



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:27 AM UTC

PDB ID : 6BAT / pdb_00006bat
Title : Crystal Structure of Wild-Type GltPh in complex with L-aspartate
Authors : Font, J.; Scopelliti, A.J.; Vandenberg, R.J.; Boudker, O.; Ryan, R.M.
Deposited on : 2017-10-15
Resolution : 3.40 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

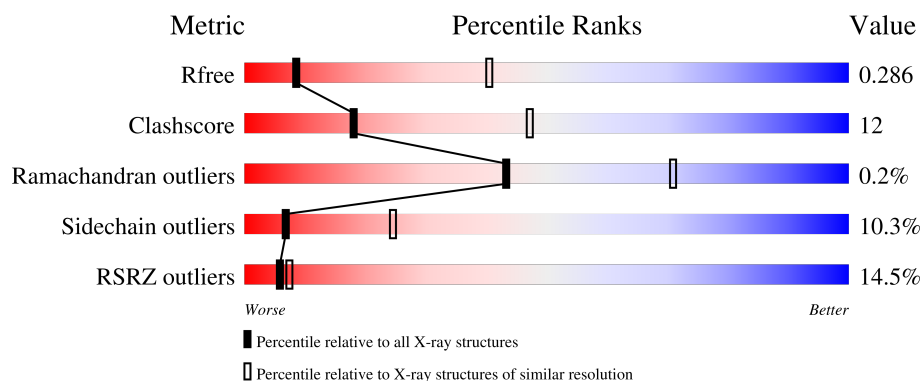
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 $\leq 5\%$. 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	420	11% 69% 25% • •
1	B	420	12% 65% 30% • •
1	C	420	19% 66% 28% • •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ASP	A	503	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9051 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 Glutamate transporter homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3006	1979	477	533	17			
1	B	408	Total	C	N	O	S	0	0	0
			3006	1979	477	533	17			
1	C	408	Total	C	N	O	S	0	0	0
			3006	1979	477	533	17			

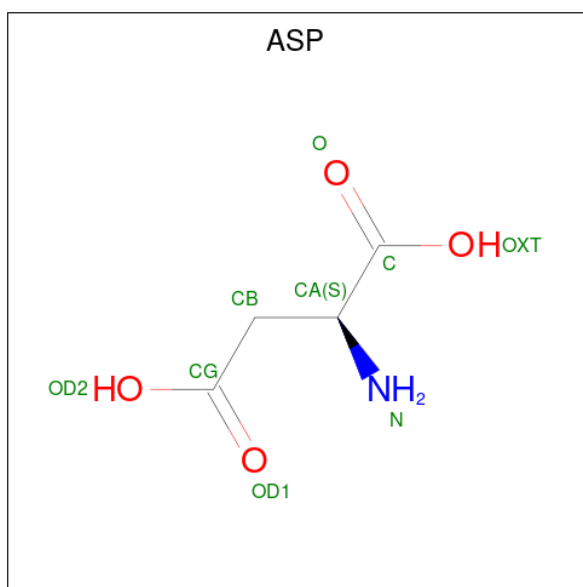
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	418	THR	-	expression tag	UNP O59010
A	419	LEU	-	expression tag	UNP O59010
A	420	VAL	-	expression tag	UNP O59010
B	418	THR	-	expression tag	UNP O59010
B	419	LEU	-	expression tag	UNP O59010
B	420	VAL	-	expression tag	UNP O59010
C	418	THR	-	expression tag	UNP O59010
C	419	LEU	-	expression tag	UNP O59010
C	420	VAL	-	expression tag	UNP O59010

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Na	0	0
			2	2		
2	B	2	Total	Na	0	0
			2	2		
2	C	2	Total	Na	0	0
			2	2		

- Molecule 3 is ASPARTIC ACID (CCD ID: ASP) (formula: C₄H₇NO₄).

