



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:24 PM GMT

PDB ID : 3GEB
Title : Crystal Structure of edeya2
Authors : Kim, S.J.
Deposited on : 2009-02-25
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

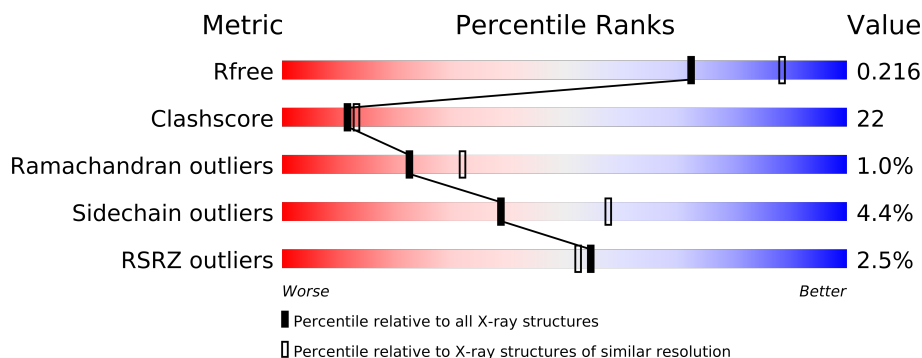
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	274	
1	B	274	
1	C	274	
1	D	274	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	701	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8355 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Eyes absent homolog 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2078	1322	355	389	12			
1	B	253	Total	C	N	O	S	0	0	0
			2049	1305	350	383	11			
1	C	258	Total	C	N	O	S	0	0	0
			2078	1322	355	389	12			
1	D	256	Total	C	N	O	S	0	0	0
			2064	1314	353	386	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	SER	-	EXPRESSION TAG	UNP O00167
A	266	HIS	-	EXPRESSION TAG	UNP O00167
A	267	MET	-	EXPRESSION TAG	UNP O00167
B	265	SER	-	EXPRESSION TAG	UNP O00167
B	266	HIS	-	EXPRESSION TAG	UNP O00167
B	267	MET	-	EXPRESSION TAG	UNP O00167
C	265	SER	-	EXPRESSION TAG	UNP O00167
C	266	HIS	-	EXPRESSION TAG	UNP O00167
C	267	MET	-	EXPRESSION TAG	UNP O00167
D	265	SER	-	EXPRESSION TAG	UNP O00167
D	266	HIS	-	EXPRESSION TAG	UNP O00167
D	267	MET	-	EXPRESSION TAG	UNP O00167

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

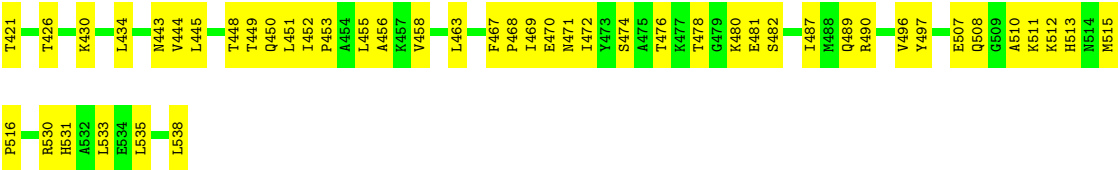
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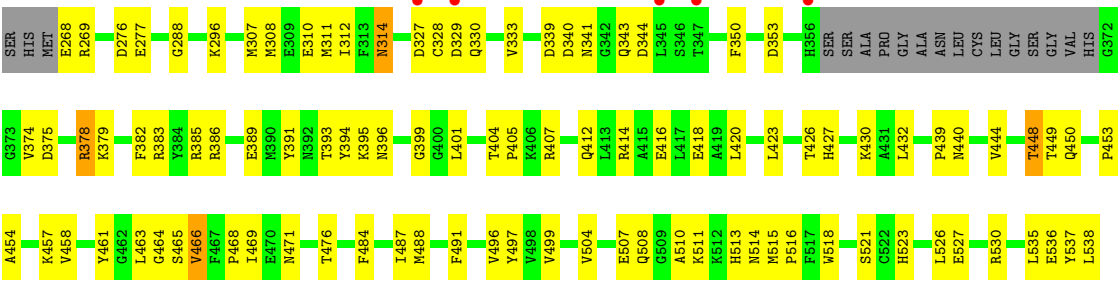
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total 28	O 28	0	0
3	B	12	Total 12	O 12	0	0
3	C	13	Total 13	O 13	0	0
3	D	29	Total 29	O 29	0	0



● Molecule 1: Eyes absent homolog 2



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	183.61Å 183.61Å 120.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 67.79 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-2.40) 99.2 (67.79-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 2.40Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.171 , 0.218 0.171 , 0.216	Depositor DCC
R_{free} test set	3694 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 26.9	EDS
Estimated twinning fraction	0.650 for h,k,l 0.350 for h,-k,-l 0.356 for -k,-h,-l	Xtriage
Reported twinning fraction	0.650 for h,k,l 0.350 for h,-k,-l	Depositor
L-test for twinning	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 77276 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8355	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.43	0/2121	0.63	0/2867
1	B	0.39	0/2092	0.59	0/2829
1	C	0.40	0/2121	0.59	0/2867
1	D	0.42	0/2107	0.61	0/2849
All	All	0.41	0/8441	0.61	0/11412

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2078	0	2041	71	0
