Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2022 – 06:55 AM JST

PDB ID	:	7ESG
Title	:	Crystal structure of Haloarcula marismortui CheB with Glutathione S-transferase expression tag
Authors	:	Chen, K.L.; Yang, C.S.
Deposited on	:	2021-05-10
Resolution	:	2.53 Å(reported)

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

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

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

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

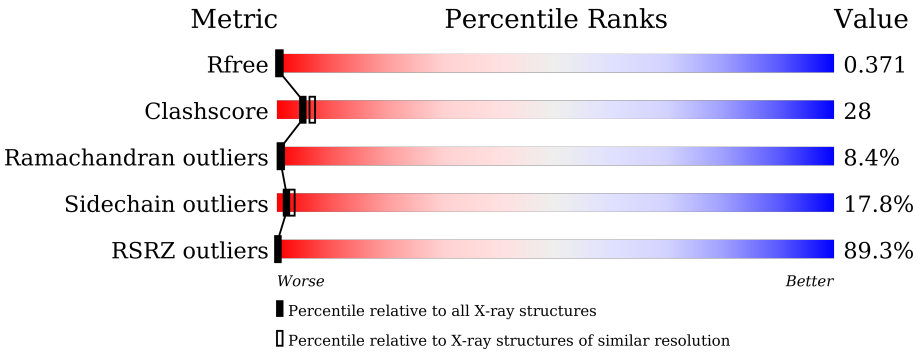
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.53 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	598	88% 38% 48% 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4553 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 Glutathione S-transferase,Protein-glutamate methylesterase/ protein-glutamine glutaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	589	4514	2822	767	895	30	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	SER	-	linker	UNP P08515
A	220	ASP	-	linker	UNP P08515
A	221	LEU	-	linker	UNP P08515
A	222	VAL	-	linker	UNP P08515
A	223	PRO	-	linker	UNP P08515
A	224	ARG	-	linker	UNP P08515
A	225	GLY	-	linker	UNP P08515
A	226	SER	-	linker	UNP P08515
A	227	PRO	-	linker	UNP P08515
A	228	GLU	-	linker	UNP P08515
A	229	PHE	-	linker	UNP P08515

- Molecule 2 is water.

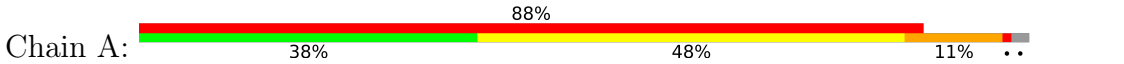
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	39	39	39	0	0

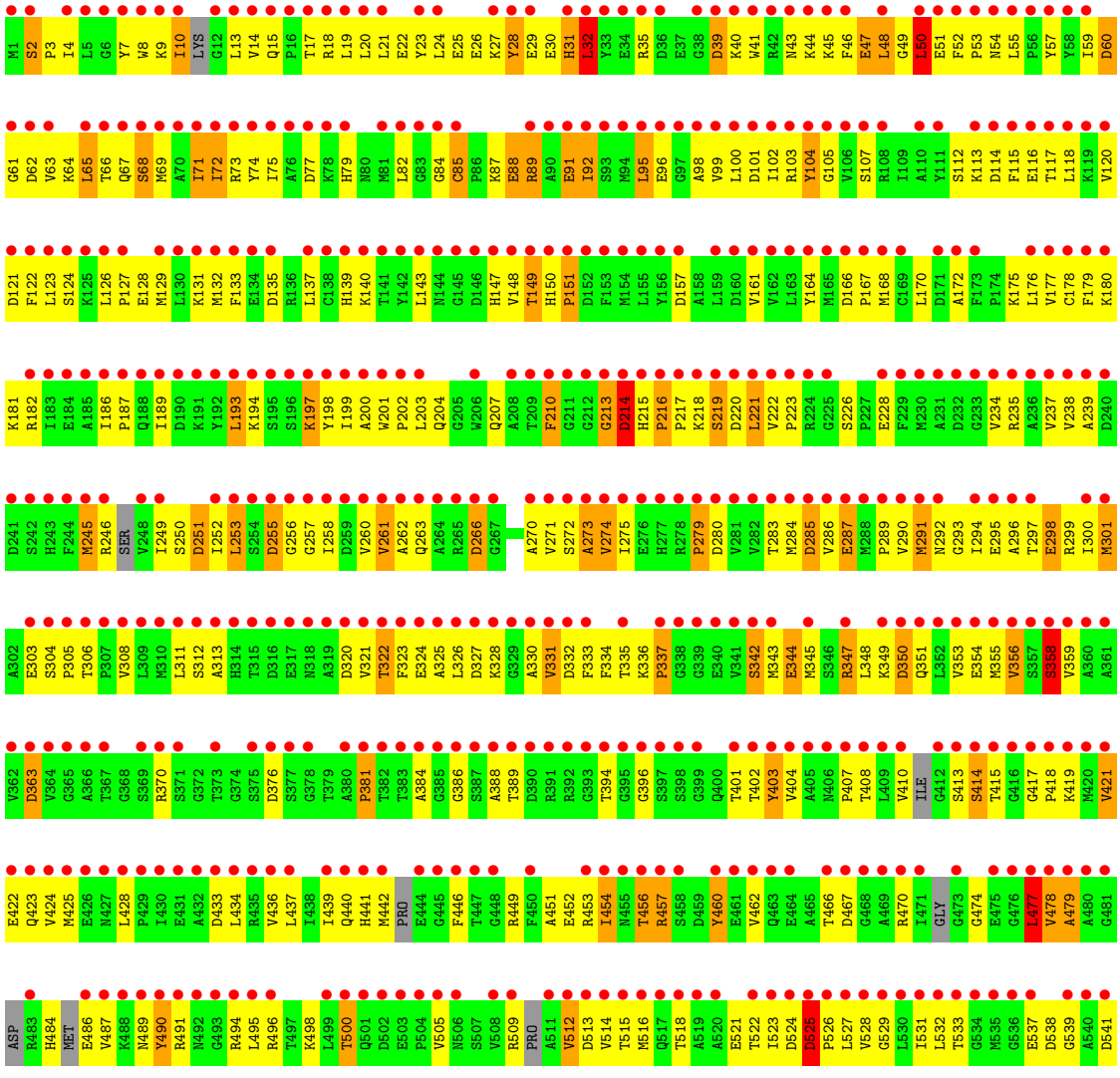
3 Residue-property plots (i)

