:139:TYR:OH	1:B:143:ARG:NH1	2.47	0.47
1:C:25:ILE:HD11	1:C:138:LEU:HD22	1.95	0.47
1:C:372:VAL:HG13	1:C:373:PHE:N	2.28	0.47
1:D:549:ASN:HB3	5:D:758:HOH:O	2.14	0.47
1:B:504:LYS:HE2	5:B:775:HOH:O	2.14	0.47
1:C:42:LEU:HD22	1:C:73:GLU:HB3	1.95	0.47
1:D:25:ILE:HD13	1:D:153:LEU:HD23	1.97	0.47
1:D:82:GLU:C	1:D:83:THR:OG1	2.53	0.47
1:D:348:LEU:HD22	1:D:376:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:PRO:O	1:B:144:ARG:NH1	2.48	0.47
1:C:457:ASN:O	1:C:461:VAL:HG13	2.13	0.47
1:D:558:CYS:O	1:D:563:LYS:HE3	2.14	0.47
1:B:409:ARG:NH2	2:B:601:PGE:H22	2.30	0.47
1:B:416:GLN:CD	1:B:416:GLN:H	2.17	0.47
1:C:59:HIS:HB3	1:C:62:CYS:SG	2.54	0.47
1:C:159:LYS:O	1:C:160:TYR:C	2.53	0.47
1:C:36:PHE:HB2	1:C:139:TYR:CD2	2.50	0.47
1:C:547:MET:HE2	2:C:602:PGE:O4	2.13	0.47
1:D:304:LEU:C	1:D:306:ALA:H	2.18	0.47
1:A:29:GLN:HG2	1:A:146:PRO:HA	1.97	0.47
1:A:35:PRO:HA	1:A:139:TYR:OH	2.15	0.47
1:A:44:LYS:O	1:A:48:GLU:N	2.48	0.47
1:A:531:LEU:HD21	1:A:546:VAL:CG1	2.45	0.47
1:B:22:LEU:CD2	1:B:150:ALA:HB1	2.45	0.47
1:C:395:GLU:OE1	1:C:395:GLU:CA	2.62	0.47
1:B:519:GLU:OE2	1:B:519:GLU:CA	2.61	0.47
1:C:160:TYR:HB2	1:C:184:MET:HE1	1.96	0.47
1:D:219:SER:HB2	1:D:334:SER:HB2	1.96	0.47
1:D:52:THR:O	1:D:55:ALA:N	2.45	0.47
1:D:382:GLU:OE1	1:D:383:PRO:CD	2.63	0.47
1:C:79:THR:HG22	1:C:82:GLU:HB3	1.96	0.47
1:D:219:SER:HB2	1:D:334:SER:CB	2.45	0.46
1:D:553:PHE:HE1	1:D:570:GLU:HB2	1.80	0.46
1:A:82:GLU:OE2	1:A:88:ALA:HB1	2.14	0.46
1:A:93:LYS:HE2	1:A:97:GLU:CD	2.35	0.46
1:B:414:ALA:HB1	1:B:417:VAL:CG2	2.45	0.46
1:D:66:LEU:HD13	1:D:250:LEU:HD12	1.97	0.46
1:A:86:ASP:HB2	1:A:105:HIS:ND1	2.29	0.46
1:B:264:CYS:O	1:B:267:GLN:HB3	2.16	0.46
1:C:421:THR:HG23	1:C:462:LEU:CD1	2.44	0.46
1:D:386:LEU:HD12	1:D:386:LEU:HA	1.78	0.46
1:A:40:VAL:O	1:A:44:LYS:HG2	2.15	0.46
1:A:256:ARG:CZ	1:A:286:SER:CB	2.93	0.46
1:A:282:VAL:HG13	1:A:283:LEU:HG	1.98	0.46
1:A:511:ASP:CG	1:B:175:ALA:HA	2.35	0.46
1:C:223:PRO:HD2	1:C:295:ASP:HB3	1.97	0.46
1:D:151:PRO:HB2	1:D:256:ARG:NH1	2.31	0.46
1:A:66:LEU:HA	1:A:66:LEU:HD23	1.57	0.46
1:A:138:LEU:HD21	1:A:157:ALA:CB	2.45	0.46
1:B:501:PHE:CD2	1:B:502:ASP:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:528:LEU:O	1:D:528:LEU:HD12	2.15	0.46
1:A:122:LEU:HD23	1:A:125:GLU:OE1	2.15	0.46
1:A:414:ALA:O	1:A:416:GLN:N	2.48	0.46
1:A:506:PHE:O	1:A:508:PHE:CD2	2.68	0.46
1:B:35:PRO:O	1:B:38:GLU:HG2	2.15	0.46
1:A:139:TYR:O	1:A:143:ARG:CG	2.64	0.46
1:A:531:LEU:CD2	1:A:546:VAL:HG11	2.45	0.46
1:B:224:LYS:HG2	5:B:717:HOH:O	2.16	0.46
1:C:69:LEU:O	1:C:73:GLU:HG2	2.16	0.46
1:C:332:GLU:OE1	1:C:332:GLU:HA	2.15	0.46
1:C:421:THR:HG23	1:C:462:LEU:HD12	1.98	0.46
1:C:439:LYS:HB3	1:C:440:PRO:HD2	1.96	0.46
2:C:602:PGE:H6	2:C:602:PGE:H42	1.70	0.46
