Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 06:57 PM JST

PDB ID	:	5ZZJ
Title	:	Crystal structure of a enzyme from Santalum album
Authors	:	Han, X.; Liu, W.D.; Chen, C.C.; Guo, R.T.
Deposited on	:	2018-06-01
Resolution	:	2.60 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 (1)) were used in the production of this report:

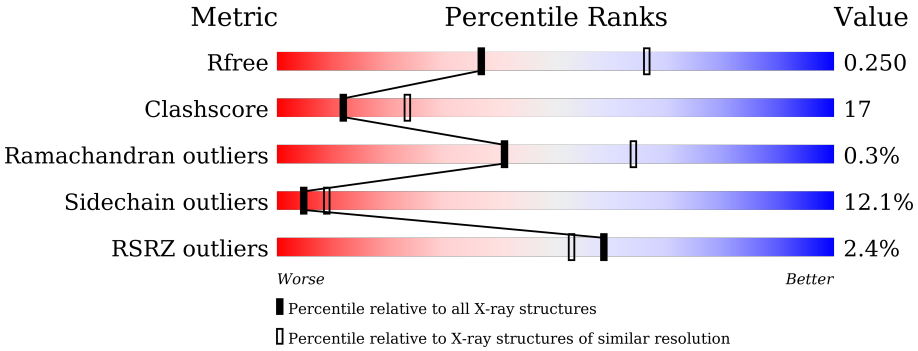
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	569	%, 66%, 22%, •, 8%
1	B	569	2%, 61%, 26%, •, 9%
1	C	569	3%, 62%, 24%, 6%, 9%
1	D	569	3%, 58%, 28%, 6%, 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17019 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 Santalene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	522	4231	2736	707	769	19	0	0	0
1	B	520	4215	2728	704	764	19	0	0	0
1	C	519	4211	2726	703	763	19	0	0	0
1	D	521	4227	2734	706	768	19	0	0	0

- Molecule 2 is water.

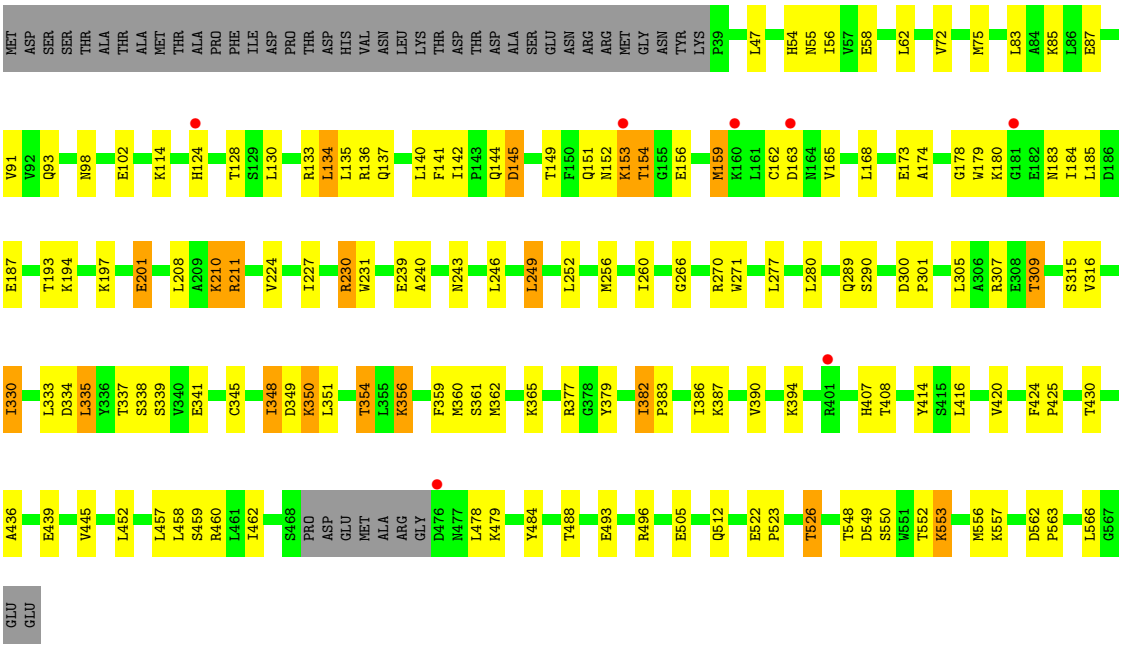
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	45	45	45	0	0
2	B	45	45	45	0	0
2	C	35	35	35	0	0
2	D	10	10	10	0	0

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.

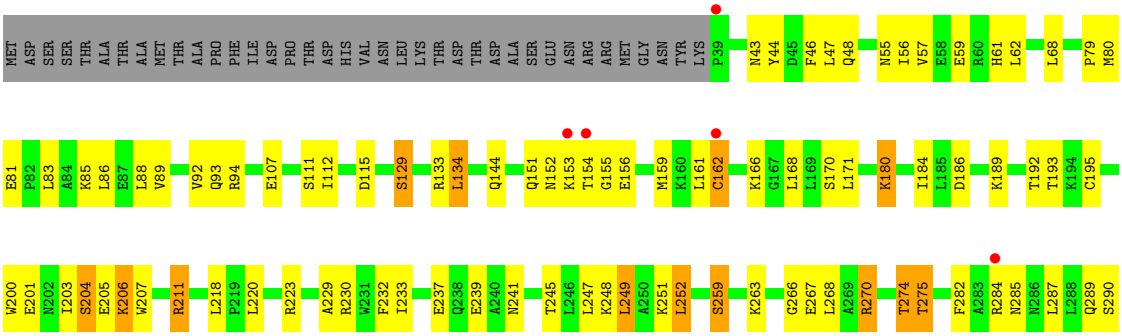
• Molecule 1: Santalene synthase

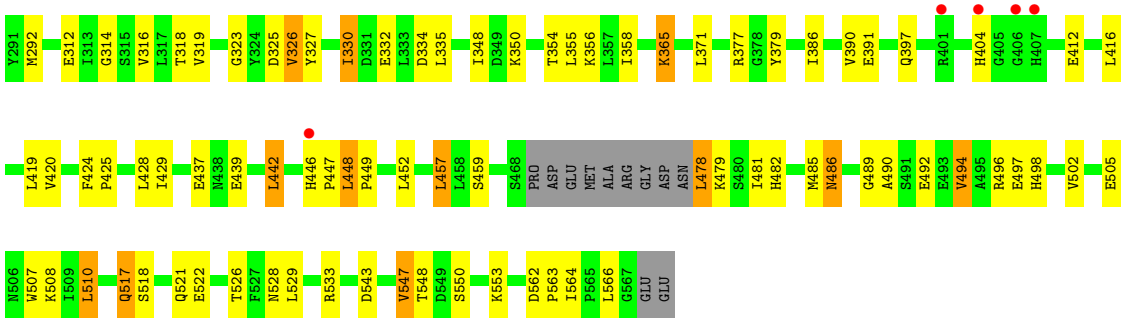
Chain A:



• Molecule 1: Santalene synthase

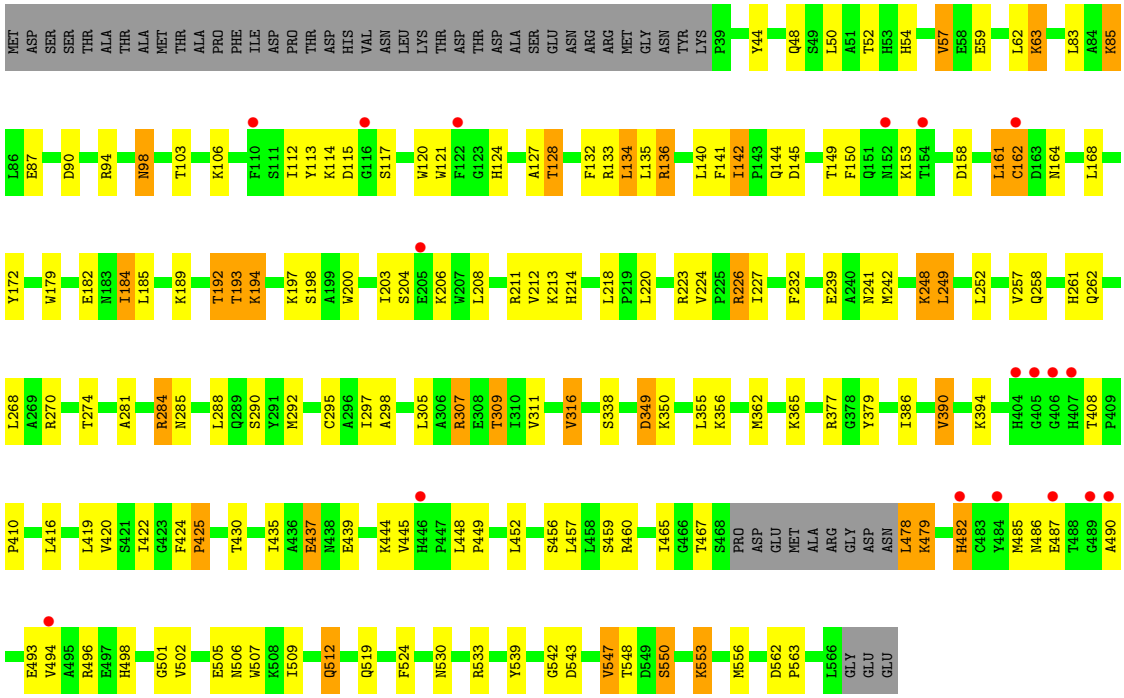
Chain B:





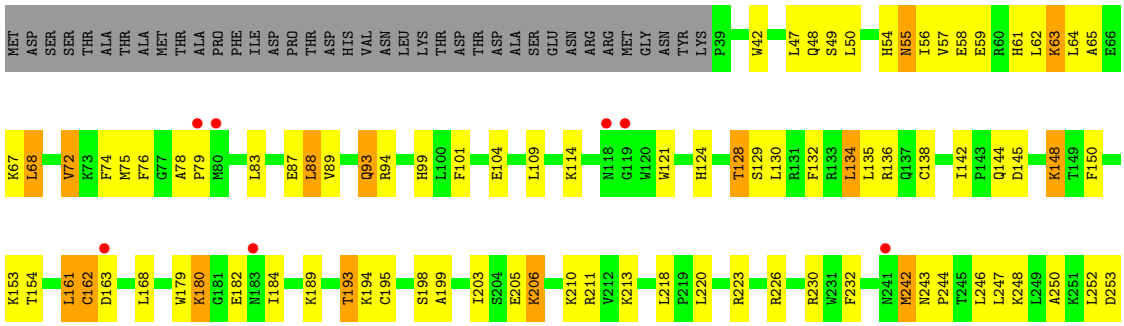
- Molecule 1: Santalene synthase

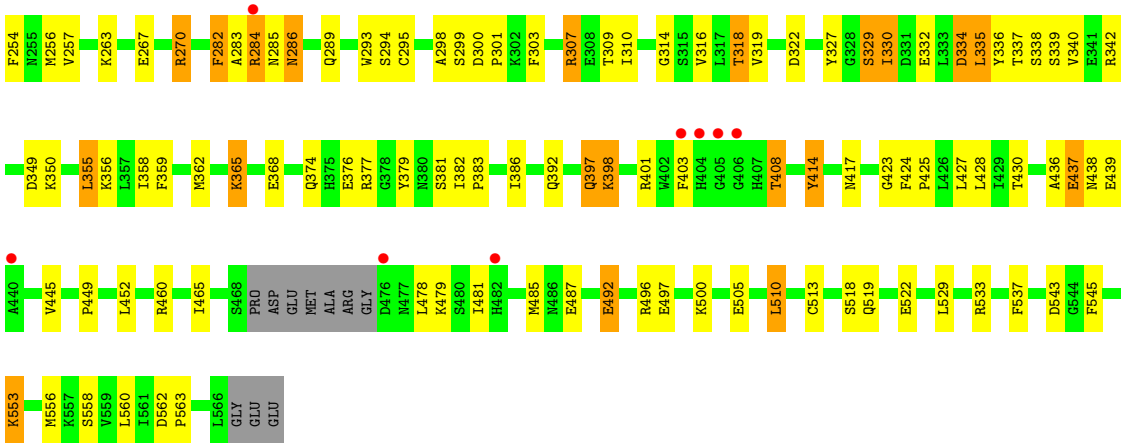
Chain C:



- Molecule 1: Santalene synthase

Chain D:




F254
N255
M256
V257
K263
E267
R270
F282
A283
R284
N285
N286
Q289
W293
S294
C295
A298
S299
D300
P301
K302
F303
R307
E308
T309
I310
G314
S315
V316
L317
T318
V319
D322
Y327
G328
S329
I330
D331
E332
L333
D334
L335
Y336
T337
S338
S339
V340
E341
R342
D349
K350
L355
K356
L357
I358
F359
M362
K365
E368
Q374
H375
E376
R377
G378
Y379
N380
S381
I382
P383
I386
Q392
Q397
K398
R401
W402
F403
H404
G405
G406
H407
T408
Y414
N417
G423
F424
P425
L426
L427
L428
I429
T430
A436
E437
N438
E439
A440
V445
P449
L452
R460
I465
S468
PRO
ASP
GLU
MET
ALA
ARG
GLY
D476
M477
L478
K479
S480
I481
H482
M485
M486
E487
E492
R496
E497
K500
E505
L510
C513
S518
Q519
E522
L529
R533
F537
D543
G544
F545
K553
M556
K557
S558
V559
L560
I561
D562
P563
L566
GLY
GLU
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.51Å 155.11Å 164.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.60 24.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (25.00-2.60) 99.1 (24.99-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.43 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.189 , 0.234 0.217 , 0.250	Depositor DCC
R_{free} test set	4938 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	59.5	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17019	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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)

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	0.82	0/4341	0.69	0/5879
1	B	0.79	0/4325	0.69	0/5857
1	C	0.76	0/4321	0.68	0/5852
1	D	0.72	0/4337	0.71	0/5874
All	All	0.77	0/17324	0.69	0/23462

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	4231	0	4176	107	0
1	B	4215	0	4166	144	0
1	C	4211	0	4161	149	0
1	D	4227	0	4173	187	0
2	A	45	0	0	3	0
2	B	45	0	0	2	0
2	C	35	0	0	2	0
2	D	10	0	0	1	0
All	All	17019	0	16676	580	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 17.