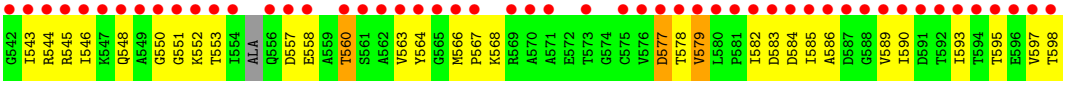
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glutathione S-transferase,Protein-glutamate methylesterase/protein-glutamine glutaminase

Chain A:






G542
I543
R544
R545
I546
K547
Q548
A549
G550
G551
K552
T553
I554
ALA
Q556
D557
E558
A559
T560
S561
A562
V563
Y564
G565
M566
P567
K568
R569
A570
A571
E572
T573
G574
C575
V576
D577
T578
V579
L580
P581
I582
D583
D584
I585
A586
D587
G588
V589
I590
D591
T592
I593
T594
T595
E596
V597
T598

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.06Å 93.91Å 93.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.86 – 2.53 23.86 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.5 (23.86-2.53) 98.9 (23.86-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	120.76 (at 2.53Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.349 , 0.372 0.346 , 0.371	Depositor DCC
R_{free} test set	1753 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.14 , 19.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.318 for -h,l,k	Xtriage
F_o,F_c correlation	0.75	EDS
Total number of atoms	4553	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.26	0/4585	0.54	0/6191

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

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	4514	0	4445	253	0
2	A	39	0	0	11	0
All	All	4553	0	4445	253	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 28.