1:D:29:GLN:HG2	1:D:146:PRO:HA	1.97	0.46
1:A:504:LYS:HE3	1:A:505:PHE:CZ	2.51	0.46
2:A:601:PGE:H4	2:A:601:PGE:O4	2.15	0.46
1:B:395:GLU:HG3	5:B:789:HOH:O	2.16	0.46
1:C:501:PHE:HB2	1:C:534:HIS:CE1	2.50	0.46
1:A:564:GLU:HG2	5:B:786:HOH:O	2.15	0.46
1:A:572:PRO:O	1:A:573:LYS:C	2.54	0.46
1:B:318:TYR:OH	1:B:357:GLU:OE1	2.34	0.46
1:C:219:SER:O	1:C:335:ARG:HA	2.15	0.46
1:A:489:ASP:O	1:A:490:LEU:C	2.53	0.45
1:D:80:LEU:HG	1:D:81:ARG:N	2.31	0.45
1:C:179:PRO:HB3	1:D:510:ALA:HB3	1.98	0.45
1:C:572:PRO:HB2	5:C:722:HOH:O	2.16	0.45
1:D:393:LEU:HD23	1:D:402:PHE:CD1	2.51	0.45
1:D:409:ARG:HB2	4:D:603:PRO:CG	2.37	0.45
1:D:509:HIS:HB2	1:D:511:ASP:OD1	2.16	0.45
1:A:36:PHE:CD2	1:A:136:LYS:HG3	2.51	0.45
1:B:242:LYS:O	1:B:242:LYS:HG2	2.16	0.45
1:C:175:ALA:HA	1:D:511:ASP:OD1	2.15	0.45
1:C:510:ALA:HB3	1:D:179:PRO:HB3	1.97	0.45
1:A:408:VAL:HG12	1:A:412:ARG:HD2	1.98	0.45
1:D:24:LEU:HD12	1:D:24:LEU:O	2.17	0.45
1:D:46:LEU:HD23	1:D:46:LEU:HA	1.67	0.45
1:A:61:GLY:C	1:A:63:ASP:N	2.70	0.45
1:A:416:GLN:N	1:A:416:GLN:OE1	2.39	0.45
1:B:93:LYS:HG2	1:B:94:GLN:N	2.19	0.45
1:D:528:LEU:HD22	1:D:547:MET:SD	2.55	0.45
1:A:344:VAL:HG11	1:A:445:MET:HE1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:MET:HB2	1:B:105:HIS:CE1	2.51	0.45
1:B:487:PHE:O	1:B:490:LEU:HB2	2.17	0.45
1:C:482:ASN:C	1:C:485:PRO:HD2	2.37	0.45
1:A:375:LYS:HD3	1:A:376:LEU:N	2.32	0.45
1:A:417:VAL:HG12	1:A:418:SER:O	2.17	0.45
1:A:516:PRO:HG2	1:A:519:GLU:HG3	1.98	0.45
1:A:553:PHE:HA	1:A:556:LYS:HG2	1.98	0.45
1:B:390:ASN:OD1	1:B:409:ARG:NH1	2.28	0.45
1:D:509:HIS:O	1:D:512:ILE:HG22	2.17	0.45
1:D:516:PRO:HG2	1:D:519:GLU:HG3	1.98	0.45
1:A:198:ARG:HD3	1:A:241:HIS:CD2	2.52	0.45
1:A:215:VAL:HG23	1:A:234:VAL:HG11	1.99	0.45
1:B:517:ASP:O	1:B:518:THR:C	2.54	0.45
1:C:4:LYS:NZ	1:C:57:GLU:CB	2.80	0.45
1:A:36:PHE:HB2	1:A:139:TYR:CD2	2.51	0.45
1:A:71:GLY:O	1:A:75:CYS:HB2	2.17	0.45
1:C:88:ALA:O	1:C:91:CYS:HB3	2.17	0.45
1:D:101:CYS:O	1:D:104:ASN:HB2	2.16	0.45
1:A:456:LEU:O	1:A:459:LEU:HB3	2.17	0.45
1:A:458:ARG:O	1:A:459:LEU:C	2.55	0.45
1:D:27:PHE:CE1	1:D:42:LEU:HB3	2.51	0.45
1:A:546:VAL:HG23	1:A:582:LEU:HD22	1.99	0.44
1:C:470:GLU:OE1	1:C:470:GLU:N	2.29	0.44
1:A:177:LEU:HD12	1:A:178:LEU:N	2.32	0.44
1:B:44:LYS:HG3	1:B:45:GLU:N	2.31	0.44
1:C:332:GLU:OE1	1:C:336:ARG:NH2	2.50	0.44
1:C:413:LYS:HD3	1:C:490:LEU:HB2	2.00	0.44
1:A:275:LYS:HD2	1:A:275:LYS:HA	1.60	0.44
1:B:402:PHE:HZ	2:B:601:PGE:H6	1.82	0.44
1:D:514:THR:O	1:D:514:THR:CG2	2.65	0.44
1:B:11:PHE:CD1	1:B:54:VAL:HG21	2.52	0.44
1:B:399:GLU:O	1:B:403:GLN:HG3	2.18	0.44
1:D:387:ILE:HG22	1:D:444:ARG:HD3	1.98	0.44
1:A:66:LEU:O	1:A:70:PHE:HD2	2.00	0.44
1:A:399:GLU:HG2	5:A:729:HOH:O	2.18	0.44
1:B:457:ASN:O	1:B:461:VAL:HG13	2.17	0.44