All (580) 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:B:162:CYS:HB3	1:B:195:CYS:SG	1.47	1.50
1:C:141:PHE:O	1:C:142:ILE:HD13	1.30	1.26
1:D:76:PHE:CD2	1:D:104:GLU:HB3	1.71	1.25
1:B:162:CYS:CB	1:B:195:CYS:SG	2.31	1.17
1:C:208:LEU:O	1:C:212:VAL:HG23	1.45	1.16
1:C:124:HIS:O	1:C:128:THR:HB	1.42	1.16
1:A:289:GLN:HA	1:A:556:MET:HE3	1.29	1.14
1:C:94:ARG:HE	1:C:220:LEU:CD2	1.61	1.13
1:C:172:TYR:HB2	1:C:192:THR:CG2	1.78	1.11
1:B:330:ILE:HD11	1:B:404:HIS:NE2	1.64	1.10
1:C:172:TYR:HB2	1:C:192:THR:HG21	1.11	1.10
1:C:141:PHE:C	1:C:142:ILE:HD13	1.72	1.09
1:C:284:ARG:HG3	1:C:284:ARG:HH11	1.04	1.09
1:B:152:ASN:HD21	1:B:156:GLU:HG2	0.95	1.08
1:D:206:LYS:H	1:D:206:LYS:HD2	1.19	1.07
1:C:172:TYR:CB	1:C:192:THR:HG21	1.85	1.06
1:B:152:ASN:ND2	1:B:156:GLU:HG2	1.71	1.05
1:B:159:MET:HG3	1:B:162:CYS:SG	1.97	1.04
1:B:206:LYS:H	1:B:206:LYS:HD2	1.14	1.04
1:D:226:ARG:NH1	1:D:254:PHE:CD2	2.26	1.03
1:C:94:ARG:HE	1:C:220:LEU:HD22	1.21	1.03
1:B:94:ARG:NH1	1:B:211:ARG:HH11	1.56	1.02
1:B:386:ILE:O	1:B:390:VAL:HG13	1.60	1.02
1:D:330:ILE:HD12	1:D:330:ILE:H	1.25	1.01
1:C:281:ALA:HB1	1:C:284:ARG:NH1	1.75	1.00
1:C:284:ARG:HH11	1:C:284:ARG:CG	1.73	0.99
1:C:141:PHE:O	1:C:142:ILE:CD1	2.11	0.98
1:C:94:ARG:NE	1:C:220:LEU:HD22	1.78	0.98
1:D:298:ALA:O	1:D:307:ARG:HD3	1.63	0.97
1:C:298:ALA:O	1:C:307:ARG:HD3	1.64	0.97
1:B:330:ILE:HD11	1:B:404:HIS:CD2	1.99	0.96
1:D:76:PHE:HD2	1:D:104:GLU:HB3	1.04	0.96
1:B:152:ASN:HD21	1:B:156:GLU:CG	1.80	0.94
1:D:529:LEU:O	1:D:533:ARG:HG3	1.67	0.94
1:B:44:TYR:O	1:B:48:GLN:HG3	1.68	0.94
1:D:89:VAL:O	1:D:93:GLN:HG3	1.68	0.93
1:D:226:ARG:NH1	1:D:254:PHE:CE2	2.36	0.93
1:D:76:PHE:CE1	1:D:88:LEU:HD23	2.03	0.93
1:C:144:GLN:NE2	1:C:184:ILE:HB	1.85	0.92
1:C:386:ILE:O	1:C:390:VAL:HG13	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:PHE:CE1	1:D:88:LEU:CD2	2.53	0.91
1:B:289:GLN:HE22	1:B:548:THR:HG22	1.34	0.91
1:D:94:ARG:HH12	1:D:211:ARG:NH2	1.68	0.91
1:A:289:GLN:HA	1:A:556:MET:CE	1.99	0.91
1:B:94:ARG:HH12	1:B:211:ARG:HH11	1.13	0.91
1:B:449:PRO:HG2	1:B:452:LEU:HD13	1.50	0.90
1:D:72:VAL:HG11	1:D:101:PHE:CZ	2.08	0.89
1:D:104:GLU:N	1:D:104:GLU:OE1	2.07	0.87
1:B:201:GLU:N	1:B:201:GLU:OE1	2.08	0.87
1:D:365:LYS:O	1:D:365:LYS:HD3	1.73	0.86
1:C:284:ARG:HG3	1:C:284:ARG:NH1	1.86	0.86
1:D:132:PHE:HZ	1:D:136:ARG:HH11	1.20	0.86
1:B:94:ARG:NH1	1:B:211:ARG:NH1	2.23	0.86
1:D:76:PHE:HE1	1:D:88:LEU:CD2	1.89	0.85
1:D:253:ASP:O	1:D:257:VAL:HG23	1.76	0.85
1:D:162:CYS:HB2	1:D:195:CYS:SG	2.16	0.85
1:B:206:LYS:HD2	1:B:206:LYS:N	1.87	0.85
1:B:270:ARG:O	1:B:274:THR:HB	1.75	0.84
1:B:289:GLN:NE2	1:B:548:THR:HG22	1.93	0.83
1:C:281:ALA:HB1	1:C:284:ARG:HH12	1.42	0.83
1:D:76:PHE:HE1	1:D:88:LEU:HD23	1.44	0.82
1:A:305:LEU:O	1:A:309:THR:HB	1.78	0.82
1:C:200:TRP:HA	1:C:203:ILE:HD12	1.62	0.81
1:C:305:LEU:O	1:C:309:THR:HB	1.80	0.81
1:D:132:PHE:HZ	1:D:136:ARG:NH1	1.79	0.81
1:D:513:CYS:O	1:D:518:SER:HB3	1.81	0.81
1:A:309:THR:CG2	1:A:430:THR:HG22	2.12	0.80
1:D:72:VAL:HG12	1:D:101:PHE:CE2	2.16	0.80
1:B:162:CYS:CB	1:B:195:CYS:HG	1.82	0.80
1:D:94:ARG:NH1	1:D:211:ARG:NH2	2.29	0.80
1:C:144:GLN:HB2	1:C:184:ILE:CG2	2.11	0.79
1:C:179:TRP:CD2	1:C:512:GLN:HG3	2.17	0.79
1:D:206:LYS:H	1:D:206:LYS:CD	1.95	0.78
1:A:87:GLU:O	1:A:91:VAL:HG13	1.83	0.78
1:A:345:CYS:HB3	1:A:360:MET:HE1	1.64	0.78
1:C:208:LEU:O	1:C:212:VAL:CG2	2.27	0.78
1:D:56:ILE:HD12	1:D:56:ILE:O	1.83	0.78
1:D:206:LYS:HD2	1:D:206:LYS:N	1.99	0.78
1:B:386:ILE:O	1:B:390:VAL:CG1	2.32	0.78
1:C:482:HIS:HA	1:C:485:MET:HE2	1.66	0.77
1:A:83:LEU:O	1:A:87:GLU:HG3	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:O	1:B:92:VAL:HG23	1.85	0.77
1:D:76:PHE:CE2	1:D:104:GLU:HB3	2.19	0.77
1:D:58:GLU:O	1:D:61:HIS:HB2	1.84	0.77
1:A:345:CYS:CB	1:A:360:MET:HE3	2.14	0.77
1:A:345:CYS:HB2	1:A:360:MET:HE3	1.66	0.76
1:C:460:ARG:O	1:C:460:ARG:HD3	1.85	0.76
1:A:345:CYS:HB3	1:A:360:MET:CE	2.15	0.76
1:D:300:ASP:HB2	1:D:303:PHE:CD2	2.21	0.75
1:B:263:LYS:O	1:B:267:GLU:HG3	1.86	0.75
1:C:150:PHE:HB3	1:C:161:LEU:HD21	1.68	0.75
1:B:55:ASN:OD1	1:B:563:PRO:HG3	1.87	0.74
1:A:309:THR:HG23	1:A:430:THR:CG2	2.18	0.74
1:C:226:ARG:HH22	1:C:257:VAL:HB	1.51	0.74
1:D:335:LEU:O	1:D:335:LEU:HD12	1.88	0.73
1:A:349:ASP:HA	1:A:356:LYS:NZ	2.04	0.73
1:C:94:ARG:HE	1:C:220:LEU:HD21	1.51	0.73
1:B:80:MET:SD	1:D:282:PHE:HE2	2.11	0.73
1:C:179:TRP:CE3	1:C:512:GLN:HG3	2.24	0.72
1:D:94:ARG:HH21	1:D:220:LEU:HD22	1.54	0.72
1:D:72:VAL:CG1	1:D:101:PHE:CZ	2.73	0.72
1:A:386:ILE:O	1:A:390:VAL:HG13	1.88	0.72
1:C:281:ALA:CB	1:C:284:ARG:HH12	2.03	0.72
1:B:543:ASP:O	1:B:547:VAL:HG13	1.90	0.71
1:D:338:SER:OG	1:D:342:ARG:NH2	2.23	0.71
1:B:207:TRP:CE3	1:B:239:GLU:HG2	2.26	0.71
1:B:334:ASP:OD1	1:B:397:GLN:NE2	2.23	0.71
1:C:490:ALA:HB1	1:C:494:VAL:CG1	2.21	0.71
1:D:144:GLN:HG3	1:D:184:ILE:HD12	1.70	0.71
1:B:485:MET:O	1:B:489:GLY:N	2.24	0.70
1:A:55:ASN:OD1	1:A:563:PRO:HG3	1.92	0.70
1:D:42:TRP:HH2	1:D:553:LYS:HB2	1.56	0.70
1:D:72:VAL:HG22	1:D:75:MET:HE1	1.74	0.70
1:B:543:ASP:O	1:B:547:VAL:CG1	2.39	0.70
1:B:162:CYS:HB3	1:B:195:CYS:HG	0.87	0.70
1:C:94:ARG:NE	1:C:220:LEU:CD2	2.41	0.70
1:D:72:VAL:HA	1:D:75:MET:HE2	1.74	0.70
1:A:309:THR:CG2	1:A:430:THR:CG2	2.70	0.70
1:A:345:CYS:CB	1:A:360:MET:CE	2.70	0.70
1:A:345:CYS:HA	1:A:348:ILE:HG21	1.72	0.70
1:B:159:MET:CG	1:B:162:CYS:SG	2.80	0.69
1:C:90:ASP:OD1	1:C:133:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:VAL:CG1	1:D:101:PHE:CE2	2.76	0.69
1:C:270:ARG:O	1:C:274:THR:HB	1.93	0.68
1:D:76:PHE:CE1	1:D:88:LEU:HD21	2.28	0.68
1:C:144:GLN:HB2	1:C:184:ILE:HG21	1.74	0.68
1:D:76:PHE:CD2	1:D:104:GLU:CB	2.65	0.68
1:C:144:GLN:OE1	1:C:182:GLU:HA	1.93	0.68
1:C:410:PRO:HA	1:C:487:GLU:HG3	1.75	0.68
1:A:289:GLN:CA	1:A:556:MET:CE	2.72	0.68
1:A:56:ILE:HD12	1:A:56:ILE:O	1.94	0.68
1:C:115:ASP:OD2	1:C:120:TRP:NE1	2.25	0.67
1:D:94:ARG:HB3	1:D:232:PHE:CD2	2.30	0.67
1:D:101:PHE:HB3	1:D:104:GLU:HB2	1.76	0.67
1:D:365:LYS:HE3	1:D:368:GLU:OE1	1.94	0.67
1:D:337:THR:HG21	1:D:397:GLN:NE2	2.08	0.67
1:A:153:LYS:HD3	1:A:153:LYS:N	2.10	0.67
1:D:382:ILE:N	1:D:383:PRO:CD	2.57	0.67
1:D:298:ALA:O	1:D:307:ARG:CD	2.41	0.67
1:D:109:LEU:CD1	1:D:138:CYS:SG	2.83	0.67
1:A:180:LYS:HE3	1:A:505:GLU:OE1	1.94	0.66
1:C:543:ASP:O	1:C:547:VAL:HG13	1.95	0.66
1:D:130:LEU:CD1	1:D:134:LEU:HD22	2.25	0.66
1:A:309:THR:HG22	1:A:430:THR:HG22	1.78	0.66
1:D:319:VAL:HG12	1:D:358:ILE:HG23	1.77	0.66
1:D:294:SER:HB2	1:D:310:ILE:HG22	1.76	0.66
1:C:94:ARG:CZ	1:C:220:LEU:HD22	2.26	0.66