All (253) 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:A:295:GLU:OE1	2:A:601:HOH:O	1.85	0.94
1:A:140:LYS:HA	1:A:143:LEU:HB2	1.51	0.92
1:A:161:VAL:O	2:A:602:HOH:O	1.91	0.89
1:A:137:LEU:HB3	1:A:151:PRO:HB3	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ARG:H	1:A:249:ILE:HB	1.41	0.85
1:A:586:ALA:HA	1:A:589:VAL:HG12	1.57	0.85
1:A:172:ALA:HA	1:A:175:LYS:HB3	1.61	0.83
1:A:71:ILE:HA	1:A:210:PHE:HB3	1.61	0.82
1:A:53:PRO:HB3	1:A:199:ILE:HD11	1.62	0.81
1:A:178:CYS:SG	2:A:618:HOH:O	2.38	0.81
1:A:238:VAL:HG13	1:A:246:ARG:HB3	1.61	0.80
1:A:126:LEU:HD12	1:A:129:MET:HG2	1.64	0.80
1:A:521:GLU:O	2:A:603:HOH:O	2.01	0.79
1:A:53:PRO:HG2	1:A:222:VAL:HG22	1.64	0.79
1:A:72:ILE:HG21	1:A:216:PRO:HD2	1.65	0.79
1:A:101:ASP:HA	1:A:104:TYR:HB3	1.64	0.78
1:A:327:ASP:OD1	2:A:604:HOH:O	2.01	0.78
1:A:148:VAL:O	1:A:150:HIS:N	2.16	0.77
1:A:531:ILE:HD11	1:A:539:GLY:HA3	1.67	0.77
1:A:298:GLU:HA	1:A:301:MET:HB2	1.67	0.76
1:A:168:MET:HA	1:A:172:ALA:HB3	1.69	0.75
1:A:35:ARG:HB3	1:A:39:ASP:HB2	1.69	0.75
1:A:347:ARG:NH2	2:A:607:HOH:O	2.16	0.72
1:A:29:GLU:HA	1:A:32:LEU:HD13	1.71	0.71
1:A:98:ALA:O	1:A:102:ILE:N	2.23	0.71
1:A:2:SER:H	1:A:3:PRO:HD2	1.56	0.71
1:A:252:ILE:HG23	1:A:253:LEU:HG	1.72	0.71
1:A:246:ARG:HH22	1:A:253:LEU:HD21	1.56	0.70
1:A:167:PRO:O	1:A:172:ALA:N	2.20	0.70
1:A:337:PRO:HG2	1:A:348:LEU:HD21	1.74	0.70
1:A:417:GLY:HA2	1:A:421:VAL:HB	1.73	0.69
1:A:31:HIS:O	1:A:43:ASN:ND2	2.26	0.69
1:A:135:ASP:O	1:A:139:HIS:NE2	2.25	0.69
1:A:320:ASP:O	1:A:324:GLU:N	2.26	0.69
1:A:95:LEU:HD23	1:A:98:ALA:HB3	1.74	0.68
1:A:410:VAL:HA	1:A:437:LEU:H	1.57	0.68
1:A:200:ALA:HA	1:A:203:LEU:HB3	1.76	0.68
1:A:73:ARG:HD3	1:A:217:PRO:HG3	1.76	0.67
1:A:424:VAL:HG22	1:A:585:ILE:HG13	1.76	0.67
1:A:54:ASN:OD1	2:A:605:HOH:O	2.12	0.67
1:A:186:ILE:HA	1:A:189:ILE:HG12	1.75	0.66
1:A:578:THR:HG22	1:A:579:VAL:H	1.60	0.66
1:A:87:LYS:HB3	1:A:509:ARG:HE	1.60	0.66
1:A:44:LYS:O	1:A:46:PHE:N	2.29	0.64
1:A:193:LEU:HD23	1:A:199:ILE:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:HA	1:A:126:LEU:HB2	1.78	0.64
1:A:355:MET:O	1:A:359:VAL:N	2.31	0.63
1:A:286:VAL:HG23	1:A:321:VAL:HG11	1.80	0.63
1:A:414:SER:OG	1:A:415:THR:N	2.29	0.62
1:A:283:THR:HG22	1:A:311:LEU:HD21	1.81	0.62
1:A:79:HIS:HD2	1:A:537:GLU:H	1.48	0.62
1:A:297:THR:O	1:A:301:MET:N	2.32	0.61
1:A:24:LEU:HD11	1:A:218:LYS:HE3	1.82	0.61
1:A:237:VAL:HG23	1:A:279:PRO:HG2	1.82	0.61
1:A:518:THR:O	1:A:522:THR:OG1	2.18	0.61
1:A:237:VAL:HG21	1:A:274:VAL:HA	1.82	0.61
1:A:238:VAL:HB	1:A:263:GLN:HA	1.83	0.61
1:A:99:VAL:HA	1:A:102:ILE:HB	1.83	0.61
1:A:10:ILE:HG23	1:A:13:LEU:HB3	1.84	0.60
1:A:545:ARG:HA	1:A:548:GLN:HB2	1.84	0.60
1:A:72:ILE:HD13	1:A:216:PRO:HG2	1.84	0.60
1:A:543:ILE:HG22	1:A:546:ILE:HD12	1.84	0.60
1:A:15:GLN:O	1:A:19:LEU:HB2	2.01	0.60
1:A:8:TRP:HD1	1:A:234:VAL:HG22	1.67	0.59
1:A:442:MET:HB3	1:A:446:PHE:HD2	1.68	0.59
1:A:200:ALA:O	1:A:204:GLN:N	2.31	0.58
1:A:546:ILE:HG22	1:A:551:GLY:HA3	1.86	0.58
1:A:531:ILE:HG23	1:A:566:MET:HE3	1.85	0.58
1:A:408:THR:HB	1:A:528:VAL:HG12	1.86	0.58
1:A:437:LEU:HD12	1:A:477:LEU:HD22	1.86	0.58
1:A:466:THR:OG1	1:A:467:ASP:N	2.37	0.57
1:A:199:ILE:HG13	1:A:200:ALA:N	2.20	0.57
1:A:419:LYS:NZ	1:A:423:GLN:OE1	2.37	0.57
1:A:454:ILE:HG22	1:A:460:TYR:HE1	1.70	0.57
1:A:528:VAL:HG23	1:A:552:LYS:HB2	1.87	0.56
1:A:113:LYS:HA	1:A:116:GLU:HB2	1.87	0.56
1:A:394:THR:HG22	1:A:396:GLY:H	1.70	0.56
1:A:179:PHE:HA	1:A:182:ARG:HB2	1.87	0.55
1:A:239:ALA:HB3	1:A:284:MET:HA	1.86	0.55
1:A:67:GLN:O	1:A:71:ILE:HG13	2.06	0.55
1:A:577:ASP:OD1	1:A:577:ASP:N	2.39	0.55
1:A:424:VAL:HG21	1:A:532:LEU:HD11	1.89	0.55
1:A:72:ILE:CG2	1:A:216:PRO:HD2	2.34	0.54
1:A:73:ARG:NE	1:A:77:ASP:OD2	2.40	0.54
1:A:344:GLU:O	1:A:348:LEU:N	2.36	0.54
1:A:53:PRO:HD2	1:A:222:VAL:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:O	1:A:129:MET:HG3	2.07	0.54
1:A:478:VAL:HG12	1:A:479:ALA:H	1.73	0.54
1:A:20:LEU:O	1:A:24:LEU:HD12	2.08	0.54
1:A:332:ASP:OD2	1:A:415:THR:OG1	2.25	0.54
1:A:180:LYS:O	1:A:180:LYS:NZ	2.33	0.53
1:A:286:VAL:HG13	1:A:287:GLU:H	1.72	0.53
1:A:255:ASP:OD1	2:A:608:HOH:O	2.17	0.53
1:A:477:LEU:N	2:A:611:HOH:O	2.40	0.52
1:A:452:GLU:O	1:A:456:THR:OG1	2.27	0.52
1:A:50:LEU:HB3	1:A:219:SER:HB3	1.91	0.52
1:A:470:ARG:HD2	1:A:496:ARG:HG2	1.90	0.52
1:A:558:GLU:HA	1:A:564:TYR:CZ	2.44	0.52
1:A:88:GLU:HG3	1:A:509:ARG:H	1.72	0.52
1:A:418:PRO:O	1:A:422:GLU:HG3	2.09	0.52
1:A:101:ASP:HA	1:A:104:TYR:CB	2.37	0.52
1:A:4:ILE:HA	1:A:7:TYR:HB2	1.92	0.52
1:A:22:GLU:O	1:A:26:GLU:HB2	2.10	0.52
1:A:193:LEU:HD23	1:A:199:ILE:CD1	2.40	0.51
1:A:214:ASP:OD1	1:A:215:HIS:N	2.42	0.51
1:A:63:VAL:O	1:A:66:THR:HG22	2.11	0.51
1:A:222:VAL:HG11	1:A:226:SER:OG	2.10	0.51
1:A:235:ARG:HE	1:A:279:PRO:HA	1.75	0.51
1:A:381:PRO:HG3	1:A:584:ASP:OD1	2.11	0.51
1:A:4:ILE:O	1:A:8:TRP:N	2.41	0.50
1:A:179:PHE:CD1	1:A:182:ARG:HD3	2.46	0.50
1:A:82:LEU:HD22	1:A:350:ASP:HB2	1.92	0.50
1:A:137:LEU:HD13	1:A:151:PRO:HA	1.93	0.50
1:A:326:LEU:HD12	1:A:327:ASP:N	2.27	0.50
1:A:54:ASN:HB3	1:A:55:LEU:HD12	1.94	0.50
1:A:285:ASP:OD1	1:A:286:VAL:HG12	2.12	0.50
1:A:304:SER:O	1:A:304:SER:OG	2.30	0.50
1:A:213:GLY:O	1:A:214:ASP:HB3	2.11	0.50
1:A:525:ASP:HB3	1:A:526:PRO:CD	2.42	0.50
1:A:271:VAL:HG22	1:A:300:ILE:HB	1.94	0.49
1:A:320:ASP:HB2	1:A:449:ARG:HH11	1.77	0.49
1:A:238:VAL:HG22	1:A:246:ARG:HH11	1.77	0.49
1:A:304:SER:O	1:A:306:THR:N	2.45	0.49
1:A:350:ASP:O	1:A:354:GLU:HB3	2.13	0.49
1:A:293:GLY:HA2	1:A:296:ALA:HB3	1.95	0.49
1:A:541:ASP:HA	1:A:544:ARG:HD2	1.95	0.49