1:B:512:ILE:O	1:B:520:LYS:HE3	2.17	0.44
1:B:402:PHE:CE1	1:B:406:LEU:HD21	2.53	0.44
1:D:213:TRP:CD1	1:D:213:TRP:C	2.90	0.44
1:D:341:ALA:HA	1:D:446:PRO:HA	1.99	0.44
1:D:347:ARG:CZ	1:D:485:PRO:HD3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TYR:CD1	1:A:87:MET:CG	3.01	0.44
1:B:511:ASP:OD1	1:B:511:ASP:N	2.49	0.44
1:D:42:LEU:HA	1:D:45:GLU:HG2	2.00	0.44
1:D:167:CYS:HB3	1:D:177:LEU:CD1	2.48	0.44
1:D:514:THR:O	1:D:514:THR:HG23	2.18	0.44
1:A:23:VAL:HG12	1:A:43:VAL:HG22	2.00	0.44
1:A:66:LEU:HD12	1:A:251:GLU:OE2	2.18	0.44
1:A:421:THR:O	1:A:422:LEU:C	2.54	0.44
1:C:480:LEU:O	1:C:483:ARG:HG3	2.17	0.44
1:D:35:PRO:HA	1:D:139:TYR:OH	2.17	0.44
1:D:195:GLN:NE2	1:D:245:CYS:SG	2.91	0.44
1:D:341:ALA:HB3	1:D:344:VAL:HG23	1.99	0.44
1:A:148:PHE:HD1	1:A:153:LEU:HB2	1.81	0.43
1:A:457:ASN:HB3	5:A:717:HOH:O	2.18	0.43
1:C:505:PHE:HB3	1:C:530:GLU:HG3	2.00	0.43
1:D:33:GLN:CB	1:D:84:TYR:OH	2.66	0.43
1:D:81:ARG:HD2	1:D:81:ARG:O	2.17	0.43
1:D:211:LYS:O	1:D:215:VAL:HG23	2.17	0.43
1:B:267:GLN:NE2	1:B:278:CYS:SG	2.91	0.43
1:B:289:ILE:O	1:B:292:VAL:CG1	2.66	0.43
1:B:507:THR:O	1:B:508:PHE:CD2	2.71	0.43
1:B:564:GLU:O	1:B:568:VAL:HG23	2.18	0.43
1:C:175:ALA:HA	1:D:511:ASP:CG	2.39	0.43
1:A:140:GLU:OE1	1:A:143:ARG:NH1	2.43	0.43
1:A:537:LYS:HA	1:A:537:LYS:HD2	1.78	0.43
1:A:555:ASP:O	1:A:556:LYS:C	2.57	0.43
1:C:31:LEU:HD13	1:C:80:LEU:HD21	2.00	0.43
1:C:318:TYR:OH	1:C:357:GLU:OE1	2.35	0.43
1:D:101:CYS:O	1:D:104:ASN:N	2.51	0.43
1:D:151:PRO:O	1:D:154:LEU:HB2	2.18	0.43
1:D:152:GLU:O	1:D:152:GLU:HG3	2.17	0.43
1:D:173:LYS:O	1:D:177:LEU:CD1	2.66	0.43
1:D:502:ASP:HB2	5:D:764:HOH:O	2.17	0.43
1:D:21:GLY:O	1:D:25:ILE:HG13	2.19	0.43
1:A:223:PRO:HB2	1:A:298:PRO:HD3	2.00	0.43
1:B:404:ASN:OD1	1:B:525:GLN:HG2	2.18	0.43
1:C:95:GLU:OE2	1:C:98:ARG:NE	2.52	0.43
1:D:6:GLU:O	1:D:10:ARG:HG2	2.19	0.43
1:B:222:PHE:CE1	1:B:274:LEU:HD11	2.54	0.43
1:D:118:GLU:HB3	1:D:121:THR:OG1	2.19	0.43
1:D:403:GLN:O	1:D:407:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:LYS:HA	1:B:242:LYS:HE2	2.00	0.43
1:C:112:LEU:HD13	1:C:143:ARG:CZ	2.48	0.43
1:C:119:PRO:CB	4:C:605:PRO:HD3	2.47	0.43
1:C:131:LYS:HD2	1:C:131:LYS:C	2.39	0.43
1:D:220:GLN:HG2	1:D:334:SER:O	2.19	0.43
1:D:407:ILE:HD13	1:D:426:SER:CB	2.49	0.43
1:A:86:ASP:CB	1:A:105:HIS:CE1	3.02	0.43
1:A:150:ALA:HB3	1:A:151:PRO:CD	2.48	0.43
1:B:367:ALA:O	1:B:368:CYS:C	2.56	0.43
1:D:82:GLU:HA	1:D:88:ALA:HB2	2.01	0.43
1:D:409:ARG:CA	4:D:603:PRO:HG3	2.48	0.43
1:D:512:ILE:HD12	1:D:512:ILE:HA	1.76	0.43
1:A:479:SER:OG	1:A:482:ASN:HB2	2.19	0.43
1:B:126:PHE:HD1	1:B:133:PHE:CD2	2.36	0.43
1:D:400:TYR:OH	1:D:524:LYS:HD2	2.19	0.43
1:A:155:TYR:CD2	1:A:155:TYR:C	2.92	0.42
1:B:118:GLU:HA	1:B:119:PRO:HD3	1.75	0.42