1	B	2049	0	2012	119	0
1	C	2078	0	2041	100	0
1	D	2064	0	2027	79	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	0	0	0
3	B	12	0	0	0	0
3	C	13	0	0	0	0
3	D	29	0	0	2	0
All	All	8355	0	8121	360	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (360) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:402:ILE:HG23	1:A:406:LYS:HB2	1.53	0.87
1:B:509:GLY:HA2	1:B:512:LYS:HD2	1.57	0.87
1:D:427:HIS:HD2	1:D:523:HIS:HE1	1.20	0.85
1:B:516:PRO:HB3	1:C:538:LEU:HD23	1.57	0.85
1:D:427:HIS:HD2	1:D:523:HIS:CE1	1.95	0.84
1:B:332:HIS:CD2	1:B:333:VAL:H	1.97	0.82
1:B:502:ASP:HB3	1:B:520:ILE:O	1.80	0.82
1:C:478:THR:HB	1:C:482:SER:OG	1.80	0.81
1:B:336:VAL:O	1:B:338:SER:N	2.16	0.78
1:C:316:ALA:HA	1:C:320:LEU:HD12	1.64	0.78
1:D:312:ILE:HD13	1:D:457:LYS:HG2	1.66	0.77
1:D:427:HIS:CD2	1:D:523:HIS:HE1	2.04	0.76
1:B:310:GLU:O	1:B:314:ASN:HB2	1.86	0.74
1:C:507:GLU:O	1:C:511:LYS:HD3	1.88	0.73
1:A:341:ASN:HD21	1:A:343:GLN:NE2	1.87	0.73
1:C:373:GLY:HA2	1:C:376:TRP:HE3	1.53	0.72
1:B:481:GLU:O	1:B:485:GLU:HG2	1.90	0.72
1:D:269:ARG:HG2	1:D:496:VAL:HG22	1.70	0.72
1:A:404:THR:HG23	1:A:408:GLU:OE2	1.89	0.71
1:B:311:MET:HE1	1:B:413:LEU:HD23	1.72	0.71
1:B:350:PHE:HA	1:B:353:ASP:OD1	1.90	0.71
1:C:343:GLN:HG2	1:C:344:ASP:H	1.55	0.71
1:C:385:ARG:O	1:C:389:GLU:HG3	1.91	0.71
1:C:508:GLN:HE21	1:C:512:LYS:NZ	1.90	0.70
1:C:350:PHE:HD2	1:C:383:ARG:HH11	1.38	0.70
1:B:275:LEU:HD11	1:B:280:ILE:HD12	1.74	0.70
1:C:291:ALA:HA	1:C:296:LYS:HB2	1.72	0.70
1:D:385:ARG:O	1:D:389:GLU:HG3	1.92	0.69
1:B:311:MET:CE	1:B:413:LEU:HD23	2.22	0.68
1:A:386:ARG:O	1:A:390:MET:HG2	1.93	0.68
1:D:389:GLU:O	1:D:393:THR:HG23	1.94	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:491:PHE:HB2	1:B:497:TYR:OH	1.93	0.68
1:D:412:GLN:O	1:D:416:GLU:HG3	1.94	0.68
1:A:385:ARG:O	1:A:389:GLU:HG3	1.94	0.67
1:D:276:ASP:HB3	1:D:277:GLU:OE1	1.94	0.67
1:A:523:HIS:O	1:A:527:GLU:HG3	1.94	0.67
1:C:404:THR:HG23	1:C:405:PRO:HA	1.77	0.67
1:C:389:GLU:O	1:C:393:THR:HG23	1.94	0.66
1:C:383:ARG:O	1:C:387:VAL:HG23	1.96	0.66
1:C:343:GLN:HG2	1:C:344:ASP:N	2.11	0.66
1:B:516:PRO:HB3	1:C:538:LEU:CD2	2.25	0.66
1:B:508:GLN:HG3	1:B:512:LYS:HE3	1.78	0.65
1:D:327:ASP:OD1	1:D:328:CYS:N	2.28	0.65
1:C:409:THR:HA	1:C:412:GLN:HE21	1.61	0.65
1:C:350:PHE:HD2	1:C:383:ARG:NH1	1.95	0.65
1:B:452:ILE:HB	1:B:453:PRO:HD3	1.78	0.64
1:A:452:ILE:HB	1:A:453:PRO:HD3	1.79	0.64
1:A:402:ILE:HG23	1:A:406:LYS:CB	2.27	0.64
1:D:308:MET:CE	1:D:312:ILE:HD11	2.27	0.64
1:C:408:GLU:O	1:C:412:GLN:HG3	1.99	0.63
1:C:448:THR:HG22	1:C:480:LYS:HE3	1.81	0.63
1:B:510:ALA:HA	1:B:515:MET:CE	2.28	0.63
1:B:427:HIS:HD2	1:B:523:HIS:HE1	1.47	0.63
1:B:339:ASP:HB3	1:B:377:MET:HB3	1.79	0.63
1:A:269:ARG:NH2	1:D:537:TYR:O	2.32	0.63