1:A:172:ALA:O	1:A:176:LEU:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLU:O	1:A:32:LEU:N	2.46	0.48
1:A:193:LEU:HB3	1:A:199:ILE:HD13	1.96	0.48
1:A:294:ILE:HD11	1:A:321:VAL:HG22	1.96	0.48
1:A:453:ARG:HD2	1:A:457:ARG:HD2	1.96	0.48
1:A:514:VAL:O	1:A:518:THR:HG23	2.13	0.48
1:A:258:ILE:HD12	1:A:353:VAL:HB	1.95	0.48
1:A:120:VAL:O	1:A:124:SER:N	2.46	0.48
1:A:59:ILE:O	1:A:61:GLY:N	2.46	0.48
1:A:79:HIS:CD2	1:A:537:GLU:H	2.31	0.48
1:A:85:CYS:SG	1:A:88:GLU:N	2.87	0.48
1:A:235:ARG:HB2	1:A:279:PRO:HA	1.96	0.47
1:A:404:VAL:HG12	1:A:597:VAL:HB	1.96	0.47
1:A:486:GLU:N	1:A:500:THR:HG1	2.13	0.47
1:A:2:SER:N	1:A:3:PRO:HD2	2.28	0.47
1:A:177:VAL:O	1:A:181:LYS:N	2.30	0.47
1:A:75:ILE:HG13	1:A:79:HIS:CG	2.50	0.47
1:A:199:ILE:O	1:A:202:PRO:HD2	2.14	0.47
1:A:593:ILE:HG13	1:A:597:VAL:HG11	1.96	0.46
1:A:356:VAL:HA	1:A:359:VAL:HB	1.98	0.46
1:A:358:SER:O	1:A:563:VAL:HG21	2.16	0.46
1:A:384:ALA:HA	1:A:388:ALA:HB3	1.97	0.46
1:A:91:GLU:O	1:A:92:ILE:HG13	2.16	0.46
1:A:326:LEU:HA	1:A:330:ALA:HB3	1.97	0.46
1:A:148:VAL:HG13	1:A:150:HIS:CD2	2.50	0.46
1:A:428:LEU:HD22	1:A:434:LEU:HD13	1.97	0.46
1:A:21:LEU:HA	1:A:24:LEU:HD13	1.97	0.46
1:A:505:VAL:HG21	1:A:514:VAL:HB	1.97	0.46
1:A:69:MET:HB2	1:A:216:PRO:O	2.16	0.46
1:A:326:LEU:HB2	1:A:418:PRO:HB3	1.96	0.46
1:A:63:VAL:O	1:A:67:GLN:HG3	2.16	0.46
1:A:91:GLU:C	1:A:92:ILE:HG13	2.36	0.46
1:A:566:MET:HB3	1:A:567:PRO:HD3	1.98	0.46
1:A:403:TYR:HA	1:A:598:THR:HA	1.98	0.45
1:A:410:VAL:O	1:A:436:VAL:HG23	2.15	0.45
1:A:266:ASP:HA	1:A:289:PRO:HG2	1.99	0.45
1:A:334:PHE:CE2	1:A:337:PRO:HD3	2.52	0.45
1:A:424:VAL:HG13	1:A:585:ILE:HB	1.99	0.45
1:A:487:VAL:HG23	1:A:496:ARG:H	1.82	0.45
1:A:47:GLU:O	1:A:49:GLY:N	2.49	0.45
1:A:75:ILE:HG13	1:A:79:HIS:ND1	2.32	0.45
1:A:478:VAL:HG12	1:A:479:ALA:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PHE:HD2	1:A:55:LEU:HB2	1.81	0.45
1:A:64:LYS:O	1:A:68:SER:N	2.34	0.45
1:A:161:VAL:HA	1:A:164:TYR:HB3	1.98	0.45
1:A:262:ALA:HB1	1:A:273:ALA:HB1	1.98	0.45
1:A:590:ILE:O	1:A:593:ILE:HG22	2.16	0.45
1:A:523:ILE:HG21	1:A:527:LEU:HD13	1.97	0.45
1:A:65:LEU:HD13	1:A:65:LEU:HA	1.83	0.44
1:A:112:SER:HA	1:A:115:PHE:HD2	1.82	0.44
1:A:292:ASN:OD1	1:A:293:GLY:N	2.51	0.44
1:A:370:ARG:NH2	1:A:560:THR:O	2.50	0.44
1:A:50:LEU:HB2	1:A:51:GLU:H	1.51	0.44
1:A:557:ASP:OD1	1:A:558:GLU:N	2.51	0.44
1:A:177:VAL:HA	1:A:180:LYS:HB3	2.00	0.44
1:A:270:ALA:O	1:A:273:ALA:N	2.51	0.44
1:A:326:LEU:HD13	1:A:418:PRO:O	2.18	0.44
1:A:437:LEU:HD21	1:A:515:THR:HG23	1.99	0.44
1:A:79:HIS:HD2	1:A:537:GLU:N	2.15	0.43
1:A:127:PRO:O	1:A:131:LYS:HB2	2.17	0.43
1:A:525:ASP:HB3	1:A:526:PRO:HD2	2.00	0.43
1:A:532:LEU:HD23	1:A:532:LEU:HA	1.86	0.43
1:A:121:ASP:OD1	1:A:122:PHE:N	2.51	0.43
1:A:126:LEU:HD12	1:A:126:LEU:HA	1.87	0.43
1:A:349:LYS:O	1:A:353:VAL:HG22	2.18	0.43
1:A:23:TYR:O	1:A:27:LYS:HB2	2.17	0.43
1:A:197:LYS:HB2	1:A:197:LYS:HE3	1.80	0.43
1:A:126:LEU:N	1:A:127:PRO:HD2	2.34	0.43
1:A:331:VAL:HG13	1:A:332:ASP:H	1.83	0.43
1:A:238:VAL:HG23	1:A:260:VAL:HG23	2.00	0.43
1:A:245:MET:SD	1:A:245:MET:N	2.88	0.43
1:A:336:LYS:HA	1:A:337:PRO:HD3	1.84	0.43
1:A:297:THR:OG1	1:A:308:VAL:HG11	2.19	0.43
1:A:404:VAL:HG22	1:A:494:ARG:HH22	1.84	0.43
1:A:133:PHE:HD1	1:A:133:PHE:HA	1.75	0.43
1:A:356:VAL:C	1:A:358:SER:H	2.21	0.43
1:A:484:HIS:N	1:A:500:THR:O	2.52	0.43
1:A:79:HIS:NE2	1:A:537:GLU:HB3	2.34	0.43
1:A:118:LEU:HD22	1:A:178:CYS:HB2	2.00	0.43
1:A:193:LEU:HA	1:A:199:ILE:HG21	2.00	0.43
1:A:24:LEU:HD22	1:A:48:LEU:HD13	2.00	0.43
1:A:166:ASP:HB3	1:A:167:PRO:HD2	2.00	0.43
1:A:182:ARG:O	1:A:186:ILE:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ASP:O	1:A:222:VAL:N	2.49	0.42
1:A:148:VAL:HG12	1:A:149:THR:N	2.34	0.42
1:A:386:GLY:HA3	1:A:590:ILE:HG22	2.01	0.42
1:A:19:LEU:HD23	2:A:607:HOH:O	2.20	0.42
1:A:275:ILE:HG23	1:A:300:ILE:HD11	2.01	0.42
1:A:287:GLU:O	1:A:287:GLU:HG3	2.20	0.42
1:A:251:ASP:OD1	1:A:251:ASP:N	2.52	0.42
1:A:529:GLY:O	1:A:553:THR:HA	2.20	0.42
1:A:582:ILE:HA	1:A:585:ILE:HD11	2.02	0.42
1:A:313:ALA:N	1:A:336:LYS:HB3	2.35	0.42
1:A:454:ILE:H	1:A:454:ILE:HG13	1.57	0.42
1:A:166:ASP:O	1:A:170:LEU:N	2.51	0.42
1:A:234:VAL:O	1:A:258:ILE:HA	2.19	0.42
1:A:326:LEU:HD22	1:A:418:PRO:HA	2.01	0.42
1:A:292:ASN:O	1:A:296:ALA:N	2.52	0.42
1:A:140:LYS:HG2	1:A:143:LEU:HD22	2.02	0.42
1:A:271:VAL:HA	1:A:300:ILE:HD12	2.02	0.42
1:A:347:ARG:HH11	1:A:347:ARG:HB2	1.85	0.42
1:A:407:PRO:HB3	1:A:434:LEU:HA	2.02	0.42
1:A:24:LEU:O	1:A:28:TYR:HB3	2.20	0.41
1:A:425:MET:SD	1:A:425:MET:N	2.94	0.41
1:A:513:ASP:HB2	1:A:538:ASP:HB3	2.01	0.41
1:A:148:VAL:C	1:A:150:HIS:N	2.73	0.41
1:A:228:GLU:OE1	1:A:228:GLU:N	2.53	0.41
1:A:322:THR:HB	1:A:323:PHE:CD1	2.55	0.41
1:A:394:THR:HG22	1:A:396:GLY:N	2.35	0.41
1:A:486:GLU:O	1:A:498:LYS:HB3	2.20	0.41
1:A:531:ILE:HD13	1:A:566:MET:HE3	2.03	0.41
1:A:96:GLU:O	1:A:100:LEU:HB2	2.21	0.41
1:A:512:VAL:O	1:A:516:MET:HG3	2.20	0.41
1:A:89:ARG:NH1	1:A:351:GLN:OE1	2.54	0.41
1:A:215:HIS:NE2	2:A:607:HOH:O	2.15	0.41
1:A:235:ARG:HB3	1:A:261:VAL:CG2	2.51	0.41
1:A:342:SER:HB2	1:A:343:MET:H	1.54	0.41
1:A:413:SER:O	1:A:440:GLN:HA	2.21	0.41
1:A:564:TYR:O	1:A:568:LYS:HB2	2.21	0.40
1:A:10:ILE:HG21	1:A:221:LEU:HD22	2.02	0.40
1:A:128:GLU:O	1:A:132:MET:HB2	2.21	0.40
1:A:325:ALA:HA	1:A:328:LYS:HB2	2.03	0.40
1:A:410:VAL:CA	1:A:437:LEU:H	2.29	0.40
1:A:451:ALA:HB1	1:A:462:VAL:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ARG:HE	1:A:491:ARG:HB3	1.74	0.40
1:A:417:GLY:N	1:A:418:PRO:HD2	2.36	0.40
1:A:495:LEU:HD11	1:A:523:ILE:HB	2.03	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	569/598 (95%)	399 (70%)	122 (21%)	48 (8%)	1 0