1:C:144:GLN:OE1	1:C:182:GLU:HB3	1.97	0.65
1:A:300:ASP:O	1:A:307:ARG:NH2	2.28	0.65
1:C:298:ALA:O	1:C:307:ARG:CD	2.43	0.65
1:D:180:LYS:CE	1:D:505:GLU:HG3	2.26	0.65
1:A:162:CYS:HA	1:A:168:LEU:HD11	1.78	0.65
1:B:94:ARG:HH11	1:B:211:ARG:NH1	1.94	0.65
1:C:50:LEU:O	1:C:54:HIS:HB3	1.96	0.65
1:D:64:LEU:HD12	1:D:64:LEU:O	1.96	0.65
1:C:316:VAL:HG11	1:C:362:MET:HA	1.78	0.65
1:D:243:ASN:HB2	1:D:246:LEU:HD12	1.79	0.65
1:D:161:LEU:O	1:D:168:LEU:HD11	1.97	0.64
1:C:172:TYR:CA	1:C:192:THR:HG21	2.26	0.64
1:A:550:SER:O	1:A:553:LYS:HG2	1.98	0.64
1:C:144:GLN:HB2	1:C:184:ILE:HG22	1.78	0.64
1:C:309:THR:HG22	1:C:430:THR:HG22	1.80	0.64
1:B:159:MET:HG3	1:B:159:MET:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:GLN:OE1	1:C:182:GLU:CA	2.46	0.63
1:B:419:LEU:C	1:B:419:LEU:HD12	2.18	0.63
1:B:83:LEU:HD12	1:B:83:LEU:O	1.98	0.63
1:B:452:LEU:N	1:B:452:LEU:HD12	2.13	0.63
1:D:132:PHE:CZ	1:D:136:ARG:NH1	2.63	0.63
1:B:152:ASN:ND2	1:B:156:GLU:CG	2.49	0.63
1:B:517:GLN:HA	1:B:517:GLN:NE2	2.12	0.63
1:D:109:LEU:HD12	1:D:138:CYS:SG	2.39	0.63
1:D:284:ARG:NH1	1:D:286:ASN:OD1	2.32	0.63
1:D:226:ARG:NH2	1:D:257:VAL:HB	2.14	0.62
1:B:161:LEU:O	1:B:168:LEU:HD21	1.98	0.62
1:A:522:GLU:OE1	1:A:522:GLU:HA	1.99	0.62
1:A:478:LEU:O	1:A:479:LYS:HE2	1.98	0.62
1:D:83:LEU:O	1:D:87:GLU:HG3	2.00	0.61
1:A:348:ILE:O	1:A:348:ILE:HG13	1.98	0.61
1:D:64:LEU:O	1:D:68:LEU:HG	2.00	0.61
1:B:319:VAL:HG12	1:B:358:ILE:HG23	1.82	0.61
1:C:386:ILE:O	1:C:390:VAL:CG1	2.43	0.61
1:C:57:VAL:CG2	1:C:62:LEU:CD2	2.79	0.61
1:D:109:LEU:HD13	1:D:138:CYS:SG	2.41	0.61
1:D:124:HIS:O	1:D:128:THR:HB	2.01	0.61
1:D:397:GLN:O	1:D:401:ARG:HG3	2.00	0.61
1:C:309:THR:CG2	1:C:430:THR:HG22	2.30	0.60
1:D:130:LEU:HD12	1:D:134:LEU:HD22	1.82	0.60
1:D:365:LYS:CE	1:D:368:GLU:OE1	2.50	0.60
1:A:289:GLN:N	1:A:556:MET:HE1	2.17	0.60
1:C:193:THR:CG2	1:C:194:LYS:N	2.64	0.60
1:C:490:ALA:HB1	1:C:494:VAL:HG12	1.82	0.60
1:D:68:LEU:N	1:D:68:LEU:HD23	2.17	0.59
1:D:42:TRP:CH2	1:D:553:LYS:HB2	2.36	0.59
1:D:76:PHE:CD1	1:D:88:LEU:CD2	2.85	0.59
1:D:334:ASP:HA	1:D:397:GLN:OE1	2.02	0.59
1:D:465:ILE:HD13	1:D:481:ILE:HD11	1.83	0.59
1:C:193:THR:HG22	1:C:194:LYS:N	2.17	0.59
1:D:319:VAL:HG13	1:D:358:ILE:HG12	1.85	0.59
1:D:286:ASN:HA	1:D:289:GLN:OE1	2.02	0.59
1:B:448:LEU:HD22	1:B:449:PRO:HD2	1.85	0.59
1:D:543:ASP:OD1	1:D:545:PHE:O	2.20	0.59
1:A:58:GLU:OE2	1:A:58:GLU:HA	2.03	0.58
1:B:133:ARG:NH2	2:B:604:HOH:O	2.35	0.58
1:B:159:MET:O	1:B:162:CYS:SG	2.61	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:ARG:HB3	1:C:496:ARG:NH1	2.18	0.58
1:D:284:ARG:O	1:D:284:ARG:HG2	2.01	0.58
1:C:211:ARG:HH21	1:C:232:PHE:HE1	1.43	0.58
1:A:271:TRP:CZ2	1:A:365:LYS:HE3	2.39	0.58
1:D:223:ARG:O	1:D:533:ARG:HD3	2.03	0.58
1:D:424:PHE:O	1:D:428:LEU:HB2	2.04	0.58
1:C:390:VAL:O	1:C:394:LYS:HG3	2.04	0.58
1:C:226:ARG:HD2	1:C:226:ARG:O	2.04	0.58
1:B:252:LEU:HD11	1:B:566:LEU:HD13	1.86	0.57
1:D:76:PHE:HD2	1:D:104:GLU:CB	1.98	0.57
1:B:332:GLU:O	1:B:335:LEU:HB2	2.04	0.57
1:C:284:ARG:NH1	1:C:284:ARG:CG	2.43	0.57
1:C:144:GLN:CB	1:C:184:ILE:HG21	2.35	0.57
1:C:172:TYR:HB2	1:C:192:THR:HG23	1.81	0.57
1:A:180:LYS:NZ	1:A:505:GLU:HB3	2.20	0.57
1:D:529:LEU:HD13	1:D:533:ARG:HH21	1.70	0.57
1:A:379:TYR:HB2	1:A:439:GLU:HB2	1.86	0.57
1:D:299:SER:O	1:D:307:ARG:NH1	2.38	0.57
1:D:330:ILE:H	1:D:330:ILE:CD1	2.03	0.57
1:B:162:CYS:HA	1:B:168:LEU:HD11	1.87	0.57
1:D:199:ALA:O	1:D:203:ILE:HG13	2.05	0.57
1:A:382:ILE:HB	1:A:383:PRO:HD3	1.87	0.56
1:D:180:LYS:HE3	1:D:505:GLU:HG3	1.86	0.56
1:D:522:GLU:OE1	1:D:522:GLU:HA	2.05	0.56
1:B:229:ALA:O	1:B:233:ILE:HG13	2.05	0.56
1:D:449:PRO:HG2	1:D:452:LEU:HD12	1.86	0.56
1:B:482:HIS:HA	1:B:485:MET:HE2	1.87	0.56
1:D:65:ALA:HB3	1:D:256:MET:HE1	1.86	0.56
1:A:349:ASP:HA	1:A:356:LYS:HZ1	1.69	0.56
1:A:460:ARG:HD3	1:A:460:ARG:C	2.25	0.56
1:B:151:GLN:NE2	1:B:155:GLY:O	2.39	0.56
1:D:510:LEU:O	1:D:510:LEU:HD22	2.05	0.56
1:A:335:LEU:HB3	1:A:351:LEU:HD11	1.87	0.56
1:B:144:GLN:HG2	2:B:603:HOH:O	2.04	0.56
1:A:460:ARG:HD3	1:A:460:ARG:O	2.05	0.55
1:D:179:TRP:N	1:D:182:GLU:OE1	2.31	0.55
1:D:314:GLY:O	1:D:318:THR:HG23	2.06	0.55
1:A:549:ASP:OD1	1:A:553:LYS:HE2	2.06	0.55
1:B:162:CYS:HB2	1:B:195:CYS:SG	2.42	0.55
1:C:179:TRP:CE3	1:C:512:GLN:CG	2.89	0.55
1:C:543:ASP:O	1:C:547:VAL:CG1	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:GLN:HA	1:B:517:GLN:HE21	1.72	0.55
1:D:54:HIS:ND1	1:D:55:ASN:O	2.26	0.55
1:A:133:ARG:HD2	1:A:137:GLN:OE1	2.06	0.55
1:A:144:GLN:OE1	1:A:184:ILE:HB	2.06	0.55
1:C:121:TRP:HE3	1:C:128:THR:HG1	1.55	0.55
1:D:337:THR:HG21	1:D:397:GLN:HE22	1.71	0.55
1:C:57:VAL:CG2	1:C:62:LEU:HD21	2.37	0.55
1:C:132:PHE:CZ	1:C:136:ARG:CZ	2.89	0.55
1:C:135:LEU:HD22	1:C:140:LEU:HD12	1.88	0.55
1:A:224:VAL:HG22	1:A:227:ILE:HG13	1.89	0.54
1:B:425:PRO:O	1:B:429:ILE:HG13	2.07	0.54
1:A:124:HIS:O	1:A:128:THR:OG1	2.21	0.54
1:B:314:GLY:O	1:B:318:THR:HG23	2.07	0.54
1:B:485:MET:O	1:B:489:GLY:CA	2.55	0.54
1:C:113:TYR:HB2	1:C:140:LEU:HD13	1.88	0.54
1:C:490:ALA:HB1	1:C:494:VAL:HG11	1.89	0.54
1:D:50:LEU:O	1:D:54:HIS:HB3	2.07	0.54
1:D:162:CYS:O	1:D:162:CYS:SG	2.65	0.54
1:B:94:ARG:HB3	1:B:232:PHE:CD2	2.43	0.54
1:B:68:LEU:HD22	1:B:245:THR:HG23	1.88	0.54
1:D:230:ARG:NH1	1:D:558:SER:O	2.40	0.54
1:B:223:ARG:O	1:B:533:ARG:HD3	2.08	0.54
1:D:529:LEU:HD13	1:D:533:ARG:NH2	2.23	0.54
1:B:249:LEU:HD22	1:B:249:LEU:O	2.08	0.53
1:C:258:GLN:O	1:C:262:GLN:HG3	2.08	0.53
1:D:330:ILE:HD12	1:D:330:ILE:N	2.10	0.53
1:B:490:ALA:HB1	1:B:494:VAL:CG1	2.37	0.53
1:C:437:GLU:HG2	2:C:606:HOH:O	2.07	0.53
1:D:94:ARG:HH12	1:D:211:ARG:HH21	1.52	0.53
1:A:211:ARG:NH2	1:A:239:GLU:OE1	2.42	0.53
1:B:439:GLU:O	1:B:442:LEU:HB2	2.09	0.53
1:B:479:LYS:H	1:B:482:HIS:CE1	2.25	0.53
1:A:47:LEU:O	1:A:266:GLY:HA2	2.08	0.53
1:B:43:ASN:OD1	1:B:46:PHE:N	2.40	0.53
1:C:44:TYR:CE1	1:C:285:ASN:OD1	2.62	0.53
1:D:377:ARG:NH2	1:D:436:ALA:O	2.41	0.53
1:D:76:PHE:HE1	1:D:88:LEU:HD21	1.66	0.53
1:D:72:VAL:HG22	1:D:75:MET:CE	2.37	0.53
1:B:56:ILE:N	1:B:56:ILE:HD12	2.24	0.52
1:D:65:ALA:CB	1:D:256:MET:CE	2.87	0.52
1:C:144:GLN:OE1	1:C:182:GLU:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ARG:O	1:C:533:ARG:HD3	2.09	0.52
1:D:339:SER:HB2	1:D:359:PHE:CE2	2.45	0.52
1:B:189:LYS:O	1:B:193:THR:OG1	2.20	0.52
1:D:65:ALA:CB	1:D:256:MET:HE3	2.39	0.52
1:B:252:LEU:CD1	1:B:566:LEU:HD13	2.40	0.51
1:A:349:ASP:HA	1:A:356:LYS:HZ3	1.75	0.51
1:B:478:LEU:C	1:B:478:LEU:HD22	2.30	0.51
1:B:330:ILE:CD1	1:B:330:ILE:N	2.73	0.51