1:B:339:ASP:O	1:B:378:ARG:HA	1.99	0.63
1:D:432:LEU:HB3	1:D:466:VAL:HG11	1.80	0.63
1:C:397:ASN:ND2	1:C:400:GLY:HA3	2.15	0.62
1:B:350:PHE:HB3	1:B:383:ARG:HH12	1.63	0.62
1:D:450:GLN:O	1:D:453:PRO:HD2	2.00	0.62
1:B:350:PHE:HD2	1:B:383:ARG:NH1	1.98	0.62
1:D:308:MET:HE3	1:D:312:ILE:HD11	1.82	0.62
1:B:510:ALA:HA	1:B:515:MET:HE2	1.82	0.62
1:A:308:MET:HE3	1:A:312:ILE:HG13	1.82	0.61
1:B:278:THR:HG23	1:B:520:ILE:HD12	1.82	0.61
1:B:427:HIS:CD2	1:B:523:HIS:HE1	2.18	0.61
1:C:267:MET:HB3	1:C:538:LEU:HD22	1.82	0.61
1:A:291:ALA:HA	1:A:296:LYS:HB2	1.82	0.61
1:C:481:GLU:HG3	1:C:513:HIS:HE1	1.65	0.61
1:C:268:GLU:O	1:C:496:VAL:HG22	2.00	0.61
1:C:508:GLN:HE21	1:C:512:LYS:HZ3	1.48	0.61
1:B:385:ARG:O	1:B:389:GLU:HG3	2.00	0.61
1:B:333:VAL:HG21	1:B:469:ILE:HG12	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:321:PHE:CE1	1:A:386:ARG:HG2	2.36	0.61
1:C:322:PHE:O	1:C:326:GLU:HB2	2.01	0.61
1:A:510:ALA:HA	1:A:515:MET:CE	2.31	0.61
1:B:402:ILE:N	1:B:402:ILE:HD12	2.16	0.61
1:B:496:VAL:HG11	1:C:267:MET:CE	2.31	0.60
1:B:291:ALA:HA	1:B:296:LYS:HB2	1.84	0.60
1:D:427:HIS:CD2	1:D:523:HIS:CE1	2.83	0.60
1:C:339:ASP:N	1:C:339:ASP:OD2	2.35	0.60
1:D:458:VAL:HG13	1:D:463:LEU:HB2	1.84	0.60
1:B:268:GLU:HA	1:B:440:ASN:O	2.02	0.59
1:A:510:ALA:HA	1:A:515:MET:HE2	1.83	0.59
1:D:513:HIS:HB2	1:D:515:MET:HE2	1.84	0.59
1:A:321:PHE:HE1	1:A:386:ARG:HG2	1.68	0.59
1:C:445:LEU:HD23	1:C:472:ILE:HG23	1.85	0.59
1:C:391:TYR:O	1:C:395:LYS:HB3	2.03	0.59
1:B:312:ILE:HD13	1:B:457:LYS:HG2	1.85	0.59
1:A:389:GLU:O	1:A:393:THR:HG23	2.03	0.59
1:B:399:GLY:HA3	1:B:407:ARG:HD2	1.85	0.59
1:B:402:ILE:HG22	1:B:406:LYS:HB2	1.85	0.58
1:D:343:GLN:HG2	1:D:344:ASP:N	2.18	0.58
1:C:508:GLN:NE2	1:C:512:LYS:NZ	2.51	0.58
1:D:468:PRO:HG2	1:D:471:ASN:HB2	1.86	0.58
1:C:373:GLY:HA2	1:C:376:TRP:CE3	2.37	0.58
1:B:527:GLU:OE1	1:B:530:ARG:NH2	2.36	0.58
1:D:399:GLY:HA3	1:D:407:ARG:HG3	1.85	0.58
1:C:481:GLU:HG3	1:C:513:HIS:CE1	2.39	0.57
1:C:508:GLN:NE2	1:C:512:LYS:HZ2	2.01	0.57
1:B:276:ASP:O	1:B:277:GLU:HB2	2.04	0.57
1:A:333:VAL:HG21	1:A:469:ILE:HG12	1.87	0.57
1:B:402:ILE:O	1:B:402:ILE:HG22	2.04	0.57
1:C:507:GLU:HG3	1:C:511:LYS:NZ	2.20	0.57
1:D:468:PRO:HG2	1:D:471:ASN:CG	2.25	0.57
1:D:374:VAL:HG12	1:D:378:ARG:HD3	1.86	0.57
1:D:444:VAL:HG11	1:D:487:ILE:HD13	1.86	0.57
1:A:444:VAL:HG11	1:A:487:ILE:HD13	1.86	0.57
1:B:481:GLU:OE2	1:B:513:HIS:HE1	1.88	0.57
1:A:458:VAL:HG13	1:A:463:LEU:HB2	1.85	0.56
1:B:450:GLN:O	1:B:453:PRO:HD2	2.05	0.56
1:C:394:TYR:CG	1:C:401:LEU:HB2	2.40	0.56
1:C:355:PHE:HD1	1:C:355:PHE:O	1.89	0.56
1:C:452:ILE:HB	1:C:453:PRO:HD3	1.88	0.56
1:B:340:ASP:OD1	1:B:341:ASN:N	2.38	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:497:TYR:O	1:A:516:PRO:HG2	2.06	0.56