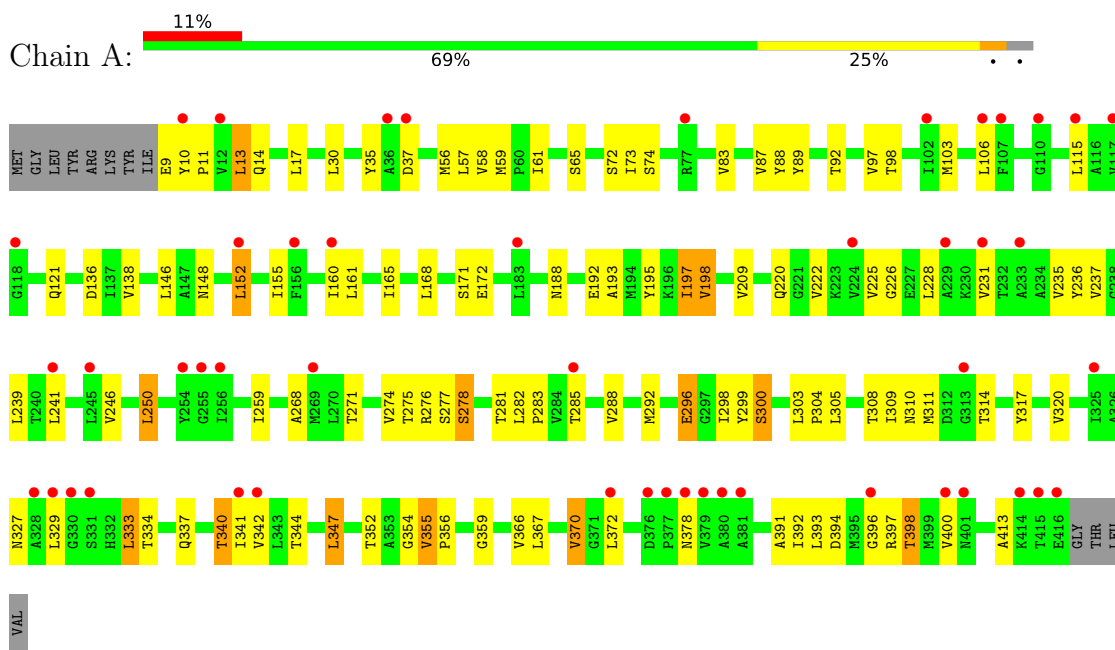


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	4	1	4		
3	B	1	Total	C	N	O	0	0
			9	4	1	4		
3	C	1	Total	C	N	O	0	0
			9	4	1	4		

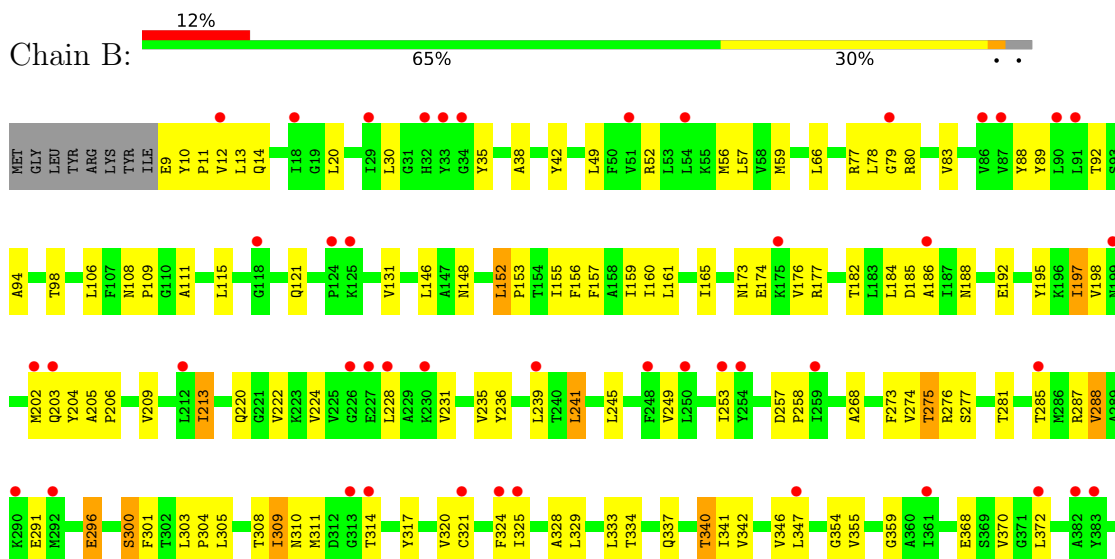
3 Residue-property plots [i](#)