1:B:515:LEU:HB3	1:B:519:GLU:HB2	2.00	0.42
1:C:1:ASP:N	1:C:10:ARG:HH22	2.18	0.42
1:C:106:LYS:HD3	1:C:146:PRO:O	2.19	0.42
1:C:289:ILE:C	1:C:291:GLU:H	2.22	0.42
1:D:224:LYS:O	1:D:224:LYS:HG2	2.19	0.42
1:A:289:ILE:O	1:A:290:ALA:C	2.57	0.42
1:B:350:LYS:NZ	1:B:479:SER:OG	2.52	0.42
1:D:308:PHE:HB2	1:D:373:PHE:HZ	1.84	0.42
1:A:221:LYS:HE3	1:A:290:ALA:O	2.19	0.42
1:A:316:LYS:O	1:A:317:ASN:C	2.57	0.42
1:B:46:LEU:HA	1:B:49:PHE:HB3	2.01	0.42
1:C:509:HIS:O	1:C:512:ILE:HG22	2.19	0.42
1:A:441:GLU:OE2	1:A:444:ARG:HD3	2.19	0.42
1:B:35:PRO:HB2	1:B:38:GLU:OE1	2.19	0.42
1:C:72:ASP:N	1:C:98:ARG:HH22	2.18	0.42
1:D:79:THR:O	1:D:83:THR:N	2.53	0.42
1:D:159:LYS:HA	1:D:159:LYS:HD3	1.81	0.42
1:D:177:LEU:O	1:D:180:LYS:N	2.53	0.42
1:D:512:ILE:CD1	1:D:520:LYS:HA	2.49	0.42
1:B:528:LEU:HD12	1:B:528:LEU:HA	1.77	0.42
1:D:42:LEU:HA	1:D:45:GLU:HG3	2.00	0.42
1:A:282:VAL:HG13	1:A:283:LEU:H	1.82	0.42
1:B:372:VAL:O	1:B:376:LEU:HG	2.20	0.42
1:B:414:ALA:HB1	1:B:417:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:LYS:HG3	1:B:582:LEU:HB3	2.02	0.42
1:C:558:CYS:O	1:C:563:LYS:HE3	2.19	0.42
1:D:205:PHE:CE2	1:D:480:LEU:HD13	2.54	0.42
1:A:289:ILE:O	1:A:291:GLU:N	2.52	0.42
1:A:305:THR:O	1:A:310:GLU:HG3	2.20	0.42
1:A:456:LEU:HD23	1:A:456:LEU:HA	1.86	0.42
1:C:178:LEU:HD23	1:C:178:LEU:HA	1.78	0.42
1:C:410:TYR:HE1	2:C:601:PGE:H2	1.85	0.42
1:C:410:TYR:OH	2:C:601:PGE:H1	2.19	0.42
1:A:179:PRO:HB3	1:B:510:ALA:HB3	2.01	0.42
1:A:220:GLN:O	1:A:223:PRO:HD3	2.20	0.42
1:B:112:LEU:HD13	1:B:143:ARG:CZ	2.49	0.42
1:B:482:ASN:O	1:B:483:ARG:C	2.58	0.42
1:C:248:ASP:OD1	1:C:248:ASP:N	2.52	0.42
1:D:463:HIS:O	1:D:463:HIS:CG	2.73	0.42
1:A:545:THR:HG21	1:A:582:LEU:HD21	2.01	0.42
1:A:570:GLU:O	1:A:573:LYS:HB3	2.20	0.42
1:B:306:ALA:HA	1:B:310:GLU:OE1	2.19	0.42
1:C:27:PHE:CD2	1:C:74:LEU:HD21	2.55	0.42
1:D:203:GLN:OE1	1:D:203:GLN:CA	2.67	0.42
1:D:334:SER:HA	1:D:345:LEU:HD13	2.02	0.42
1:A:65:SER:O	1:A:68:THR:HB	2.20	0.42
1:A:412:ARG:HB3	1:A:492:LEU:HD12	2.02	0.42
1:B:112:LEU:CD1	1:B:143:ARG:NE	2.82	0.42
1:B:208:ARG:NH2	5:B:719:HOH:O	2.52	0.42
1:C:36:PHE:CZ	1:C:40:VAL:HG21	2.54	0.42
1:D:32:GLN:NE2	1:D:107:ASP:O	2.53	0.42
1:D:260:ALA:HB1	1:D:285:LYS:HD3	2.02	0.42
1:A:422:LEU:O	1:A:426:SER:HB2	2.20	0.41
1:A:466:THR:O	1:A:467:PRO:C	2.56	0.41
1:A:509:HIS:N	5:A:716:HOH:O	2.45	0.41
1:A:582:LEU:O	1:A:583:ALA:OXT	2.37	0.41
1:B:415:PRO:HD2	1:B:416:GLN:CD	2.41	0.41
1:D:110:PRO:O	1:D:111:ASP:C	2.58	0.41
1:D:511:ASP:C	1:D:513:CYS:H	2.24	0.41
1:A:78:ALA:O	1:A:80:LEU:HG	2.20	0.41
1:A:82:GLU:O	1:A:84:TYR:O	2.38	0.41
1:B:2:THR:O	1:B:3:HIS:ND1	2.53	0.41
1:B:406:LEU:O	1:B:407:ILE:C	2.58	0.41
1:C:312:LYS:HE3	1:C:366:HIS:CG	2.55	0.41