1:B:522:GLU:OE1	1:B:526:THR:OG1	2.20	0.51
1:C:211:ARG:NH2	1:C:232:PHE:CZ	2.77	0.51
1:D:59:GLU:OE2	1:D:59:GLU:HA	2.08	0.51
1:B:61:HIS:NE2	1:B:566:LEU:HD12	2.25	0.51
1:D:298:ALA:O	1:D:307:ARG:HG3	2.10	0.51
1:D:382:ILE:O	1:D:386:ILE:HG13	2.10	0.51
1:A:130:LEU:HG	1:A:134:LEU:HD22	1.91	0.51
1:B:312:GLU:HB3	1:B:365:LYS:HD2	1.93	0.51
1:D:67:LYS:C	1:D:68:LEU:HD23	2.31	0.51
1:C:98:ASN:OD1	1:C:98:ASN:N	2.36	0.51
1:B:59:GLU:HA	1:B:62:LEU:HD12	1.92	0.50
1:B:282:PHE:O	1:B:284:ARG:HG3	2.11	0.50
1:B:485:MET:O	1:B:489:GLY:HA2	2.12	0.50
1:C:59:GLU:O	1:C:59:GLU:HG3	2.11	0.50
1:C:435:ILE:HD11	1:C:524:PHE:HB2	1.92	0.50
1:C:437:GLU:CG	2:C:606:HOH:O	2.58	0.50
1:C:449:PRO:HG2	1:C:452:LEU:HD13	1.93	0.50
1:C:94:ARG:HH21	1:C:220:LEU:CD2	2.24	0.50
1:C:295:CYS:HA	1:C:307:ARG:HD2	1.94	0.50
1:C:288:LEU:HG	1:C:556:MET:CE	2.41	0.50
1:A:407:HIS:HE1	2:A:629:HOH:O	1.94	0.50
1:C:94:ARG:NH2	1:C:220:LEU:HD22	2.27	0.50
1:C:150:PHE:HB3	1:C:161:LEU:CD2	2.37	0.50
1:A:145:ASP:OD1	1:A:145:ASP:N	2.42	0.50
1:D:295:CYS:HA	1:D:307:ARG:HD2	1.93	0.50
1:D:329:SER:HB3	1:D:332:GLU:OE2	2.12	0.50
1:A:102:GLU:OE1	1:A:102:GLU:HA	2.11	0.50
1:B:354:THR:O	1:B:358:ILE:HG13	2.11	0.50
1:C:298:ALA:O	1:C:307:ARG:HG3	2.12	0.50
1:A:249:LEU:O	1:A:249:LEU:HD22	2.12	0.50
1:B:200:TRP:O	1:B:203:ILE:HG13	2.12	0.50
1:C:57:VAL:HG21	1:C:62:LEU:CD2	2.42	0.50
1:C:132:PHE:O	1:C:136:ARG:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:HIS:CE1	1:C:223:ARG:NH1	2.80	0.50
1:A:136:ARG:NH2	1:A:141:PHE:CE1	2.80	0.50
1:B:452:LEU:HD12	1:B:452:LEU:H	1.76	0.49
1:C:292:MET:CE	1:C:556:MET:HA	2.42	0.49
1:D:76:PHE:CE2	1:D:104:GLU:CB	2.92	0.49
1:D:379:TYR:HB2	1:D:439:GLU:HB2	1.94	0.49
1:A:452:LEU:N	1:A:452:LEU:HD12	2.28	0.49
1:C:57:VAL:HG21	1:C:62:LEU:HD23	1.95	0.49
1:D:381:SER:C	1:D:383:PRO:HD2	2.33	0.49
1:D:329:SER:HB3	1:D:332:GLU:CD	2.33	0.49
1:A:338:SER:HA	1:A:341:GLU:HG3	1.93	0.49
1:D:382:ILE:N	1:D:383:PRO:HD3	2.27	0.49
1:A:424:PHE:N	1:A:425:PRO:CD	2.76	0.49
1:B:79:PRO:HG2	1:D:327:TYR:HA	1.94	0.49
1:C:144:GLN:CD	1:C:184:ILE:HB	2.31	0.49
1:C:200:TRP:C	1:C:200:TRP:CD1	2.85	0.49
1:D:56:ILE:HD12	1:D:56:ILE:C	2.34	0.49
1:C:248:LYS:HD3	1:C:248:LYS:HA	1.52	0.49
1:D:286:ASN:C	1:D:286:ASN:HD22	2.16	0.49
1:D:154:THR:O	1:D:154:THR:HG22	2.11	0.48
1:A:152:ASN:OD1	1:A:154:THR:HG23	2.12	0.48
1:B:61:HIS:CD2	1:B:566:LEU:HD12	2.48	0.48
1:A:133:ARG:HG3	1:A:174:ALA:HA	1.94	0.48
1:B:490:ALA:HB1	1:B:494:VAL:HG12	1.96	0.48
1:A:420:VAL:HA	1:A:425:PRO:HG2	1.95	0.48
1:B:180:LYS:HE2	1:B:505:GLU:HB3	1.95	0.48
1:B:171:LEU:HD23	1:B:192:THR:CG2	2.44	0.48
1:D:392:GLN:OE1	1:D:423:GLY:HA2	2.14	0.48
1:A:151:GLN:OE1	1:A:184:ILE:HG23	2.14	0.48
1:B:94:ARG:HE	1:B:220:LEU:HD22	1.78	0.48
1:C:502:VAL:HG12	1:C:506:ASN:HD22	1.77	0.48
1:A:277:LEU:HD23	1:A:280:LEU:HD12	1.95	0.48
1:A:386:ILE:O	1:A:390:VAL:CG1	2.58	0.48
1:B:330:ILE:N	1:B:330:ILE:HD12	2.29	0.48
1:C:281:ALA:CB	1:C:284:ARG:NH1	2.58	0.48
1:D:162:CYS:HA	1:D:168:LEU:HD11	1.95	0.48
1:A:135:LEU:HD23	1:A:142:ILE:HD11	1.96	0.48
1:D:374:GLN:O	1:D:374:GLN:HG3	2.14	0.48
1:A:458:LEU:O	1:A:462:ILE:HG13	2.13	0.48
1:C:349:ASP:OD1	1:C:356:LYS:NZ	2.47	0.47
1:D:424:PHE:N	1:D:425:PRO:CD	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:GLN:CA	1:A:556:MET:HE1	2.43	0.47
1:A:159:MET:O	1:A:159:MET:HG3	2.14	0.47
1:B:159:MET:CG	1:B:162:CYS:HG	2.23	0.47
1:C:193:THR:HG22	1:C:194:LYS:H	1.79	0.47
1:D:449:PRO:CG	1:D:452:LEU:HD12	2.44	0.47
1:C:379:TYR:HB2	1:C:439:GLU:HG3	1.96	0.47
1:A:390:VAL:O	1:A:394:LYS:HG3	2.15	0.47
1:B:55:ASN:HB2	1:B:259:SER:HB2	1.97	0.47
1:B:86:LEU:HD22	1:B:134:LEU:HD23	1.96	0.47
1:C:435:ILE:CD1	1:C:524:PHE:HB2	2.45	0.47
1:D:270:ARG:HG2	1:D:270:ARG:HH21	1.78	0.47
1:B:289:GLN:OE1	1:B:289:GLN:N	2.42	0.47
1:B:517:GLN:HE21	1:B:517:GLN:CA	2.27	0.47
1:D:487:GLU:O	1:D:487:GLU:HG3	2.15	0.47
1:B:412:GLU:HA	1:B:412:GLU:OE1	2.15	0.47
1:D:282:PHE:CD1	1:D:282:PHE:N	2.82	0.47
1:A:153:LYS:N	1:A:153:LYS:CD	2.73	0.47
1:B:129:SER:HB2	1:B:170:SER:HB3	1.96	0.47
1:B:517:GLN:NE2	1:B:517:GLN:CA	2.78	0.47
1:C:113:TYR:CB	1:C:140:LEU:HD13	2.45	0.47
1:D:76:PHE:CD1	1:D:88:LEU:HD21	2.48	0.47
1:A:414:TYR:CD1	1:A:414:TYR:C	2.88	0.46
1:B:529:LEU:O	1:B:533:ARG:HG3	2.16	0.46
1:C:224:VAL:HB	1:C:227:ILE:HD12	1.97	0.46
1:B:330:ILE:CD1	1:B:404:HIS:CD2	2.84	0.46
1:A:211:ARG:NH2	1:A:239:GLU:OE2	2.49	0.46
1:B:334:ASP:HA	1:B:397:GLN:HE22	1.80	0.46
1:B:547:VAL:O	1:B:547:VAL:HG22	2.14	0.46
1:D:218:LEU:HB2	1:D:223:ARG:NH2	2.30	0.46
1:D:193:THR:HG22	1:D:194:LYS:N	2.30	0.46
1:D:242:MET:HE2	1:D:242:MET:HB2	1.69	0.46
1:B:241:ASN:ND2	1:D:283:ALA:HA	2.31	0.46
1:C:208:LEU:O	1:C:208:LEU:HD12	2.16	0.46
1:D:62:LEU:HD12	1:D:62:LEU:HA	1.77	0.46
1:D:99:HIS:NE2	1:D:253:ASP:OD2	2.39	0.46
1:D:379:TYR:CB	1:D:439:GLU:HB2	2.45	0.46
1:D:537:PHE:O	2:D:601:HOH:O	2.21	0.46
1:A:178:GLY:HA2	1:A:185:LEU:CD1	2.46	0.46
1:A:330:ILE:HD13	1:A:330:ILE:HA	1.74	0.46
1:C:158:ASP:HB2	1:C:161:LEU:HD22	1.98	0.46
1:C:218:LEU:HB2	1:C:223:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:LEU:HA	1:C:449:PRO:HD2	1.71	0.46
1:C:539:TYR:HA	1:C:542:GLY:O	2.15	0.46
1:D:242:MET:O	1:D:244:PRO:HD3	2.16	0.46
1:D:398:LYS:HD3	1:D:417:ASN:OD1	2.15	0.46
1:B:562:ASP:HA	1:B:563:PRO:HD3	1.76	0.46
1:C:420:VAL:HA	1:C:425:PRO:HG2	1.98	0.46
1:D:148:LYS:HD3	1:D:148:LYS:HA	1.76	0.46
1:A:179:TRP:CD2	1:A:512:GLN:HB2	2.51	0.46
1:A:523:PRO:HB2	2:A:625:HOH:O	2.15	0.46
1:B:89:VAL:O	1:B:93:GLN:HG3	2.15	0.46
1:A:354:THR:HB	1:B:518:SER:OG	2.16	0.46
1:C:149:THR:HG22	1:C:149:THR:O	2.16	0.46
1:A:526:THR:HG22	2:A:625:HOH:O	2.16	0.45
1:C:257:VAL:HG12	1:C:261:HIS:CE1	2.51	0.45
1:D:242:MET:HE1	1:D:247:LEU:HB2	1.99	0.45
1:B:237:GLU:HG3	1:B:247:LEU:HD21	1.98	0.45
1:C:309:THR:CG2	1:C:430:THR:CG2	2.94	0.45
1:D:286:ASN:HD22	1:D:286:ASN:H	1.64	0.45
1:A:335:LEU:HB3	1:A:351:LEU:CD1	2.46	0.45
1:B:323:GLY:HA2	1:B:327:TYR:HB2	1.98	0.45
1:B:325:ASP:OD1	1:B:326:VAL:HG23	2.17	0.45
1:D:300:ASP:HA	1:D:301:PRO:HD3	1.76	0.45
1:B:428:LEU:HD13	1:B:528:ASN:OD1	2.16	0.45
1:D:403:PHE:O	1:D:403:PHE:CD1	2.70	0.45
1:D:335:LEU:HD12	1:D:335:LEU:C	2.35	0.45
1:D:427:LEU:O	1:D:430:THR:HB	2.17	0.45
1:A:289:GLN:N	1:A:556:MET:CE	2.80	0.45
1:A:365:LYS:HA	1:A:365:LYS:HD3	1.72	0.45
1:A:377:ARG:NH2	1:A:436:ALA:O	2.50	0.45
1:D:460:ARG:C	1:D:460:ARG:HD3	2.35	0.45
1:A:93:GLN:HA	1:A:98:ASN:HB3	1.99	0.45
1:B:241:ASN:HD21	1:D:283:ALA:HA	1.82	0.45
1:C:121:TRP:HE3	1:C:128:THR:OG1	2.00	0.45
1:A:55:ASN:OD1	1:A:563:PRO:CG	2.60	0.44