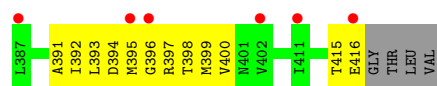
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glutamate transporter homolog

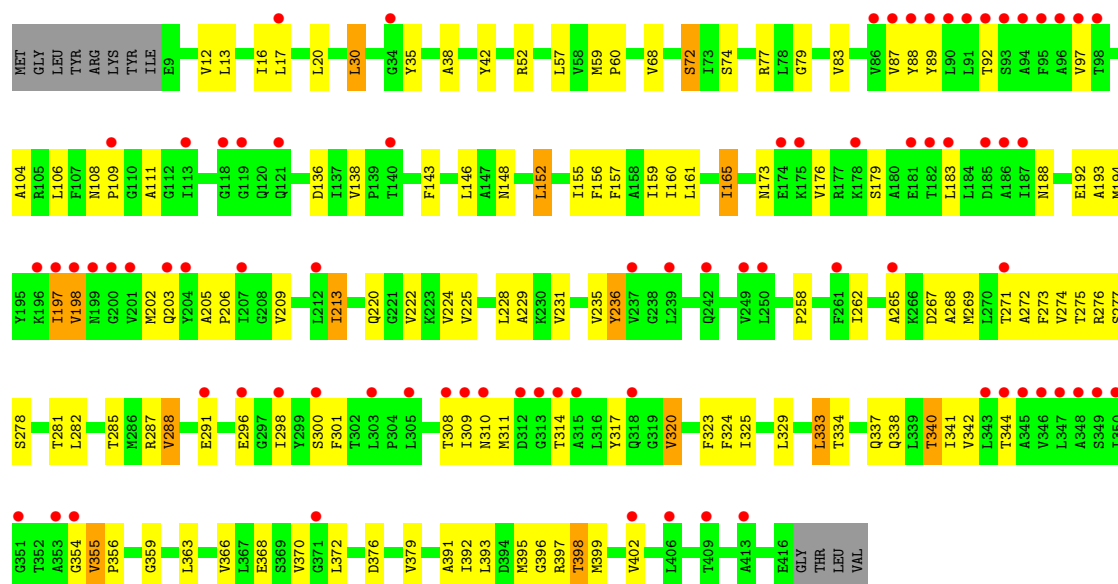


- Molecule 1: Glutamate transporter homolog





● Molecule 1: Glutamate transporter homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	114.73Å 114.73Å 322.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.40 40.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.1 (40.00-3.40) 97.0 (40.00-3.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.247 , 0.286 0.249 , 0.286	Depositor DCC
R_{free} test set	1566 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	120.4	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.077 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9051	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.53	0/3058	0.93	0/4168
1	B	0.56	0/3058	0.93	0/4168
1	C	0.58	0/3058	0.97	2/4168 (0.0%)
All	All	0.56	0/9174	0.94	2/12504 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	376	ASP	CA-C-N	7.87	129.67	119.84
1	C	376	ASP	C-N-CA	7.87	129.67	119.84

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	3006	0	3198	74	0
1	B	3006	0	3198	80	0
1	C	3006	0	3198	89	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	9	0	3	5	0
3	B	9	0	3	2	0
3	C	9	0	3	2	0
All	All	9051	0	9603	227	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 12.