1:C:320:LEU:HD22	1:C:387:VAL:HG13	1.88	0.56
1:A:311:MET:CE	1:A:413:LEU:HD23	2.36	0.56
1:B:508:GLN:O	1:B:512:LYS:HG3	2.07	0.55
1:A:375:ASP:HA	1:A:378:ARG:HG3	1.89	0.55
1:B:485:GLU:O	1:B:489:GLN:HG2	2.06	0.55
1:D:418:GLU:OE1	1:D:423:LEU:HA	2.07	0.55
1:C:451:LEU:O	1:C:455:LEU:HG	2.06	0.55
1:A:339:ASP:HA	1:A:378:ARG:HH21	1.72	0.54
1:A:266:HIS:HD2	1:D:514:ASN:HB3	1.72	0.54
1:B:483:CYS:O	1:B:487:ILE:HG13	2.07	0.54
1:B:480:LYS:HE2	1:B:506:GLU:HG3	1.88	0.54
1:D:379:LYS:O	1:D:383:ARG:HG2	2.07	0.54
1:D:310:GLU:O	1:D:314:ASN:HB2	2.08	0.54
1:C:333:VAL:HG13	1:C:334:ASP:N	2.23	0.54
1:D:269:ARG:HG2	1:D:496:VAL:CG2	2.36	0.54
1:A:496:VAL:HG23	1:A:496:VAL:O	2.07	0.54
1:D:391:TYR:O	1:D:395:LYS:HB3	2.08	0.54
1:C:513:HIS:HB2	1:C:515:MET:HE2	1.90	0.54
1:C:513:HIS:HB2	1:C:515:MET:CE	2.38	0.53
1:A:355:PHE:N	1:A:355:PHE:CD2	2.76	0.53
1:A:508:GLN:HE21	1:A:512:LYS:HE3	1.73	0.53
1:D:510:ALA:HA	1:D:515:MET:CE	2.39	0.53
1:C:443:ASN:HB3	1:C:467:PHE:CE2	2.44	0.53
1:A:285:LEU:HD11	1:A:417:LEU:HD11	1.90	0.53
1:A:432:LEU:HB3	1:A:466:VAL:HG21	1.91	0.53
1:C:474:SER:OG	1:C:476:THR:HG23	2.08	0.53
1:A:303:ARG:NH2	1:A:416:GLU:OE1	2.42	0.53
1:B:320:LEU:O	1:B:322:PHE:N	2.42	0.53
1:B:509:GLY:HA2	1:B:512:LYS:CD	2.34	0.52
1:D:513:HIS:HB2	1:D:515:MET:CE	2.39	0.52
1:D:527:GLU:HG2	1:D:530:ARG:HH12	1.74	0.52
1:D:535:LEU:O	1:D:536:GLU:HB2	2.09	0.52
1:A:538:LEU:CD2	1:D:516:PRO:HB3	2.40	0.52
1:B:426:THR:O	1:B:430:LYS:HG2	2.09	0.52
1:C:277:GLU:OE2	1:C:284:SER:HB2	2.10	0.52
1:C:399:GLY:HA3	1:C:407:ARG:HD2	1.91	0.52
1:C:348:TYR:HE2	1:C:350:PHE:HA	1.74	0.52
1:D:391:TYR:OH	1:D:464:GLY:HA2	2.10	0.52
1:C:434:LEU:HD23	1:C:533:LEU:HB2	1.92	0.51
1:B:402:ILE:HG22	1:B:406:LYS:CB	2.40	0.51
1:D:426:THR:O	1:D:430:LYS:HG2	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:375:ASP:O	1:D:379:LYS:HG3	2.10	0.51
1:B:396:ASN:OD1	1:B:465:SER:HB2	2.10	0.51
1:D:499:VAL:HG21	1:D:510:ALA:HB2	1.93	0.51
1:B:330:GLN:HB2	1:B:451:LEU:CD2	2.41	0.51
1:C:375:ASP:HA	1:C:378:ARG:CZ	2.40	0.51
1:B:444:VAL:HG11	1:B:487:ILE:HD13	1.92	0.51
1:A:285:LEU:HD11	1:A:417:LEU:CD1	2.40	0.51
1:D:507:GLU:O	1:D:511:LYS:HG3	2.10	0.51
1:A:315:LEU:HD22	1:A:456:ALA:CB	2.41	0.51
1:B:386:ARG:HG2	1:B:386:ARG:HH11	1.75	0.51
1:A:315:LEU:C	1:A:315:LEU:HD23	2.30	0.51
1:B:349:ASN:O	1:B:352:ALA:HB3	2.11	0.50
1:A:311:MET:HE2	1:A:413:LEU:HD23	1.93	0.50
1:B:427:HIS:HD2	1:B:523:HIS:CE1	2.27	0.50
1:D:399:GLY:CA	1:D:407:ARG:HG3	2.42	0.50
1:D:308:MET:CE	1:D:461:TYR:CE1	2.95	0.50
1:C:397:ASN:HD21	1:C:400:GLY:HA3	1.75	0.50
1:A:468:PRO:HG2	1:A:471:ASN:CG	2.30	0.50
1:B:466:VAL:HG23	1:B:467:PHE:CD1	2.47	0.50
1:B:404:THR:N	1:B:405:PRO:HD2	2.26	0.50
1:D:269:ARG:NH1	1:D:538:LEU:O	2.44	0.50