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	LYS
1	A	149	THR
1	A	216	PRO
1	A	358	SER
1	A	381	PRO
1	A	478	VAL
1	A	490	TYR
1	A	17	THR
1	A	31	HIS
1	A	32	LEU
1	A	60	ASP
1	A	72	ILE
1	A	261	VAL
1	A	279	PRO
1	A	303	GLU
1	A	337	PRO
1	A	363	ASP
1	A	414	SER

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Mol	Chain	Res	Type
1	A	477	LEU
1	A	71	ILE
1	A	105	GLY
1	A	214	ASP
1	A	219	SER
1	A	223	PRO
1	A	479	ALA
1	A	525	ASP
1	A	48	LEU
1	A	187	PRO
1	A	256	GLY
1	A	273	ALA
1	A	290	VAL
1	A	583	ASP
1	A	91	GLU
1	A	210	PHE
1	A	213	GLY
1	A	221	LEU
1	A	344	GLU
1	A	50	LEU
1	A	151	PRO
1	A	291	MET
1	A	257	GLY
1	A	439	ILE
1	A	474	GLY
1	A	2	SER
1	A	84	GLY
1	A	92	ILE
1	A	305	PRO
1	A	550	GLY

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	488/495 (99%)	401 (82%)	87 (18%)	2 3

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	10	ILE
1	A	14	VAL
1	A	18	ARG
1	A	25	GLU
1	A	28	TYR
1	A	32	LEU
1	A	39	ASP
1	A	40	LYS
1	A	41	TRP
1	A	47	GLU
1	A	50	LEU
1	A	57	TYR
1	A	60	ASP
1	A	62	ASP
1	A	65	LEU
1	A	68	SER
1	A	74	TYR
1	A	85	CYS
1	A	88	GLU
1	A	89	ARG
1	A	95	LEU
1	A	103	ARG
1	A	104	TYR
1	A	107	SER
1	A	114	ASP
1	A	117	THR
1	A	147	HIS
1	A	157	ASP
1	A	193	LEU
1	A	194	LYS
1	A	197	LYS
1	A	198	TYR
1	A	201	TRP
1	A	207	GLN
1	A	214	ASP
1	A	245	MET
1	A	250	SER
1	A	251	ASP
1	A	253	LEU
1	A	255	ASP
1	A	266	ASP