1:D:140:GLU:OE1	1:D:144:ARG:NH1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASN:HA	5:A:774:HOH:O	2.20	0.41
1:C:499:LYS:HA	1:C:500:PRO:HD3	1.91	0.41
1:A:581:ALA:HB3	1:A:582:LEU:HD12	2.03	0.41
1:C:345:LEU:HA	1:C:348:LEU:HD12	2.01	0.41
1:A:123:CYS:SG	1:A:173:LYS:HD3	2.60	0.41
1:A:366:HIS:HA	1:A:369:TYR:CZ	2.56	0.41
1:B:36:PHE:CD2	1:B:136:LYS:HD2	2.56	0.41
1:C:280:LYS:H	1:C:280:LYS:HG3	1.53	0.41
1:C:522:ILE:O	1:C:526:THR:N	2.42	0.41
1:C:543:LEU:O	1:C:547:MET:HG3	2.20	0.41
1:D:123:CYS:O	1:D:124:ALA:C	2.58	0.41
1:A:3:HIS:NE2	4:A:605:PRO:HA	2.35	0.41
1:A:412:ARG:HG2	1:A:492:LEU:HD12	2.03	0.41
1:B:32:GLN:NE2	1:B:146:PRO:HG3	2.36	0.41
1:B:80:LEU:HD23	1:B:91:CYS:HB2	2.02	0.41
1:B:395:GLU:CG	5:B:789:HOH:O	2.68	0.41
1:D:177:LEU:O	1:D:178:LEU:C	2.59	0.41
1:D:564:GLU:O	1:D:564:GLU:HG3	2.20	0.41
1:A:539:THR:N	1:A:542:GLN:OE1	2.51	0.41
1:B:341:ALA:CB	1:B:449:GLU:HB2	2.51	0.41
1:D:532:LEU:HD22	1:D:532:LEU:N	2.35	0.41
1:A:9:HIS:O	1:A:13:ASP:HB2	2.21	0.41
1:A:177:LEU:O	1:A:178:LEU:C	2.58	0.41
1:A:242:LYS:NZ	1:D:169:GLN:OE1	2.54	0.41
1:D:484:ARG:HB3	1:D:485:PRO:HD3	2.02	0.41
1:A:36:PHE:HB2	1:A:139:TYR:CE2	2.56	0.41
1:A:173:LYS:O	1:A:176:CYS:HB3	2.21	0.41
1:B:505:PHE:HB3	1:B:530:GLU:HG3	2.03	0.41
1:C:71:GLY:HA3	1:C:98:ARG:NH2	2.36	0.41
1:C:173:LYS:O	1:C:174:GLY:C	2.59	0.41
1:C:387:ILE:HD12	1:C:448:THR:HG21	2.03	0.41
1:D:49:PHE:CE2	1:D:69:LEU:HD11	2.55	0.41
1:D:460:CYS:O	1:D:464:GLU:HB3	2.21	0.41
1:C:1:ASP:C	1:C:3:HIS:CE1	2.94	0.41
1:C:283:LEU:C	1:C:285:LYS:N	2.73	0.41
1:C:565:GLY:O	1:C:569:LEU:HD13	2.20	0.41
1:A:297:VAL:HA	1:A:298:PRO:HD3	1.91	0.40
1:B:270:LEU:HD23	1:B:270:LEU:HA	1.97	0.40
1:D:314:VAL:HG12	1:D:315:CYS:N	2.36	0.40
1:A:93:LYS:O	1:A:98:ARG:HB2	2.20	0.40
1:A:266:HIS:ND1	1:A:266:HIS:N	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ARG:CA	1:B:88:ALA:HB2	2.51	0.40
1:B:259:LEU:O	1:B:259:LEU:HD12	2.21	0.40
1:B:561:ASP:O	1:B:563:LYS:NZ	2.54	0.40
1:D:31:LEU:HD23	1:D:31:LEU:N	2.35	0.40
1:D:94:GLN:OE1	1:D:98:ARG:NH1	2.54	0.40
1:D:140:GLU:HA	1:D:143:ARG:HD3	2.03	0.40
1:A:5:SER:HB2	1:A:62:CYS:O	2.21	0.40
1:C:305:THR:HG22	1:C:373:PHE:CD1	2.57	0.40
1:D:87:MET:O	1:D:88:ALA:C	2.59	0.40
1:D:93:LYS:O	1:D:94:GLN:OE1	2.39	0.40
1:D:408:VAL:HG12	4:D:603:PRO:HG2	2.04	0.40
1:B:80:LEU:HD12	1:B:84:TYR:HD2	1.87	0.40
1:B:225:ALA:CB	1:B:270:LEU:HD23	2.50	0.40
1:D:90:CYS:C	1:D:92:GLU:N	2.74	0.40
1:D:499:LYS:HD3	1:D:533:LYS:HB3	2.04	0.40
1:A:436:CYS:HA	1:A:439:LYS:HG2	2.02	0.40
1:C:7:ILE:HG23	1:C:8:ALA:N	2.35	0.40
1:C:30:TYR:CE2	1:C:74:LEU:HD11	2.57	0.40
1:C:196:ARG:HA	1:C:196:ARG:HD2	1.82	0.40
1:C:547:MET:HE3	1:C:547:MET:HB2	1.91	0.40
1:D:280:LYS:HB3	1:D:281:PRO:CD	2.51	0.40
1:D:543:LEU:HA	1:D:543:LEU:HD23	1.88	0.40