All (227) 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:268:ALA:HB1	1:A:285:THR:HG22	1.43	1.00
1:B:296:GLU:O	1:B:300:SER:HB2	1.77	0.85
1:C:275:THR:HG23	1:C:277:SER:H	1.43	0.84
1:A:296:GLU:O	1:A:300:SER:HB2	1.79	0.83
1:A:275:THR:HG23	1:A:277:SER:H	1.44	0.82
1:C:57:LEU:HD13	1:C:198:VAL:HG12	1.62	0.81
1:A:235:VAL:HG22	1:A:320:VAL:HG11	1.65	0.79
1:C:398:THR:HG1	3:C:503:ASP:N	1.81	0.79
1:A:56:MET:HE3	1:B:157:PHE:HD1	1.48	0.77
1:A:344:THR:HB	1:A:366:VAL:HG23	1.68	0.75
1:A:209:VAL:HA	1:A:274:VAL:HG11	1.69	0.74
1:A:299:TYR:HB2	1:A:303:LEU:HD12	1.71	0.73
1:C:194:MET:O	1:C:198:VAL:HG13	1.88	0.73
1:A:155:ILE:HD11	1:A:304:PRO:HB2	1.71	0.72
1:A:161:LEU:O	1:A:165:ILE:HG12	1.90	0.72
1:C:235:VAL:HG22	1:C:320:VAL:HG11	1.71	0.71
1:B:161:LEU:O	1:B:165:ILE:HG12	1.89	0.71
1:C:12:VAL:HG12	1:C:203:GLN:HE22	1.55	0.71
1:B:268:ALA:HB1	1:B:285:THR:HG22	1.73	0.70
1:B:305:LEU:HD21	1:B:309:ILE:HD12	1.75	0.69
1:A:160:ILE:HG22	1:C:197:ILE:HD12	1.73	0.69
1:A:393:LEU:O	1:A:397:ARG:HG3	1.97	0.65
1:C:209:VAL:HA	1:C:274:VAL:HG11	1.80	0.64
1:B:20:LEU:HA	1:B:213:ILE:CD1	2.28	0.64
1:A:209:VAL:HG13	1:A:274:VAL:HG21	1.79	0.64
1:C:89:TYR:CG	1:C:310:ASN:HB2	2.33	0.64
1:A:160:ILE:CG2	1:C:197:ILE:HD12	2.29	0.63
1:B:59:MET:HE2	1:B:146:LEU:HA	1.80	0.62
1:A:225:VAL:HG12	1:A:226:GLY:H	1.65	0.62
1:B:52:ARG:NH2	1:C:136:ASP:HA	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ASN:O	1:B:192:GLU:HG2	2.00	0.62
1:C:193:ALA:O	1:C:197:ILE:HG12	1.99	0.61
1:C:268:ALA:HB1	1:C:285:THR:HG22	1.81	0.61
1:B:276:ARG:HD2	1:B:394:ASP:HB3	1.81	0.61
1:A:276:ARG:O	3:A:503:ASP:N	2.33	0.61
1:A:311:MET:HE2	3:A:503:ASP:O	2.00	0.61
1:C:57:LEU:CD1	1:C:198:VAL:HG12	2.31	0.60
1:B:287:ARG:O	1:B:291:GLU:HG2	2.02	0.59
1:A:220:GLN:HE22	1:A:391:ALA:N	2.01	0.59
1:A:397:ARG:NE	3:A:503:ASP:OD1	2.35	0.59
1:B:20:LEU:HA	1:B:213:ILE:HD11	1.85	0.59
1:A:231:VAL:O	1:A:235:VAL:HG23	2.03	0.58
1:B:155:ILE:HD11	1:B:304:PRO:HB2	1.86	0.58