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Mol	Chain	Res	Type
1	A	272	SER
1	A	274	VAL
1	A	280	ASP
1	A	285	ASP
1	A	287	GLU
1	A	291	MET
1	A	298	GLU
1	A	299	ARG
1	A	301	MET
1	A	312	SER
1	A	322	THR
1	A	331	VAL
1	A	333	PHE
1	A	335	THR
1	A	342	SER
1	A	345	MET
1	A	347	ARG
1	A	350	ASP
1	A	356	VAL
1	A	358	SER
1	A	363	ASP
1	A	376	ASP
1	A	389	THR
1	A	401	THR
1	A	402	THR
1	A	403	TYR
1	A	421	VAL
1	A	433	ASP
1	A	441	HIS
1	A	454	ILE
1	A	456	THR
1	A	457	ARG
1	A	460	TYR
1	A	477	LEU
1	A	489	ASN
1	A	490	TYR
1	A	500	THR
1	A	512	VAL
1	A	524	ASP
1	A	525	ASP
1	A	533	THR
1	A	560	THR

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Mol	Chain	Res	Type
1	A	577	ASP
1	A	579	VAL
1	A	595	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	589/598 (98%)	4.32	526 (89%)	0	0	23, 27, 31, 35	0

All (526) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	VAL	15.0
1	A	286	VAL	14.5
1	A	523	ILE	14.3
1	A	258	ILE	13.6
1	A	275	ILE	13.6
1	A	505	VAL	12.3
1	A	137	LEU	12.2
1	A	212	GLY	11.3
1	A	297	THR	11.1
1	A	54	ASN	11.0
1	A	441	HIS	10.6
1	A	233	GLY	10.6
1	A	229	PHE	10.5
1	A	183	ILE	10.0
1	A	221	LEU	10.0
1	A	471	ILE	9.7
1	A	522	THR	9.6
1	A	185	ALA	9.4
1	A	216	PRO	9.4
1	A	167	PRO	9.2
1	A	260	VAL	9.0
1	A	273	ALA	8.9
1	A	90	ALA	8.8
1	A	525	ASP	8.7
1	A	133	PHE	8.7
1	A	57	TYR	8.6
1	A	390	ASP	8.6

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Mol	Chain	Res	Type	RSRZ
1	A	598	THR	8.6
1	A	506	ASN	8.5
1	A	453	ARG	8.5
1	A	329	GLY	8.5
1	A	462	VAL	8.4
1	A	262	ALA	8.3
1	A	213	GLY	8.3
1	A	430	ILE	8.2
1	A	330	ALA	8.2
1	A	516	MET	8.1
1	A	244	PHE	8.1
1	A	111	TYR	8.1
1	A	201	TRP	8.0
1	A	535	MET	7.9
1	A	186	ILE	7.9
1	A	340	GLU	7.8
1	A	70	ALA	7.8
1	A	404	VAL	7.7
1	A	257	GLY	7.7
1	A	579	VAL	7.7
1	A	23	TYR	7.6
1	A	592	THR	7.6
1	A	448	GLY	7.6
1	A	593	ILE	7.4
1	A	178	CYS	7.4
1	A	151	PRO	7.3
1	A	230	MET	7.3
1	A	460	TYR	7.3
1	A	75	ILE	7.2
1	A	514	VAL	7.2
1	A	177	VAL	7.2
1	A	39	ASP	7.1
1	A	565	GLY	7.1
1	A	534	GLY	7.1
1	A	557	ASP	7.1
1	A	197	LYS	7.1
1	A	166	ASP	7.1
1	A	384	ALA	7.1
1	A	200	ALA	7.0
1	A	447	THR	7.0
1	A	281	VAL	7.0
1	A	270	ALA	7.0