There are no symmetry-related clashes.

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	581/583 (100%)	502 (86%)	76 (13%)	3 (0%)	29	40
1	B	581/583 (100%)	524 (90%)	55 (10%)	2 (0%)	41	51
1	C	581/583 (100%)	527 (91%)	51 (9%)	3 (0%)	29	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	581/583 (100%)	529 (91%)	51 (9%)	1 (0%)	47	60
All	All	2324/2332 (100%)	2082 (90%)	233 (10%)	9 (0%)	34	46

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	74	LEU
1	A	415	PRO
1	A	290	ALA
1	D	494	GLU
1	B	282	VAL
1	B	289	ILE
1	C	240	VAL
1	C	342	VAL
1	A	289	ILE

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	516/516 (100%)	473 (92%)	43 (8%)	11	14
1	B	516/516 (100%)	478 (93%)	38 (7%)	13	18
1	C	516/516 (100%)	483 (94%)	33 (6%)	17	23
1	D	516/516 (100%)	471 (91%)	45 (9%)	10	12
All	All	2064/2064 (100%)	1905 (92%)	159 (8%)	13	16

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	34	CYS
1	A	49	PHE
1	A	58	SER
1	A	63	ASP

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Mol	Chain	Res	Type
1	A	81	ARG
1	A	86	ASP
1	A	92	GLU
1	A	114	LYS
1	A	115	LEU
1	A	117	PRO
1	A	120	ASP
1	A	121	THR
1	A	131	LYS
1	A	166	GLU
1	A	208	ARG
1	A	244	CYS
1	A	246	HIS
1	A	275	LYS
1	A	300	ASN
1	A	305	THR
1	A	310	GLU
1	A	312	LYS
1	A	331	TYR
1	A	374	ASP
1	A	375	LYS
1	A	425	ILE
1	A	441	GLU
1	A	444	ARG
1	A	445	MET
1	A	448	THR
1	A	450	ASP
1	A	459	LEU
1	A	468	VAL
1	A	469	SER
1	A	470	GLU
1	A	512	ILE
1	A	514	THR
1	A	532	LEU
1	A	535	LYS
1	A	544	LYS
1	A	556	LYS
1	A	582	LEU
1	B	16	GLU
1	B	34	CYS
1	B	58	SER
1	B	89	ASP

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Mol	Chain	Res	Type
1	B	104	ASN
1	B	111	ASP
1	B	131	LYS
1	B	144	ARG
1	B	159	LYS
1	B	169	GLN
1	B	221	LYS
1	B	227	PHE
1	B	239	LYS
1	B	242	LYS
1	B	251	GLU
1	B	267	GLN
1	B	268	ASP
1	B	284	GLU
1	B	319	GLN
1	B	333	TYR
1	B	336	ARG
1	B	343	SER
1	B	382	GLU
1	B	435	LYS
1	B	450	ASP
1	B	464	GLU
1	B	466	THR
1	B	468	VAL
1	B	470	GLU
1	B	484	ARG
1	B	490	LEU
1	B	508	PHE
1	B	517	ASP
1	B	532	LEU
1	B	550	PHE
1	B	553	PHE
1	B	561	ASP
1	B	569	LEU
1	C	34	CYS
1	C	77	VAL
1	C	81	ARG
1	C	111	ASP
1	C	120	ASP
1	C	131	LYS
1	C	136	LYS
1	C	144	ARG

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Mol	Chain	Res	Type
1	C	159	LYS
1	C	226	ASP
1	C	239	LYS
1	C	280	LYS
1	C	282	VAL
1	C	285	LYS
1	C	286	SER
1	C	314	VAL
1	C	319	GLN
1	C	328	SER
1	C	333	TYR
1	C	335	ARG
1	C	346	LEU
1	C	350	LYS
1	C	351	GLU
1	C	385	ASN
1	C	431	LYS
1	C	435	LYS
1	C	470	GLU
1	C	474	LYS
1	C	493	ASP
1	C	503	GLU
1	C	504	LYS
1	C	544	LYS
1	C	548	GLU
1	D	2	THR
1	D	24	LEU
1	D	45	GLU
1	D	48	GLU
1	D	58	SER
1	D	80	LEU
1	D	81	ARG
1	D	82	GLU
1	D	83	THR
1	D	87	MET
1	D	104	ASN
1	D	111	ASP
1	D	120	ASP
1	D	127	LYS
1	D	136	LYS
1	D	169	GLN
1	D	191	SER

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Mol	Chain	Res	Type
1	D	201	SER
1	D	217	ARG
1	D	224	LYS
1	D	235	THR
1	D	239	LYS
1	D	244	CYS
1	D	251	GLU
1	D	254	ASP
1	D	267	GLN
1	D	275	LYS
1	D	286	SER
1	D	333	TYR
1	D	335	ARG
1	D	362	LYS
1	D	374	ASP
1	D	378	HIS
1	D	382	GLU
1	D	384	GLN
1	D	441	GLU
1	D	444	ARG
1	D	465	LYS
1	D	484	ARG
1	D	504	LYS
1	D	511	ASP
1	D	514	THR
1	D	519	GLU
1	D	544	LYS
1	D	569	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	241	HIS
1	A	384	GLN
1	A	509	HIS
1	B	105	HIS
1	B	534	HIS
1	C	20	GLN
1	C	549	ASN
1	D	105	HIS
1	D	385	ASN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