1:B:80:MET:SD	1:D:282:PHE:CE2	3.00	0.44
1:C:377:ARG:NH1	1:C:377:ARG:HG2	2.31	0.44
1:D:128:THR:HG21	1:D:150:PHE:CE2	2.51	0.44
1:C:63:LYS:HA	1:C:63:LYS:HD3	1.39	0.44
1:D:94:ARG:HE	1:D:220:LEU:HD22	1.83	0.44
1:B:282:PHE:O	1:B:282:PHE:CD1	2.70	0.44
1:B:287:LEU:HD23	1:B:287:LEU:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:HIS:HA	1:B:485:MET:CE	2.47	0.44
1:A:224:VAL:CG2	1:A:227:ILE:HG13	2.46	0.44
1:B:248:LYS:O	1:B:252:LEU:HD22	2.17	0.44
1:A:133:ARG:O	1:A:137:GLN:HG3	2.16	0.44
1:A:211:ARG:NH2	1:A:239:GLU:CD	2.71	0.44
1:C:189:LYS:O	1:C:193:THR:HB	2.18	0.44
1:C:377:ARG:HG2	1:C:377:ARG:HH11	1.82	0.44
1:C:467:THR:O	1:C:467:THR:HG22	2.17	0.44
1:D:189:LYS:O	1:D:193:THR:HB	2.17	0.44
1:A:201:GLU:HA	1:A:201:GLU:OE1	2.18	0.44
1:D:355:LEU:HD12	1:D:355:LEU:HA	1.75	0.44
1:A:134:LEU:HD12	1:A:134:LEU:HA	1.80	0.44
1:A:211:ARG:HH21	1:A:239:GLU:CD	2.22	0.44
1:C:113:TYR:CG	1:C:140:LEU:HD13	2.53	0.44
1:A:179:TRP:CE2	1:A:512:GLN:HA	2.52	0.43
1:D:78:ALA:HB1	1:D:79:PRO:HD2	1.98	0.43
1:D:556:MET:O	1:D:560:LEU:HB2	2.19	0.43
1:B:268:LEU:HD21	1:B:287:LEU:HD22	2.00	0.43
1:B:420:VAL:HA	1:B:425:PRO:HG2	2.00	0.43
1:D:121:TRP:HE3	1:D:128:THR:OG1	2.01	0.43
1:A:193:THR:HG22	1:A:197:LYS:HD2	2.00	0.43
1:A:289:GLN:CA	1:A:556:MET:HE3	2.20	0.43
1:B:424:PHE:N	1:B:425:PRO:CD	2.82	0.43
1:C:182:GLU:HB2	1:C:185:LEU:HD12	2.00	0.43
1:C:550:SER:O	1:C:553:LYS:HG2	2.18	0.43
1:A:350:LYS:H	1:A:350:LYS:HG2	1.46	0.43
1:B:161:LEU:O	1:B:168:LEU:HD11	2.18	0.43
1:C:425:PRO:HD3	1:C:456:SER:HB3	2.01	0.43
1:D:414:TYR:CD1	1:D:414:TYR:C	2.92	0.43
1:B:204:SER:OG	1:B:205:GLU:N	2.52	0.43
1:B:457:LEU:HD22	1:B:457:LEU:O	2.19	0.43
1:C:288:LEU:HD23	1:C:556:MET:HE2	2.01	0.43
1:C:309:THR:HG23	1:C:430:THR:CG2	2.48	0.43
1:D:193:THR:CG2	1:D:194:LYS:N	2.80	0.43
1:D:130:LEU:HD11	1:D:134:LEU:HD22	1.99	0.43
1:D:247:LEU:O	1:D:250:ALA:HB3	2.19	0.43
1:D:336:TYR:O	1:D:340:VAL:HG23	2.17	0.43
1:D:408:THR:HB	1:D:478:LEU:HD11	2.00	0.43
1:C:505:GLU:O	1:C:509:ILE:HG13	2.19	0.43
1:D:298:ALA:O	1:D:307:ARG:CG	2.66	0.43
1:D:403:PHE:CD1	1:D:403:PHE:C	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:ASN:C	1:B:486:ASN:ND2	2.72	0.43
1:C:132:PHE:HZ	1:C:136:ARG:CZ	2.29	0.43
1:C:424:PHE:N	1:C:425:PRO:CD	2.82	0.43
1:B:452:LEU:H	1:B:452:LEU:CD1	2.32	0.43
1:D:293:TRP:CZ2	1:D:424:PHE:HZ	2.37	0.43
1:B:481:ILE:HG22	1:B:485:MET:HE2	2.01	0.43
1:B:522:GLU:CD	1:B:526:THR:HG1	2.18	0.43
1:C:444:LYS:HE2	1:C:519:GLN:O	2.19	0.43
1:D:437:GLU:H	1:D:437:GLU:HG3	1.69	0.43
1:A:210:LYS:HD3	1:A:231:TRP:CZ2	2.53	0.42
1:A:316:VAL:HG11	1:A:362:MET:HA	2.01	0.42
1:A:562:ASP:HA	1:A:563:PRO:HD3	1.69	0.42
1:D:134:LEU:HD12	1:D:134:LEU:HA	1.72	0.42
1:A:152:ASN:ND2	1:A:156:GLU:HB2	2.33	0.42
1:B:377:ARG:HB3	1:B:379:TYR:CE2	2.55	0.42
1:B:492:GLU:O	1:B:496:ARG:HG3	2.19	0.42
1:C:298:ALA:O	1:C:307:ARG:CG	2.67	0.42
1:D:130:LEU:HD11	1:D:134:LEU:CD2	2.49	0.42
1:B:57:VAL:HG13	1:B:57:VAL:O	2.20	0.42
1:B:85:LYS:HB3	1:B:112:ILE:HD11	2.01	0.42
1:B:144:GLN:OE1	1:B:184:ILE:HB	2.19	0.42
1:C:144:GLN:CD	1:C:184:ILE:CG2	2.88	0.42
1:B:419:LEU:HD12	1:B:419:LEU:O	2.18	0.42
1:C:419:LEU:O	1:C:422:ILE:HG22	2.19	0.42
1:A:173:GLU:HA	1:A:173:GLU:OE2	2.20	0.42
1:C:83:LEU:HD13	1:C:127:ALA:CB	2.49	0.42
1:C:498:HIS:O	1:C:501:GLY:N	2.52	0.42
1:D:300:ASP:HB2	1:D:303:PHE:HD2	1.76	0.42
1:D:381:SER:C	1:D:383:PRO:CD	2.87	0.42
1:B:452:LEU:N	1:B:452:LEU:CD1	2.80	0.42
1:C:172:TYR:HD1	1:C:192:THR:HG22	1.85	0.42
1:A:337:THR:O	1:A:341:GLU:HG3	2.20	0.42
1:B:186:ASP:OD1	1:B:508:LYS:NZ	2.37	0.42
1:B:330:ILE:CD1	1:B:330:ILE:H	2.33	0.42
1:C:134:LEU:HD12	1:C:134:LEU:HA	1.80	0.42
1:A:379:TYR:HB2	1:A:439:GLU:CB	2.49	0.42
1:D:286:ASN:HD22	1:D:286:ASN:N	2.17	0.42
1:D:365:LYS:HE2	1:D:368:GLU:HB2	2.01	0.42
1:B:218:LEU:HD23	1:B:218:LEU:HA	1.90	0.42
1:B:241:ASN:OD1	1:D:285:ASN:HB2	2.20	0.42
1:C:292:MET:HE1	1:C:556:MET:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:HD12	1:B:134:LEU:HA	1.84	0.41
1:B:348:ILE:HD12	1:B:356:LYS:HG2	2.02	0.41
1:C:211:ARG:NE	1:C:239:GLU:OE2	2.53	0.41
1:C:268:LEU:HD13	1:C:311:VAL:HG13	2.02	0.41
1:D:428:LEU:HB3	1:D:452:LEU:CD2	2.50	0.41
1:B:252:LEU:CD1	1:B:566:LEU:CD1	2.97	0.41
1:D:72:VAL:O	1:D:75:MET:HB2	2.20	0.41
1:B:365:LYS:O	1:B:365:LYS:HD3	2.20	0.41
1:C:249:LEU:HA	1:C:249:LEU:HD23	1.79	0.41
1:D:47:LEU:O	1:D:50:LEU:HB2	2.21	0.41
1:D:72:VAL:CA	1:D:75:MET:HE2	2.48	0.41
1:C:85:LYS:HB3	1:C:112:ILE:HD11	2.02	0.41
1:C:44:TYR:O	1:C:48:GLN:HB2	2.21	0.41
1:C:562:ASP:HA	1:C:563:PRO:HD3	1.93	0.41
1:C:478:LEU:HD12	1:C:479:LYS:HD2	2.01	0.41
1:D:63:LYS:HA	1:D:63:LYS:HD2	1.64	0.41
1:D:94:ARG:HE	1:D:220:LEU:CD2	2.34	0.41
1:D:263:LYS:O	1:D:267:GLU:HG3	2.20	0.41
1:A:165:VAL:HG12	1:A:208:LEU:HD21	2.02	0.41
1:A:333:LEU:O	1:A:337:THR:OG1	2.32	0.41
1:B:510:LEU:CD1	1:B:529:LEU:HD23	2.51	0.41
1:C:162:CYS:HA	1:C:168:LEU:HD11	2.02	0.41
1:A:230:ARG:HH11	1:A:230:ARG:HD2	1.74	0.41
1:A:252:LEU:HD12	1:A:252:LEU:HA	1.82	0.41
1:A:484:TYR:CE1	1:A:488:THR:HG21	2.56	0.41
1:D:460:ARG:HD3	1:D:460:ARG:O	2.21	0.41
1:A:72:VAL:O	1:A:75:MET:HB2	2.21	0.41
1:A:300:ASP:HA	1:A:301:PRO:HD3	1.84	0.41
1:B:47:LEU:O	1:B:266:GLY:HA2	2.21	0.41
1:C:144:GLN:CG	1:C:184:ILE:HG21	2.50	0.41
1:D:349:ASP:HA	1:D:356:LYS:HE2	2.03	0.41
1:B:152:ASN:OD1	1:B:155:GLY:N	2.52	0.41
1:C:242:MET:SD	1:C:242:MET:C	2.99	0.41
1:A:243:ASN:HB3	1:A:246:LEU:HD12	2.03	0.40
1:A:359:PHE:CD1	1:A:359:PHE:C	2.94	0.40
1:D:513:CYS:O	1:D:518:SER:CB	2.59	0.40
1:B:251:LYS:HG2	1:B:564:ILE:HG21	2.03	0.40
1:B:275:THR:HG23	1:B:275:THR:O	2.20	0.40
1:C:297:ILE:HA	1:C:530:ASN:HB3	2.02	0.40
1:D:319:VAL:CG1	1:D:358:ILE:HG12	2.51	0.40
1:D:322:ASP:HB3	1:D:327:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:562:ASP:HA	1:D:563:PRO:HD3	1.83	0.40
1:B:334:ASP:HA	1:B:397:GLN:NE2	2.37	0.40
1:D:485:MET:SD	1:D:492:GLU:HA	2.61	0.40
1:B:498:HIS:O	1:B:502:VAL:HG23	2.20	0.40
1:C:50:LEU:HD23	1:C:50:LEU:HA	1.98	0.40
1:C:94:ARG:HH21	1:C:220:LEU:HD23	1.85	0.40
1:D:94:ARG:NH2	1:D:220:LEU:HD22	2.28	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	518/569 (91%)	503 (97%)	14 (3%)	1 (0%)	47	71
1	B	516/569 (91%)	503 (98%)	10 (2%)	3 (1%)	25	47
1	C	515/569 (90%)	497 (96%)	17 (3%)	1 (0%)	47	71
1	D	517/569 (91%)	491 (95%)	24 (5%)	2 (0%)	34	57
All	All	2066/2276 (91%)	1994 (96%)	65 (3%)	7 (0%)	41	64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	ALA
1	B	115	ASP
1	C	164	ASN
1	D	284	ARG
1	D	55	ASN
1	B	326	VAL
1	B	447	PRO