1:D:504:VAL:HB	1:D:508:GLN:HE21	1.76	0.50
1:B:454:ALA:O	1:B:458:VAL:HG23	2.12	0.50
1:B:332:HIS:NE2	1:B:470:GLU:HA	2.27	0.50
1:A:513:HIS:HB2	1:A:515:MET:CE	2.41	0.50
1:C:450:GLN:HA	1:C:476:THR:HG21	1.94	0.50
1:B:378:ARG:N	1:B:378:ARG:HD2	2.25	0.50
1:B:390:MET:O	1:B:394:TYR:HB2	2.12	0.50
1:A:293:ARG:HD2	1:A:294:TYR:CE1	2.46	0.50
1:C:375:ASP:HA	1:C:378:ARG:NH1	2.27	0.50
1:B:427:HIS:CD2	1:B:523:HIS:CE1	3.00	0.50
1:B:378:ARG:H	1:B:378:ARG:HD2	1.77	0.50
1:A:470:GLU:H	1:A:470:GLU:CD	2.15	0.50
1:A:405:PRO:O	1:A:409:THR:HG22	2.12	0.50
1:B:308:MET:CE	1:B:460:LEU:HD13	2.42	0.49
1:D:468:PRO:HG2	1:D:471:ASN:CB	2.42	0.49
1:B:446:VAL:HG12	1:B:480:LYS:HD2	1.93	0.49
1:B:342:GLY:O	1:B:343:GLN:HB2	2.12	0.49
1:B:320:LEU:O	1:B:321:PHE:C	2.50	0.49
1:C:378:ARG:HD3	1:C:378:ARG:H	1.78	0.49
1:D:396:ASN:OD1	1:D:465:SER:HB2	2.12	0.49
1:D:308:MET:CE	1:D:461:TYR:HE1	2.26	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:444:VAL:HG11	1:C:487:ILE:HD13	1.95	0.49
1:C:414:ARG:HB3	1:C:414:ARG:HH11	1.77	0.49
1:B:469:ILE:HG22	1:B:470:GLU:OE2	2.13	0.49
1:A:435:ILE:HG23	1:A:441:CYS:HB3	1.95	0.49
1:C:404:THR:CG2	1:C:405:PRO:HA	2.43	0.48
1:A:531:HIS:O	1:A:535:LEU:HG	2.12	0.48
1:D:339:ASP:O	1:D:378:ARG:HA	2.12	0.48
1:B:493:ARG:HG2	1:B:493:ARG:O	2.12	0.48
1:A:397:ASN:HD21	1:A:400:GLY:HA3	1.77	0.48
1:A:397:ASN:ND2	1:A:400:GLY:HA3	2.28	0.48
1:A:290:PHE:CE2	1:A:421:THR:HA	2.49	0.48
1:C:497:TYR:O	1:C:516:PRO:HG2	2.14	0.48
1:B:508:GLN:HG3	1:B:512:LYS:CE	2.43	0.48
1:A:334:ASP:OD1	1:A:388:LYS:NZ	2.47	0.48
1:D:308:MET:HE2	1:D:461:TYR:CE1	2.49	0.48
1:C:340:ASP:OD1	1:C:385:ARG:NE	2.44	0.48
1:B:401:LEU:HB3	1:B:402:ILE:HD12	1.96	0.48
1:D:343:GLN:HG2	1:D:344:ASP:H	1.78	0.48
1:A:339:ASP:OD2	1:A:377:MET:HE2	2.14	0.48
1:C:392:ASN:HA	1:C:395:LYS:HE3	1.95	0.48
1:B:332:HIS:CD2	1:B:333:VAL:N	2.76	0.48
1:A:296:LYS:HE3	1:A:420:LEU:O	2.15	0.47
1:A:520:ILE:HD13	1:A:526:LEU:CD2	2.44	0.47
1:B:328:CYS:O	1:B:330:GLN:HG2	2.13	0.47
1:D:404:THR:N	1:D:405:PRO:HD2	2.28	0.47
1:B:330:GLN:HB2	1:B:451:LEU:HD23	1.96	0.47
1:C:286:LEU:HD21	1:C:305:GLY:C	2.35	0.47
1:D:308:MET:HE3	1:D:312:ILE:CD1	2.43	0.47
1:B:275:LEU:CD1	1:B:280:ILE:HD12	2.43	0.47
1:C:402:ILE:HG23	1:C:406:LYS:HB2	1.97	0.47
1:B:383:ARG:HH11	1:B:383:ARG:HG2	1.80	0.47
1:C:391:TYR:CD2	1:C:469:ILE:HB	2.49	0.47
1:C:315:LEU:HG	1:C:402:ILE:HD11	1.97	0.47
1:B:456:ALA:O	1:B:460:LEU:HG	2.15	0.46
1:C:412:GLN:O	1:C:416:GLU:HG3	2.15	0.46
1:C:388:LYS:HA	1:C:469:ILE:HD13	1.97	0.46
1:B:389:GLU:O	1:B:393:THR:HG23	2.15	0.46
1:B:307:MET:O	1:B:311:MET:HG3	2.16	0.46
1:B:394:TYR:CD2	1:B:401:LEU:HB2	2.50	0.46
1:B:340:ASP:CG	1:B:341:ASN:H	2.18	0.46
1:B:475:ALA:HB1	1:B:479:GLY:C	2.36	0.46