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Mol	Chain	Res	Type	RSRZ
1	A	214	ASP	6.9
1	A	173	PHE	6.8
1	A	289	PRO	6.8
1	A	203	LEU	6.8
1	A	191	LYS	6.8
1	A	53	PRO	6.8
1	A	234	VAL	6.7
1	A	499	LEU	6.7
1	A	581	PRO	6.7
1	A	210	PHE	6.7
1	A	532	LEU	6.7
1	A	161	VAL	6.6
1	A	123	LEU	6.6
1	A	343	MET	6.6
1	A	187	PRO	6.5
1	A	225	GLY	6.5
1	A	454	ILE	6.5
1	A	594	THR	6.4
1	A	219	SER	6.4
1	A	172	ALA	6.4
1	A	361	ALA	6.4
1	A	198	TYR	6.3
1	A	518	THR	6.3
1	A	272	SER	6.3
1	A	315	THR	6.3
1	A	55	LEU	6.2
1	A	425	MET	6.2
1	A	1	MET	6.2
1	A	597	VAL	6.1
1	A	359	VAL	6.1
1	A	141	THR	6.1
1	A	300	ILE	6.1
1	A	83	GLY	6.0
1	A	511	ALA	6.0
1	A	481	GLY	6.0
1	A	500	THR	6.0
1	A	480	ALA	6.0
1	A	554	ILE	6.0
1	A	220	ASP	6.0
1	A	311	LEU	6.0
1	A	515	THR	5.9
1	A	82	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	580	LEU	5.9
1	A	248	VAL	5.9
1	A	59	ILE	5.9
1	A	429	PRO	5.9
1	A	326	LEU	5.9
1	A	215	HIS	5.8
1	A	292	ASN	5.8
1	A	455	ASN	5.8
1	A	156	TYR	5.8
1	A	21	LEU	5.7
1	A	280	ASP	5.7
1	A	62	ASP	5.7
1	A	7	TYR	5.7
1	A	360	ALA	5.7
1	A	45	LYS	5.7
1	A	405	ALA	5.6
1	A	261	VAL	5.6
1	A	364	VAL	5.6
1	A	61	GLY	5.6
1	A	252	ILE	5.6
1	A	339	GLY	5.6
1	A	394	THR	5.6
1	A	550	GLY	5.5
1	A	10	ILE	5.5
1	A	508	VAL	5.5
1	A	575	CYS	5.5
1	A	333	PHE	5.5
1	A	584	ASP	5.5
1	A	585	ILE	5.5
1	A	558	GLU	5.5
1	A	562	ALA	5.5
1	A	427	ASN	5.4
1	A	56	PRO	5.4
1	A	100	LEU	5.4
1	A	571	ALA	5.4
1	A	143	LEU	5.3
1	A	140	LYS	5.3
1	A	256	GLY	5.3
1	A	413	SER	5.3
1	A	58	TYR	5.3
1	A	325	ALA	5.3
1	A	106	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	389	THR	5.2
1	A	456	THR	5.2
1	A	560	THR	5.2
1	A	342	SER	5.2
1	A	32	LEU	5.2
1	A	237	VAL	5.2
1	A	392	ARG	5.2
1	A	439	ILE	5.2
1	A	318	ASN	5.2
1	A	556	GLN	5.2
1	A	426	GLU	5.2
1	A	494	ARG	5.2
1	A	466	THR	5.2
1	A	509	ARG	5.2
1	A	391	ARG	5.2
1	A	44	LYS	5.1
1	A	548	GLN	5.1
1	A	104	TYR	5.1
1	A	335	THR	5.1
1	A	76	ALA	5.1
1	A	513	ASP	5.1
1	A	415	THR	5.1
1	A	566	MET	5.1
1	A	259	ASP	5.1
1	A	164	TYR	5.1
1	A	463	GLN	5.0
1	A	545	ARG	5.0
1	A	189	ILE	5.0
1	A	285	ASP	5.0
1	A	406	ASN	5.0
1	A	224	ARG	5.0
1	A	206	TRP	5.0
1	A	31	HIS	4.9
1	A	138	CYS	4.9
1	A	110	ALA	4.9
1	A	304	SER	4.9
1	A	284	MET	4.9
1	A	179	PHE	4.9
1	A	369	SER	4.9
1	A	387	SER	4.9
1	A	477	LEU	4.9
1	A	121	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	370	ARG	4.9
1	A	66	THR	4.8
1	A	450	PHE	4.8
1	A	148	VAL	4.8
1	A	249	ILE	4.8
1	A	440	GLN	4.8
1	A	65	LEU	4.8
1	A	552	LYS	4.8
1	A	355	MET	4.7
1	A	543	ILE	4.7
1	A	193	LEU	4.7
1	A	102	ILE	4.7
1	A	254	SER	4.7
1	A	241	ASP	4.7
1	A	347	ARG	4.7
1	A	130	LEU	4.7
1	A	120	VAL	4.7
1	A	296	ALA	4.7
1	A	489	ASN	4.6
1	A	271	VAL	4.6
1	A	132	MET	4.6
1	A	171	ASP	4.6
1	A	279	PRO	4.6
1	A	6	GLY	4.6
1	A	582	ILE	4.6
1	A	383	THR	4.6
1	A	16	PRO	4.5
1	A	115	PHE	4.5
1	A	242	SER	4.5
1	A	327	ASP	4.5
1	A	291	MET	4.5
1	A	218	LYS	4.5
1	A	403	TYR	4.5
1	A	95	LEU	4.5
1	A	155	LEU	4.5
1	A	433	ASP	4.5
1	A	168	MET	4.5
1	A	573	THR	4.5
1	A	19	LEU	4.5
1	A	72	ILE	4.4
1	A	144	ASN	4.4
1	A	358	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	331	VAL	4.4
1	A	288	MET	4.4
1	A	308	VAL	4.4
1	A	502	ASP	4.4
1	A	236	ALA	4.4
1	A	365	GLY	4.4
1	A	14	VAL	4.4
1	A	478	VAL	4.4
1	A	103	ARG	4.4
1	A	63	VAL	4.3
1	A	283	THR	4.3
1	A	163	LEU	4.3
1	A	145	GLY	4.3
1	A	590	ILE	4.3
1	A	8	TRP	4.3
1	A	542	GLY	4.3
1	A	52	PHE	4.3
1	A	533	THR	4.2
1	A	526	PRO	4.2
1	A	295	GLU	4.2
1	A	99	VAL	4.2
1	A	194	LYS	4.2
1	A	277	HIS	4.2
1	A	345	MET	4.2
1	A	591	ASP	4.2
1	A	24	LEU	4.1
1	A	420	MET	4.1
1	A	432	ALA	4.1
1	A	549	ALA	4.1
1	A	28	TYR	4.1
1	A	316	ASP	4.1
1	A	320	ASP	4.1
1	A	583	ASP	4.1
1	A	536	GLY	4.1
1	A	196	SER	4.1
1	A	414	SER	4.1
1	A	253	LEU	4.1
1	A	119	LYS	4.1
1	A	569	ARG	4.1
1	A	238	VAL	4.1
1	A	255	ASP	4.1
1	A	570	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	165	MET	4.1
1	A	190	ASP	4.1
1	A	491	ARG	4.1
1	A	202	PRO	4.1
1	A	314	HIS	4.1
1	A	322	THR	4.1
1	A	101	ASP	4.0
1	A	114	ASP	4.0
1	A	139	HIS	4.0
1	A	442	MET	4.0
1	A	239	ALA	4.0
1	A	84	GLY	4.0
1	A	266	ASP	4.0
1	A	377	SER	4.0
1	A	487	VAL	4.0
1	A	461	GLU	4.0
1	A	98	ALA	4.0