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	459/500 (92%)	409 (89%)	50 (11%)	6 11
1	B	457/500 (91%)	409 (90%)	48 (10%)	7 13
1	C	457/500 (91%)	395 (86%)	62 (14%)	3 6
1	D	459/500 (92%)	397 (86%)	62 (14%)	4 6
All	All	1832/2000 (92%)	1610 (88%)	222 (12%)	5 9

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	62	LEU
1	A	85	LYS
1	A	114	LYS
1	A	134	LEU
1	A	140	LEU
1	A	145	ASP
1	A	149	THR
1	A	153	LYS
1	A	154	THR
1	A	159	MET
1	A	163	ASP
1	A	183	ASN
1	A	187	GLU
1	A	194	LYS
1	A	201	GLU
1	A	210	LYS
1	A	211	ARG
1	A	230	ARG
1	A	249	LEU
1	A	256	MET
1	A	260	ILE
1	A	270	ARG
1	A	290	SER

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Mol	Chain	Res	Type
1	A	309	THR
1	A	315	SER
1	A	330	ILE
1	A	334	ASP
1	A	335	LEU
1	A	339	SER
1	A	348	ILE
1	A	350	LYS
1	A	354	THR
1	A	356	LYS
1	A	361	SER
1	A	382	ILE
1	A	387	LYS
1	A	408	THR
1	A	416	LEU
1	A	445	VAL
1	A	457	LEU
1	A	459	SER
1	A	493	GLU
1	A	496	ARG
1	A	526	THR
1	A	548	THR
1	A	552	THR
1	A	553	LYS
1	A	557	LYS
1	A	566	LEU
1	B	81	GLU
1	B	107	GLU
1	B	111	SER
1	B	129	SER
1	B	134	LEU
1	B	153	LYS
1	B	154	THR
1	B	162	CYS
1	B	166	LYS
1	B	180	LYS
1	B	204	SER
1	B	206	LYS
1	B	211	ARG
1	B	230	ARG
1	B	249	LEU
1	B	252	LEU