1:A:481:GLU:HB2	1:A:513:HIS:HE1	1.79	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:296:LYS:HE2	1:D:420:LEU:O	2.16	0.46
1:D:510:ALA:HA	1:D:515:MET:HE2	1.98	0.46
1:B:482:SER:HA	1:B:485:GLU:HG3	1.98	0.46
1:B:311:MET:HE2	1:B:413:LEU:HD23	1.98	0.46
1:D:288:GLY:HA2	3:D:215:HOH:O	2.16	0.46
1:B:312:ILE:HD13	1:B:457:LYS:CD	2.46	0.45
1:A:325:LEU:HD22	1:A:384:TYR:CE1	2.52	0.45
1:D:454:ALA:O	1:D:458:VAL:HG23	2.16	0.45
1:D:458:VAL:HG13	1:D:463:LEU:CB	2.46	0.45
1:C:407:ARG:O	1:C:411:LEU:HG	2.16	0.45
1:C:414:ARG:HB3	1:C:414:ARG:NH1	2.32	0.45
1:A:290:PHE:CZ	1:A:421:THR:HA	2.51	0.45
1:B:507:GLU:O	1:B:511:LYS:HG3	2.17	0.45
1:D:333:VAL:HG11	1:D:469:ILE:HD11	1.98	0.45
1:D:327:ASP:CG	1:D:328:CYS:H	2.19	0.45
1:C:293:ARG:HD2	1:C:294:TYR:CE1	2.52	0.45
1:C:325:LEU:HD22	1:C:384:TYR:CE1	2.52	0.45
1:A:481:GLU:HB2	1:A:513:HIS:CE1	2.51	0.45
1:B:377:MET:HB2	1:B:378:ARG:HE	1.81	0.45
1:A:304:ILE:HG23	1:A:413:LEU:HD11	1.98	0.45
1:C:290:PHE:CE2	1:C:421:THR:HA	2.51	0.45
1:C:341:ASN:OD1	1:C:343:GLN:HB2	2.16	0.44
1:C:496:VAL:HG23	1:C:496:VAL:O	2.17	0.44
1:C:332:HIS:HB3	1:C:335:ASP:OD1	2.17	0.44
1:A:341:ASN:HD21	1:A:343:GLN:HE21	1.62	0.44
1:A:308:MET:HE2	1:A:312:ILE:HD11	1.98	0.44
1:A:485:GLU:O	1:A:489:GLN:HG2	2.16	0.44
1:A:332:HIS:HB3	1:A:335:ASP:OD1	2.18	0.44
1:C:355:PHE:O	1:C:355:PHE:CD1	2.68	0.44
1:C:458:VAL:HG13	1:C:463:LEU:HB2	2.00	0.44
1:B:493:ARG:HH11	1:B:493:ARG:HG2	1.82	0.44
1:D:439:PRO:HG2	3:D:106:HOH:O	2.17	0.44
1:D:350:PHE:HA	1:D:353:ASP:OD2	2.17	0.44
1:D:268:GLU:HA	1:D:440:ASN:O	2.17	0.44
1:A:417:LEU:O	1:A:421:THR:HG23	2.17	0.44
1:B:480:LYS:CE	1:B:506:GLU:HG3	2.46	0.43
1:C:468:PRO:HG2	1:C:471:ASN:HB2	2.00	0.43
1:C:285:LEU:HD11	1:C:417:LEU:HD13	1.99	0.43
1:A:520:ILE:HD13	1:A:526:LEU:HD23	2.00	0.43
1:B:290:PHE:CZ	1:B:421:THR:HA	2.54	0.43
1:A:303:ARG:O	1:A:307:MET:HG3	2.18	0.43
1:B:332:HIS:CG	1:B:333:VAL:H	2.36	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:449:THR:HG22	1:C:450:GLN:N	2.33	0.43
1:B:315:LEU:HD23	1:B:315:LEU:C	2.38	0.43
1:A:493:ARG:HB2	1:A:493:ARG:NH1	2.33	0.43
1:C:349:ASN:OD1	1:C:352:ALA:HB2	2.18	0.43
1:B:311:MET:HE3	1:B:410:TRP:HD1	1.83	0.43
1:C:407:ARG:NH1	1:C:408:GLU:OE1	2.51	0.43
1:A:468:PRO:HG2	1:A:471:ASN:HB2	2.00	0.43
1:D:340:ASP:OD1	1:D:382:PHE:CD2	2.72	0.43
1:A:500:ILE:HD13	1:A:529:LEU:HD21	1.99	0.43
1:B:268:GLU:O	1:B:495:ALA:HA	2.19	0.43
1:C:530:ARG:HH11	1:C:530:ARG:HG2	1.84	0.43
1:A:507:GLU:HB2	1:A:517:PHE:CE2	2.53	0.43
1:B:343:GLN:O	1:B:385:ARG:NH2	2.52	0.43
1:D:340:ASP:CG	1:D:341:ASN:H	2.21	0.43
1:C:315:LEU:HG	1:C:402:ILE:CD1	2.49	0.43
1:B:350:PHE:C	1:B:352:ALA:H	2.22	0.43
1:B:510:ALA:HA	1:B:515:MET:HE3	1.98	0.43
1:C:394:TYR:CD1	1:C:401:LEU:HD12	2.53	0.43
1:C:388:LYS:HA	1:C:469:ILE:CD1	2.50	0.42