1:B:275:THR:HG23	1:B:277:SER:H	1.68	0.58
1:B:115:LEU:HD11	1:B:328:ALA:HB1	1.85	0.58
1:A:281:THR:HG22	1:A:285:THR:HG23	1.85	0.58
1:C:311:MET:HE1	1:C:354:GLY:HA2	1.86	0.58
1:B:235:VAL:HG22	1:B:320:VAL:HG11	1.85	0.58
1:A:168:LEU:HD21	1:C:192:GLU:HB2	1.86	0.57
1:B:12:VAL:HG12	1:B:203:GLN:HE22	1.69	0.57
1:B:197:ILE:HD12	1:C:160:ILE:HG22	1.86	0.57
1:C:273:PHE:HB2	1:C:399:MET:HG3	1.86	0.57
1:B:173:ASN:HD22	1:B:176:VAL:HG23	1.70	0.57
1:A:314:THR:HA	1:A:397:ARG:HD2	1.87	0.57
1:A:333:LEU:HD22	1:A:341:ILE:HD11	1.85	0.56
1:C:276:ARG:HD3	1:C:395:MET:HG2	1.87	0.56
1:A:305:LEU:HD21	1:A:309:ILE:HD12	1.87	0.56
1:C:225:VAL:HA	1:C:229:ALA:HB2	1.87	0.55
1:A:220:GLN:HE22	1:A:391:ALA:H	1.53	0.55
1:B:359:GLY:N	3:B:503:ASP:OD2	2.39	0.55
1:B:209:VAL:HA	1:B:274:VAL:HG11	1.88	0.55
1:A:152:LEU:HD12	1:A:155:ILE:HD12	1.87	0.55
1:A:188:ASN:O	1:A:192:GLU:HG2	2.07	0.55
1:B:174:GLU:OE2	1:B:177:ARG:NH2	2.41	0.54
1:B:220:GLN:HE22	1:B:391:ALA:H	1.54	0.54
1:A:136:ASP:HA	1:C:52:ARG:NH2	2.21	0.54
1:C:275:THR:HG23	1:C:277:SER:N	2.17	0.54
1:B:393:LEU:O	1:B:397:ARG:HG3	2.07	0.54
1:C:173:ASN:HB3	1:C:176:VAL:HB	1.89	0.54
1:A:11:PRO:HG2	1:A:14:GLN:HG3	1.90	0.54
1:B:276:ARG:HD3	1:B:395:MET:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:MET:HB3	1:B:314:THR:HB	1.89	0.54
1:B:66:LEU:HD13	1:B:300:SER:HB3	1.91	0.53
1:C:88:TYR:CZ	1:C:92:THR:HG21	2.44	0.53
1:C:359:GLY:N	3:C:503:ASP:OD2	2.40	0.53
1:A:97:VAL:HG11	1:A:342:VAL:HA	1.90	0.53
1:B:288:VAL:HA	1:B:291:GLU:HG3	1.91	0.53
1:A:268:ALA:CB	1:A:285:THR:HG22	2.30	0.52
1:B:88:TYR:CZ	1:B:92:THR:HG21	2.45	0.52
1:C:314:THR:HA	1:C:397:ARG:HD2	1.90	0.52
1:A:235:VAL:HG22	1:A:320:VAL:CG1	2.38	0.52
1:C:60:PRO:HB2	1:C:194:MET:HG3	1.91	0.52
1:C:104:ALA:HB1	1:C:323:PHE:CB	2.40	0.52
1:C:108:ASN:HB3	1:C:111:ALA:HB2	1.91	0.52
1:A:88:TYR:CZ	1:A:92:THR:HG21	2.45	0.52
1:A:89:TYR:CG	1:A:310:ASN:HB2	2.45	0.51
1:C:59:MET:HE2	1:C:146:LEU:HA	1.91	0.51
1:A:239:LEU:HB3	1:A:400:VAL:HG21	1.91	0.51