19 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	PGE	D	601	-	9,9,9	0.67	0	8,8,8	1.60	2 (25%)
4	PRO	A	606	-	8,8,8	0.78	0	10,10,10	1.30	1 (10%)
2	PGE	A	602	-	9,9,9	0.62	0	8,8,8	0.46	0
4	PRO	D	602	-	8,8,8	0.87	0	10,10,10	1.26	1 (10%)
3	PEG	C	603	-	6,6,6	1.90	1 (16%)	5,5,5	1.11	0
3	PEG	A	603	-	6,6,6	0.63	0	5,5,5	0.50	0
2	PGE	B	601	-	9,9,9	0.49	0	8,8,8	0.92	0
4	PRO	C	606	-	8,8,8	0.94	1 (12%)	10,10,10	1.18	1 (10%)
4	PRO	B	603	-	8,8,8	0.81	0	10,10,10	1.27	2 (20%)
2	PGE	A	601	-	9,9,9	0.73	0	8,8,8	0.63	0
4	PRO	B	604	-	8,8,8	0.67	0	10,10,10	1.41	2 (20%)
4	PRO	A	604	-	8,8,8	0.78	0	10,10,10	1.65	2 (20%)
4	PRO	C	605	-	8,8,8	0.96	0	10,10,10	1.35	1 (10%)
4	PRO	C	604	-	8,8,8	0.82	1 (12%)	10,10,10	1.42	2 (20%)
2	PGE	C	601	-	9,9,9	0.46	0	8,8,8	1.06	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PGE	C	602	-	9,9,9	0.81	0	8,8,8	0.72	0
4	PRO	D	603	-	8,8,8	1.10	0	10,10,10	1.66	1 (10%)
4	PRO	B	602	-	8,8,8	0.95	1 (12%)	10,10,10	2.13	3 (30%)
4	PRO	A	605	-	8,8,8	0.89	1 (12%)	10,10,10	1.46	2 (20%)

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
2	PGE	D	601	-	-	5/7/7/7	-
4	PRO	A	606	-	-	0/4/11/11	0/1/1/1
2	PGE	A	602	-	-	7/7/7/7	-
4	PRO	D	602	-	-	4/4/11/11	0/1/1/1
3	PEG	C	603	-	-	3/4/4/4	-
3	PEG	A	603	-	-	2/4/4/4	-
2	PGE	B	601	-	-	4/7/7/7	-
4	PRO	C	606	-	-	4/4/11/11	0/1/1/1
4	PRO	B	603	-	-	4/4/11/11	0/1/1/1
2	PGE	A	601	-	-	3/7/7/7	-
4	PRO	B	604	-	-	2/4/11/11	0/1/1/1
4	PRO	A	604	-	-	0/4/11/11	0/1/1/1
4	PRO	C	605	-	-	0/4/11/11	0/1/1/1
4	PRO	C	604	-	-	2/4/11/11	0/1/1/1
2	PGE	C	601	-	-	4/7/7/7	-
2	PGE	C	602	-	-	4/7/7/7	-
4	PRO	D	603	-	-	4/4/11/11	0/1/1/1
4	PRO	B	602	-	-	0/4/11/11	0/1/1/1
4	PRO	A	605	-	-	4/4/11/11	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	PEG	O2-C3	3.27	1.56	1.42
4	B	602	PRO	OXT-C	-2.27	1.23	1.30
4	A	605	PRO	OXT-C	-2.21	1.23	1.30
4	C	606	PRO	OXT-C	-2.02	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	604	PRO	OXT-C	-2.00	1.24	1.30

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	602	PRO	OXT-C-O	-4.97	112.81	124.09
4	D	603	PRO	OXT-C-O	-3.58	115.97	124.09
4	A	604	PRO	OXT-C-CA	3.10	123.69	113.40
2	D	601	PGE	O4-C6-C5	-3.09	93.90	111.81
4	B	602	PRO	C-CA-N	3.08	118.88	106.73
2	D	601	PGE	O3-C5-C6	-3.03	96.76	110.07
4	B	604	PRO	OXT-C-O	-2.84	117.65	124.09
4	A	605	PRO	OXT-C-O	-2.76	117.83	124.09
4	A	604	PRO	OXT-C-O	-2.73	117.90	124.09
4	A	606	PRO	OXT-C-CA	2.64	122.19	113.40
4	A	605	PRO	OXT-C-CA	2.57	121.96	113.40
4	C	605	PRO	OXT-C-CA	2.53	121.80	113.40
4	C	604	PRO	OXT-C-CA	2.51	121.75	113.40
4	C	604	PRO	OXT-C-O	-2.35	118.76	124.09
4	D	602	PRO	OXT-C-O	-2.32	118.81	124.09
4	B	604	PRO	OXT-C-CA	2.28	120.98	113.40
2	C	601	PGE	O1-C1-C2	-2.23	98.90	111.81
4	B	602	PRO	OXT-C-CA	2.22	120.80	113.40
4	B	603	PRO	CD-N-CA	2.16	113.03	107.08
4	C	606	PRO	OXT-C-O	-2.16	119.19	124.09
4	B	603	PRO	OXT-C-CA	2.01	120.09	113.40