1:B:330:GLN:HG3	1:B:384:TYR:CE1	2.54	0.42
1:D:312:ILE:CD1	1:D:457:LYS:HG2	2.44	0.42
1:B:303:ARG:NH2	1:B:416:GLU:OE1	2.39	0.42
1:B:391:TYR:CD2	1:B:469:ILE:HB	2.54	0.42
1:B:350:PHE:N	1:B:350:PHE:CD1	2.88	0.42
1:C:507:GLU:HG3	1:C:511:LYS:HZ3	1.85	0.42
1:B:312:ILE:HG12	1:B:460:LEU:HD12	2.01	0.42
1:D:504:VAL:HB	1:D:508:GLN:NE2	2.34	0.42
1:B:290:PHE:HZ	1:B:421:THR:HA	1.85	0.42
1:B:336:VAL:CG1	1:B:381:ALA:HB2	2.49	0.42
1:C:530:ARG:NH1	1:C:530:ARG:HG2	2.34	0.42
1:C:531:HIS:O	1:C:535:LEU:HG	2.20	0.42
1:D:414:ARG:HH11	1:D:414:ARG:HB3	1.85	0.42
1:B:388:LYS:O	1:B:392:ASN:ND2	2.53	0.42
1:C:453:PRO:O	1:C:456:ALA:HB3	2.20	0.42
1:D:449:THR:CG2	1:D:453:PRO:HB2	2.49	0.42
1:A:538:LEU:HD23	1:D:516:PRO:HB3	2.01	0.42
1:B:438:ARG:NH2	1:B:536:GLU:HA	2.35	0.42
1:A:508:GLN:NE2	1:A:512:LYS:HE3	2.35	0.41
1:B:332:HIS:CG	1:B:333:VAL:N	2.88	0.41
1:B:380:LEU:C	1:B:380:LEU:HD13	2.40	0.41
1:D:374:VAL:O	1:D:378:ARG:HD3	2.20	0.41
1:B:375:ASP:N	1:B:378:ARG:HD3	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:394:TYR:CG	1:D:401:LEU:HB2	2.55	0.41
1:C:349:ASN:O	1:C:352:ALA:HB3	2.19	0.41
1:B:520:ILE:HD11	1:B:529:LEU:HD22	2.02	0.41
1:B:336:VAL:HG11	1:B:380:LEU:HD12	2.02	0.41
1:C:293:ARG:HB2	1:D:423:LEU:HD11	2.03	0.41
1:A:331:ILE:N	1:A:331:ILE:HD12	2.36	0.41
1:D:518:TRP:CE2	1:D:538:LEU:HD22	2.54	0.41
1:C:343:GLN:H	1:C:385:ARG:NH2	2.19	0.41
1:B:312:ILE:HD13	1:B:457:LYS:HD3	2.02	0.41
1:D:374:VAL:O	1:D:378:ARG:CD	2.69	0.41
1:B:514:ASN:HB3	1:C:265:SER:O	2.21	0.41
1:B:388:LYS:HA	1:B:469:ILE:HD13	2.02	0.41
1:C:348:TYR:CD2	1:C:349:ASN:N	2.89	0.41
1:B:343:GLN:O	1:B:345:LEU:N	2.53	0.41
1:D:491:PHE:HB2	1:D:497:TYR:OH	2.20	0.41
1:B:334:ASP:OD2	1:B:388:LYS:HE3	2.21	0.41
1:B:312:ILE:HD13	1:B:457:LYS:CG	2.50	0.41
1:C:394:TYR:CD2	1:C:401:LEU:HB2	2.55	0.41
1:C:468:PRO:HG2	1:C:471:ASN:CG	2.41	0.41
1:B:536:GLU:C	1:B:538:LEU:N	2.74	0.41
1:C:426:THR:HG22	1:C:430:LYS:NZ	2.35	0.41
1:D:449:THR:HG22	1:D:453:PRO:HB2	2.03	0.40
1:B:341:ASN:O	1:B:342:GLY:C	2.59	0.40
1:C:339:ASP:OD1	1:C:377:MET:HB3	2.22	0.40
1:D:484:PHE:O	1:D:488:MET:HG3	2.21	0.40
1:C:510:ALA:HA	1:C:515:MET:CE	2.51	0.40
1:C:333:VAL:HG13	1:C:334:ASP:H	1.86	0.40
1:B:315:LEU:HD23	1:B:315:LEU:O	2.21	0.40
1:D:307:MET:O	1:D:311:MET:HG3	2.21	0.40
1:A:310:GLU:O	1:A:314:ASN:HB2	2.21	0.40
1:A:311:MET:HE1	1:A:413:LEU:HD23	2.03	0.40
1:C:285:LEU:HD11	1:C:417:LEU:CD1	2.51	0.40
1:B:535:LEU:HD23	1:B:535:LEU:N	2.36	0.40
1:D:448:THR:O	1:D:476:THR:HG22	2.22	0.40
1:A:485:GLU:HB2	1:A:513:HIS:NE2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	254/274 (93%)	240 (94%)	11 (4%)	3 (1%)	19	26
1	B	249/274 (91%)	224 (90%)	21 (8%)	4 (2%)	14	18
1	C	254/274 (93%)	230 (91%)	21 (8%)	3 (1%)	19	26
1	D	252/274 (92%)	235 (93%)	17 (7%)	0	100	100