1	A	276	GLU	4.0
1	A	176	LEU	3.9
1	A	328	LYS	3.9
1	A	40	LYS	3.9
1	A	527	LEU	3.9
1	A	46	PHE	3.9
1	A	195	SER	3.9
1	A	337	PRO	3.9
1	A	274	VAL	3.9
1	A	4	ILE	3.8
1	A	267	GLY	3.8
1	A	310	MET	3.8
1	A	408	THR	3.8
1	A	490	TYR	3.8
1	A	117	THR	3.8
1	A	324	GLU	3.8
1	A	5	LEU	3.8
1	A	74	TYR	3.8
1	A	524	ASP	3.8
1	A	353	VAL	3.8
1	A	153	PHE	3.8
1	A	199	ILE	3.8
1	A	519	ALA	3.8
1	A	428	LEU	3.8
1	A	312	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	188	GLN	3.7
1	A	563	VAL	3.7
1	A	12	GLY	3.7
1	A	42	ARG	3.7
1	A	319	ALA	3.7
1	A	18	ARG	3.7
1	A	530	LEU	3.7
1	A	546	ILE	3.7
1	A	113	LYS	3.7
1	A	553	THR	3.7
1	A	246	ARG	3.6
1	A	127	PRO	3.6
1	A	397	SER	3.6
1	A	159	LEU	3.6
1	A	393	GLY	3.6
1	A	589	VAL	3.6
1	A	395	GLY	3.6
1	A	367	THR	3.6
1	A	446	PHE	3.6
1	A	73	ARG	3.6
1	A	398	SER	3.6
1	A	561	SER	3.6
1	A	332	ASP	3.6
1	A	97	GLY	3.6
1	A	20	LEU	3.5
1	A	118	LEU	3.5
1	A	35	ARG	3.5
1	A	105	GLY	3.5
1	A	116	GLU	3.5
1	A	29	GLU	3.5
1	A	305	PRO	3.5
1	A	380	ALA	3.4
1	A	9	LYS	3.4
1	A	232	ASP	3.4
1	A	409	LEU	3.4
1	A	134	GLU	3.4
1	A	184	GLU	3.4
1	A	243	HIS	3.4
1	A	488	LYS	3.4
1	A	43	ASN	3.4
1	A	473	GLY	3.4
1	A	79	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	496	ARG	3.4
1	A	69	MET	3.4
1	A	349	LYS	3.4
1	A	263	GLN	3.3
1	A	362	VAL	3.3
1	A	317	GLU	3.3
1	A	475	GLU	3.3
1	A	410	VAL	3.3
1	A	467	ASP	3.3
1	A	540	ALA	3.3
1	A	162	VAL	3.3
1	A	321	VAL	3.3
1	A	81	MET	3.3
1	A	240	ASP	3.3
1	A	416	GLY	3.3
1	A	36	ASP	3.3
1	A	290	VAL	3.2
1	A	578	THR	3.2
1	A	418	PRO	3.2
1	A	211	GLY	3.2
1	A	458	SER	3.2
1	A	146	ASP	3.2
1	A	303	GLU	3.2
1	A	222	VAL	3.2
1	A	576	VAL	3.2
1	A	371	SER	3.2
1	A	366	ALA	3.1
1	A	375	SER	3.1
1	A	13	LEU	3.1
1	A	48	LEU	3.1
1	A	476	GLY	3.1
1	A	588	GLY	3.1
1	A	235	ARG	3.1
1	A	2	SER	3.1
1	A	422	GLU	3.1
1	A	126	LEU	3.1
1	A	378	GLY	3.1
1	A	492	ASN	3.1
1	A	192	TYR	3.1
1	A	91	GLU	3.1
1	A	309	LEU	3.1
1	A	245	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	169	CYS	3.0
1	A	131	LYS	3.0
1	A	17	THR	3.0
1	A	356	VAL	3.0
1	A	135	ASP	3.0
1	A	567	PRO	3.0
1	A	528	VAL	3.0
1	A	154	MET	3.0
1	A	434	LEU	2.9
1	A	493	GLY	2.9
1	A	78	LYS	2.9
1	A	436	VAL	2.9
1	A	41	TRP	2.9
1	A	350	ASP	2.9
1	A	586	ALA	2.9
1	A	142	TYR	2.9
1	A	544	ARG	2.9
1	A	382	THR	2.9
1	A	50	LEU	2.9
1	A	551	GLY	2.8
1	A	209	THR	2.8
1	A	373	THR	2.8
1	A	595	THR	2.8
1	A	354	GLU	2.8
1	A	157	ASP	2.8
1	A	381	PRO	2.8
1	A	85	CYS	2.8
1	A	152	ASP	2.8
1	A	587	ASP	2.7
1	A	306	THR	2.7
1	A	68	SER	2.7
1	A	33	TYR	2.7
1	A	94	MET	2.7
1	A	503	GLU	2.7
1	A	407	PRO	2.7
1	A	541	ASP	2.7
1	A	89	ARG	2.6
1	A	388	ALA	2.6
1	A	228	GLU	2.6
1	A	419	LYS	2.6
1	A	435	ARG	2.6
1	A	486	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	231	ALA	2.6
1	A	282	VAL	2.6
1	A	15	GLN	2.6
1	A	223	PRO	2.6
1	A	182	ARG	2.6
1	A	93	SER	2.6
1	A	479	ALA	2.6
1	A	529	GLY	2.6
1	A	547	LYS	2.6
1	A	423	GLN	2.6
1	A	217	PRO	2.6
1	A	107	SER	2.6
1	A	307	PRO	2.6
1	A	150	HIS	2.6
1	A	323	PHE	2.5
1	A	71	ILE	2.5
1	A	399	GLY	2.5
1	A	596	GLU	2.5
1	A	160	ASP	2.5
1	A	27	LYS	2.5
1	A	92	ILE	2.5
1	A	338	GLY	2.5
1	A	512	VAL	2.5
1	A	431	GLU	2.5
1	A	208	ALA	2.5
1	A	363	ASP	2.5
1	A	412	GLY	2.5
1	A	108	ARG	2.4
1	A	124	SER	2.4
1	A	444	GLU	2.4
1	A	357	SER	2.4
1	A	424	VAL	2.4
1	A	577	ASP	2.4
1	A	421	VAL	2.4
1	A	537	GLU	2.4
1	A	96	GLU	2.4
1	A	265	ARG	2.4
1	A	149	THR	2.4
1	A	469	ALA	2.4
1	A	396	GLY	2.4
1	A	464	GLU	2.4
1	A	264	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	401	THR	2.4
1	A	402	THR	2.4
1	A	564	TYR	2.4
1	A	470	ARG	2.3
1	A	468	GLY	2.3
1	A	417	GLY	2.3
1	A	34	GLU	2.3
1	A	457	ARG	2.3
1	A	287	GLU	2.3
1	A	539	GLY	2.3
1	A	51	GLU	2.2
1	A	180	LYS	2.2
1	A	385	GLY	2.2
1	A	278	ARG	2.2
1	A	386	GLY	2.2
1	A	352	LEU	2.2
1	A	125	LYS	2.2
1	A	376	ASP	2.2
1	A	437	LEU	2.2
1	A	495	LEU	2.2
1	A	520	ALA	2.2
1	A	122	PHE	2.2
1	A	517	GLN	2.1
1	A	147	HIS	2.1
1	A	129	MET	2.1
1	A	483	ARG	2.1
1	A	313	ALA	2.1
1	A	445	GLY	2.1
1	A	501	GLN	2.1
1	A	77	ASP	2.1
1	A	38	GLY	2.1
1	A	67	GLN	2.1
1	A	351	GLN	2.1
1	A	294	ILE	2.1
1	A	531	ILE	2.1
1	A	504	PRO	2.0
1	A	301	MET	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.