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	605	PRO	O-C-CA-N
4	A	605	PRO	OXT-C-CA-N
4	A	605	PRO	O-C-CA-CB
4	A	605	PRO	OXT-C-CA-CB
4	B	603	PRO	O-C-CA-N
4	B	603	PRO	OXT-C-CA-N
4	B	603	PRO	O-C-CA-CB
4	B	603	PRO	OXT-C-CA-CB
4	C	604	PRO	O-C-CA-N
4	C	604	PRO	OXT-C-CA-N
4	D	602	PRO	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
4	D	602	PRO	OXT-C-CA-N
4	D	603	PRO	O-C-CA-N
4	D	603	PRO	OXT-C-CA-N
4	D	603	PRO	O-C-CA-CB
4	D	603	PRO	OXT-C-CA-CB
2	A	601	PGE	O1-C1-C2-O2
2	B	601	PGE	O3-C5-C6-O4
3	C	603	PEG	O2-C3-C4-O4
2	C	602	PGE	O3-C5-C6-O4
2	D	601	PGE	O1-C1-C2-O2
2	C	602	PGE	C6-C5-O3-C4
3	A	603	PEG	O2-C3-C4-O4
2	C	602	PGE	O1-C1-C2-O2
2	C	601	PGE	O3-C5-C6-O4
3	C	603	PEG	O1-C1-C2-O2
3	C	603	PEG	C1-C2-O2-C3
2	A	601	PGE	O2-C3-C4-O3
2	A	602	PGE	O3-C5-C6-O4
2	C	601	PGE	O1-C1-C2-O2
2	D	601	PGE	O3-C5-C6-O4
2	C	601	PGE	C4-C3-O2-C2
2	A	602	PGE	C3-C4-O3-C5
2	C	602	PGE	C4-C3-O2-C2
2	B	601	PGE	C6-C5-O3-C4
3	A	603	PEG	C4-C3-O2-C2
2	A	602	PGE	O1-C1-C2-O2
2	A	602	PGE	C4-C3-O2-C2
2	D	601	PGE	C4-C3-O2-C2
2	D	601	PGE	O2-C3-C4-O3
2	A	602	PGE	O2-C3-C4-O3
2	A	601	PGE	C4-C3-O2-C2
4	C	606	PRO	O-C-CA-N
4	C	606	PRO	OXT-C-CA-N
2	A	602	PGE	C1-C2-O2-C3
4	B	604	PRO	O-C-CA-CB
4	B	604	PRO	OXT-C-CA-CB
4	C	606	PRO	O-C-CA-CB
4	C	606	PRO	OXT-C-CA-CB
4	D	602	PRO	OXT-C-CA-CB
2	B	601	PGE	C3-C4-O3-C5
2	B	601	PGE	O2-C3-C4-O3
4	D	602	PRO	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	D	601	PGE	C3-C4-O3-C5
2	C	601	PGE	O2-C3-C4-O3
2	A	602	PGE	C6-C5-O3-C4

There are no ring outliers.

11 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	PGE	3	0
4	A	606	PRO	2	0
2	B	601	PGE	3	0
2	A	601	PGE	1	0
4	B	604	PRO	1	0
4	A	604	PRO	1	0
4	C	605	PRO	9	0
2	C	601	PGE	4	0
2	C	602	PGE	6	0
4	D	603	PRO	6	0
4	A	605	PRO	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	583/583 (100%)	-0.24	17 (2%)	51	59	31, 54, 87, 140	0
1	B	583/583 (100%)	-0.42	3 (0%)	91	94	28, 50, 83, 110	0
1	C	583/583 (100%)	-0.40	5 (0%)	84	88	27, 50, 79, 129	0
1	D	583/583 (100%)	-0.34	7 (1%)	79	84	31, 50, 84, 121	0
All	All	2332/2332 (100%)	-0.35	32 (1%)	75	81	27, 51, 84, 140	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	MET	4.7
1	A	77	VAL	4.3
1	C	79	THR	3.8
1	A	70	PHE	3.7
1	B	583	ALA	3.7
1	C	80	LEU	3.6
1	A	546	VAL	3.6
1	A	93	LYS	3.6
1	A	89	ASP	3.5
1	A	76	LYS	3.1
1	D	442	SER	3.0
1	C	77	VAL	2.9
1	B	86	ASP	2.9
1	A	569	LEU	2.7
1	A	2	THR	2.6
1	C	96	PRO	2.6
1	A	88	ALA	2.5
1	A	91	CYS	2.5
1	D	80	LEU	2.4
1	D	503	GLU	2.4
1	C	2	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	169	GLN	2.3
1	A	547	MET	2.3
1	A	85	GLY	2.3
1	A	83	THR	2.2
1	A	7	ILE	2.2
1	A	550	PHE	2.2
1	D	569	LEU	2.2
1	A	1	ASP	2.1
1	D	70	PHE	2.1
1	D	74	LEU	2.1
1	D	66	LEU	2.1

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, 95th 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
2	PGE	C	602	10/10	0.88	0.15	46,59,67,67	0
3	PEG	A	603	7/7	0.88	0.17	52,58,65,68	0
4	PRO	C	605	8/8	0.88	0.16	70,71,77,80	0
4	PRO	D	603	8/8	0.88	0.16	59,68,72,74	0
4	PRO	D	602	8/8	0.89	0.22	71,78,87,91	0
4	PRO	C	604	8/8	0.91	0.20	69,73,80,88	0
2	PGE	A	602	10/10	0.92	0.13	55,65,71,72	0
3	PEG	C	603	7/7	0.92	0.21	32,34,37,37	0
4	PRO	A	606	8/8	0.92	0.20	58,81,91,91	0
4	PRO	B	604	8/8	0.92	0.17	58,69,74,75	0
4	PRO	C	606	8/8	0.93	0.12	56,61,66,70	0
4	PRO	A	605	8/8	0.94	0.12	71,79,81,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PRO	B	602	8/8	0.94	0.14	48,62,72,79	0
2	PGE	B	601	10/10	0.95	0.17	44,60,68,72	0
2	PGE	A	601	10/10	0.95	0.26	52,60,67,72	0
4	PRO	A	604	8/8	0.95	0.21	63,74,81,83	0
2	PGE	C	601	10/10	0.96	0.15	48,62,70,71	0
2	PGE	D	601	10/10	0.96	0.19	50,60,76,78	0
4	PRO	B	603	8/8	0.96	0.18	61,67,70,73	0

6.5 Other polymers (i)

There are no such residues in this entry.