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Mol	Chain	Res	Type
1	B	259	SER
1	B	270	ARG
1	B	274	THR
1	B	275	THR
1	B	285	ASN
1	B	290	SER
1	B	292	MET
1	B	316	VAL
1	B	330	ILE
1	B	350	LYS
1	B	355	LEU
1	B	365	LYS
1	B	371	LEU
1	B	391	GLU
1	B	416	LEU
1	B	437	GLU
1	B	442	LEU
1	B	446	HIS
1	B	448	LEU
1	B	457	LEU
1	B	459	SER
1	B	478	LEU
1	B	486	ASN
1	B	494	VAL
1	B	497	GLU
1	B	507	TRP
1	B	510	LEU
1	B	517	GLN
1	B	521	GLN
1	B	547	VAL
1	B	550	SER
1	B	553	LYS
1	C	52	THR
1	C	57	VAL
1	C	63	LYS
1	C	85	LYS
1	C	87	GLU
1	C	98	ASN
1	C	103	THR
1	C	106	LYS
1	C	114	LYS
1	C	117	SER

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Mol	Chain	Res	Type
1	C	128	THR
1	C	134	LEU
1	C	136	ARG
1	C	142	ILE
1	C	145	ASP
1	C	153	LYS
1	C	161	LEU
1	C	162	CYS
1	C	184	ILE
1	C	192	THR
1	C	193	THR
1	C	194	LYS
1	C	197	LYS
1	C	198	SER
1	C	204	SER
1	C	206	LYS
1	C	213	LYS
1	C	226	ARG
1	C	241	ASN
1	C	248	LYS
1	C	249	LEU
1	C	252	LEU
1	C	284	ARG
1	C	290	SER
1	C	307	ARG
1	C	309	THR
1	C	316	VAL
1	C	338	SER
1	C	349	ASP
1	C	350	LYS
1	C	355	LEU
1	C	365	LYS
1	C	390	VAL
1	C	408	THR
1	C	416	LEU
1	C	425	PRO
1	C	437	GLU
1	C	445	VAL
1	C	457	LEU
1	C	459	SER
1	C	465	ILE
1	C	478	LEU

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Mol	Chain	Res	Type
1	C	479	LYS
1	C	482	HIS
1	C	486	ASN
1	C	493	GLU
1	C	507	TRP
1	C	512	GLN
1	C	547	VAL
1	C	548	THR
1	C	550	SER
1	C	553	LYS
1	D	48	GLN
1	D	49	SER
1	D	57	VAL
1	D	63	LYS
1	D	68	LEU
1	D	72	VAL
1	D	74	PHE
1	D	88	LEU
1	D	93	GLN
1	D	114	LYS
1	D	128	THR
1	D	129	SER
1	D	134	LEU
1	D	135	LEU
1	D	142	ILE
1	D	145	ASP
1	D	148	LYS
1	D	153	LYS
1	D	161	LEU
1	D	162	CYS
1	D	163	ASP
1	D	180	LYS
1	D	193	THR
1	D	198	SER
1	D	205	GLU
1	D	206	LYS
1	D	210	LYS
1	D	213	LYS
1	D	242	MET
1	D	248	LYS
1	D	252	LEU
1	D	270	ARG

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Mol	Chain	Res	Type
1	D	282	PHE
1	D	286	ASN
1	D	307	ARG
1	D	309	THR
1	D	316	VAL
1	D	318	THR
1	D	329	SER
1	D	330	ILE
1	D	334	ASP
1	D	335	LEU
1	D	350	LYS
1	D	355	LEU
1	D	362	MET
1	D	365	LYS
1	D	376	GLU
1	D	397	GLN
1	D	398	LYS
1	D	408	THR
1	D	414	TYR
1	D	437	GLU
1	D	438	ASN
1	D	445	VAL
1	D	479	LYS
1	D	492	GLU
1	D	496	ARG
1	D	497	GLU
1	D	500	LYS
1	D	510	LEU
1	D	519	GLN
1	D	553	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	486	ASN
1	B	517	GLN
1	C	506	ASN
1	D	506	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)

There are no ligands in this entry.

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	522/569 (91%)	-0.29	7 (1%)	77	73	35, 55, 91, 134	0
1	B	520/569 (91%)	-0.27	10 (1%)	66	62	30, 57, 95, 134	0
1	C	519/569 (91%)	-0.13	18 (3%)	44	36	34, 66, 108, 125	0
1	D	521/569 (91%)	-0.05	15 (2%)	51	45	30, 71, 107, 138	0
All	All	2082/2276 (91%)	-0.19	50 (2%)	59	53	30, 63, 101, 138	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	446	HIS	5.9
1	B	284	ARG	4.8
1	C	405	GLY	4.5
1	C	489	GLY	4.4
1	D	404	HIS	4.3
1	C	406	GLY	4.1
1	A	401	ARG	3.5
1	A	163	ASP	3.4
1	D	440	ALA	3.3
1	B	162	CYS	3.3
1	B	406	GLY	3.3
1	D	482	HIS	3.2
1	D	241	ASN	3.2
1	D	118	ASN	3.1
1	A	153	LYS	3.1
1	C	407	HIS	3.0
1	C	110	PHE	3.0
1	D	119	GLY	3.0
1	D	183	ASN	3.0
1	C	487	GLU	2.9
1	D	405	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	284	ARG	2.9
1	C	116	GLY	2.9
1	A	476	ASP	2.9
1	C	154	THR	2.8
1	D	79	PRO	2.7
1	C	152	ASN	2.7
1	C	162	CYS	2.6
1	D	406	GLY	2.6
1	A	181	GLY	2.6
1	C	490	ALA	2.6
1	C	205	GLU	2.5
1	B	401	ARG	2.5
1	C	122	PHE	2.5
1	C	494	VAL	2.5
1	B	154	THR	2.4
1	A	160	LYS	2.4
1	C	404	HIS	2.3
1	B	39	PRO	2.3
1	C	482	HIS	2.3
1	D	403	PHE	2.2
1	C	446	HIS	2.2
1	D	80	MET	2.2
1	B	153	LYS	2.1
1	D	476	ASP	2.1
1	D	163	ASP	2.1
1	A	124	HIS	2.1
1	B	407	HIS	2.1
1	C	484	TYR	2.1
1	B	404	HIS	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.