1:C:220:GLN:HE22	1:C:391:ALA:H	1.58	0.51
1:A:59:MET:HE2	1:A:146:LEU:HA	1.92	0.51
1:C:38:ALA:O	1:C:42:TYR:HB2	2.11	0.51
1:C:296:GLU:O	1:C:300:SER:HB2	2.10	0.51
1:B:77:ARG:HD3	1:B:80:ARG:HH12	1.76	0.51
1:C:258:PRO:O	1:C:262:ILE:HG12	2.11	0.50
1:C:344:THR:HB	1:C:366:VAL:HG23	1.94	0.50
1:B:38:ALA:O	1:B:42:TYR:HB2	2.12	0.50
1:A:197:ILE:CD1	1:B:160:ILE:HG22	2.42	0.49
1:B:276:ARG:O	3:B:503:ASP:N	2.45	0.49
1:C:296:GLU:O	1:C:300:SER:CB	2.59	0.49
1:C:333:LEU:HD22	1:C:341:ILE:HD11	1.93	0.49
1:A:236:TYR:HE1	1:A:396:GLY:HA3	1.77	0.49
1:A:103:MET:HE1	1:A:237:VAL:HG12	1.94	0.49
1:C:20:LEU:HA	1:C:213:ILE:HD11	1.95	0.49
1:C:20:LEU:HA	1:C:213:ILE:CD1	2.43	0.49
1:C:276:ARG:CD	1:C:395:MET:HG2	2.43	0.49
1:C:109:PRO:HB2	1:C:324:PHE:HD1	1.77	0.49
1:A:30:LEU:O	1:A:35:TYR:HB2	2.13	0.48
1:B:311:MET:HE1	1:B:354:GLY:HA2	1.94	0.48
1:A:276:ARG:HD2	1:A:394:ASP:HB3	1.96	0.48
1:B:236:TYR:HE1	1:B:396:GLY:HA3	1.79	0.48
1:C:188:ASN:O	1:C:192:GLU:HG2	2.13	0.48
1:A:282:LEU:HD21	1:A:304:PRO:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:TYR:CG	1:A:397:ARG:HD3	2.49	0.48
1:A:271:THR:O	1:A:275:THR:HG22	2.14	0.48
1:C:269:MET:O	1:C:399:MET:HG3	2.13	0.48
1:B:273:PHE:HB2	1:B:399:MET:HG3	1.95	0.48
1:C:338:GLN:HA	1:C:341:ILE:HD12	1.96	0.48
1:C:59:MET:HB2	1:C:60:PRO:HD3	1.96	0.47
1:C:317:TYR:CG	1:C:397:ARG:HD3	2.49	0.47
1:A:305:LEU:CD2	1:A:309:ILE:HD12	2.44	0.47
1:B:109:PRO:HB2	1:B:324:PHE:HD1	1.80	0.47
1:C:271:THR:HB	1:C:281:THR:HG23	1.96	0.47
1:C:97:VAL:HG11	1:C:342:VAL:HA	1.97	0.47
1:C:89:TYR:CD1	1:C:310:ASN:HB2	2.49	0.47
1:C:198:VAL:O	1:C:202:MET:HG2	2.14	0.47
1:B:56:MET:HE3	1:C:157:PHE:HD1	1.80	0.47
1:B:275:THR:HG23	1:B:277:SER:N	2.30	0.47
1:C:159:ILE:HD11	1:C:301:PHE:CD2	2.50	0.46
1:C:209:VAL:HG13	1:C:274:VAL:HG21	1.97	0.46
1:A:57:LEU:HD13	1:A:198:VAL:HG12	1.96	0.46
1:C:202:MET:HE2	1:C:267:ASP:HB3	1.97	0.46
1:C:272:ALA:HB2	1:C:281:THR:HG21	1.97	0.46
1:A:56:MET:HE3	1:B:157:PHE:CD1	2.39	0.46
1:B:89:TYR:CG	1:B:310:ASN:HB2	2.51	0.46