All	All	1009/1096 (92%)	929 (92%)	70 (7%)	10 (1%)	22	32

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	321	PHE
1	B	337	SER
1	C	341	ASN
1	B	345	LEU
1	C	353	ASP
1	A	353	ASP
1	B	353	ASP
1	C	373	GLY
1	A	374	VAL
1	A	373	GLY

5.3.2 Protein sidechains ⓘ

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	226/237 (95%)	216 (96%)	10 (4%)	39	58
1	B	223/237 (94%)	213 (96%)	10 (4%)	38	57
1	C	226/237 (95%)	215 (95%)	11 (5%)	35	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	224/237 (94%)	215 (96%)	9 (4%)	42	63
All	All	899/948 (95%)	859 (96%)	40 (4%)	39	58

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	ASP
1	A	308	MET
1	A	326	GLU
1	A	355	PHE
1	A	378	ARG
1	A	380	LEU
1	A	386	ARG
1	A	402	ILE
1	A	409	THR
1	A	466	VAL
1	B	276	ASP
1	B	329	ASP
1	B	345	LEU
1	B	355	PHE
1	B	378	ARG
1	B	412	GLN
1	B	414	ARG
1	B	506	GLU
1	B	507	GLU
1	B	526	LEU
1	C	266	HIS
1	C	276	ASP
1	C	330	GLN
1	C	339	ASP
1	C	355	PHE
1	C	378	ARG
1	C	402	ILE
1	C	420	LEU
1	C	470	GLU
1	C	489	GLN
1	C	490	ARG
1	D	314	ASN
1	D	329	ASP
1	D	330	GLN
1	D	378	ARG
1	D	386	ARG

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Mol	Chain	Res	Type
1	D	448	THR
1	D	466	VAL
1	D	521	SER
1	D	526	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	HIS
1	A	343	GLN
1	A	349	ASN
1	A	397	ASN
1	A	412	GLN
1	A	433	ASN
1	A	440	ASN
1	A	508	GLN
1	B	330	GLN
1	B	332	HIS
1	B	343	GLN
1	B	427	HIS
1	B	514	ASN
1	B	523	HIS
1	C	266	HIS
1	C	330	GLN
1	C	397	ASN
1	C	412	GLN
1	C	436	ASN
1	C	508	GLN
1	D	319	HIS
1	D	330	GLN
1	D	427	HIS
1	D	450	GLN
1	D	489	GLN
1	D	508	GLN
1	D	514	ASN
1	D	523	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	258/274 (94%)	0.19	1 (0%) 90 90	18, 31, 55, 77	0
1	B	253/274 (92%)	0.52	12 (4%) 30 28	23, 47, 79, 80	0
1	C	258/274 (94%)	0.37	8 (3%) 47 44	21, 40, 77, 80	0
1	D	256/274 (93%)	0.24	5 (1%) 62 59	19, 36, 63, 76	0
All	All	1025/1096 (93%)	0.33	26 (2%) 54 52	18, 37, 74, 80	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	ASP	5.2
1	C	345	LEU	5.0
1	C	327	ASP	3.7
1	B	337	SER	3.7
1	B	379	LYS	3.4
1	A	355	PHE	3.3
1	B	338	SER	3.3
1	B	356	HIS	3.2
1	B	378	ARG	3.1
1	B	347	THR	3.1
1	D	329	ASP	3.0
1	B	345	LEU	2.8
1	B	355	PHE	2.7
1	C	344	ASP	2.7
1	C	376	TRP	2.7
1	C	343	GLN	2.6
1	C	347	THR	2.6
1	B	376	TRP	2.6
1	B	339	ASP	2.6
1	D	356	HIS	2.5
1	D	327	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	345	LEU	2.4
1	B	380	LEU	2.3
1	C	337	SER	2.2
1	D	347	THR	2.2
1	C	378	ARG	2.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	A	701	1/1	0.21	3.17	44,44,44,44	0
2	MG	C	703	1/1	0.19	1.86	29,29,29,29	0
2	MG	D	704	1/1	0.15	-0.38	46,46,46,46	0
2	MG	B	702	1/1	0.09	-2.89	49,49,49,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.