1:A:398:THR:HG23	3:A:503:ASP:C	2.41	0.46
1:B:415:THR:O	1:B:416:GLU:HB2	2.16	0.46
1:B:89:TYR:CD1	1:B:310:ASN:HB2	2.51	0.45
1:A:61:ILE:O	1:A:65:SER:HB2	2.15	0.45
1:B:146:LEU:HB3	1:C:143:PHE:CD2	2.52	0.45
1:A:311:MET:HE1	1:A:354:GLY:HA2	1.99	0.45
1:B:249:VAL:O	1:B:253:ILE:HG13	2.16	0.45
1:C:156:PHE:O	1:C:160:ILE:HG12	2.15	0.45
1:A:347:LEU:HD13	1:A:347:LEU:HA	1.85	0.45
1:C:213:ILE:H	1:C:213:ILE:HG13	1.54	0.45
1:A:311:MET:HB3	1:A:314:THR:HB	1.99	0.45
1:C:68:VAL:O	1:C:72:SER:HB3	2.16	0.45
1:C:355:VAL:HG13	1:C:356:PRO:HD2	1.97	0.45
1:B:198:VAL:O	1:B:202:MET:HG2	2.16	0.45
1:B:241:LEU:O	1:B:245:LEU:HB3	2.17	0.44
1:C:236:TYR:HE1	1:C:396:GLY:HA3	1.82	0.44
1:C:317:TYR:HE1	1:C:393:LEU:HD13	1.82	0.44
1:C:363:LEU:O	1:C:366:VAL:HG12	2.17	0.44
1:C:281:THR:HG22	1:C:285:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LEU:HD13	1:B:198:VAL:HG12	1.98	0.44
1:B:239:LEU:HB3	1:B:400:VAL:HG21	2.00	0.44
1:A:355:VAL:HG13	1:A:356:PRO:HD2	1.99	0.44
1:B:342:VAL:O	1:B:346:VAL:HG23	2.18	0.44
1:A:58:VAL:HG22	1:A:283:PRO:HD3	1.99	0.44
1:A:337:GLN:O	1:A:340:THR:HG22	2.17	0.44
1:C:272:ALA:HA	1:C:275:THR:HG22	1.99	0.44
1:B:228:LEU:HA	1:B:231:VAL:HG12	2.00	0.44
1:B:152:LEU:HD12	1:B:155:ILE:HD12	1.99	0.44
1:C:74:SER:HB2	1:C:77:ARG:HB2	1.99	0.44
1:A:11:PRO:CG	1:A:14:GLN:HG3	2.48	0.44
1:B:30:LEU:O	1:B:35:TYR:HB2	2.18	0.44
1:B:281:THR:HG22	1:B:285:THR:HG23	2.00	0.44
1:B:209:VAL:HG13	1:B:274:VAL:HG21	2.00	0.44
1:A:197:ILE:HD13	1:B:160:ILE:HG22	2.00	0.43
1:B:185:ASP:O	1:C:179:SER:HB2	2.18	0.43
1:B:165:ILE:HG21	1:B:184:LEU:HB2	2.00	0.43
1:C:16:ILE:HG23	1:C:209:VAL:HG21	2.00	0.43
1:C:228:LEU:HA	1:C:231:VAL:HG12	1.99	0.43
1:B:321:CYS:O	1:B:325:ILE:HG12	2.18	0.43
1:A:193:ALA:O	1:A:197:ILE:HG12	2.18	0.43
1:A:278:SER:HB2	3:A:503:ASP:OXT	2.18	0.43
1:B:257:ASP:HA	1:B:258:PRO:HD3	1.87	0.43
1:C:198:VAL:HG23	1:C:287:ARG:HD3	2.00	0.43
1:B:11:PRO:HG2	1:B:14:GLN:HG3	2.01	0.43
1:B:213:ILE:H	1:B:213:ILE:HG13	1.52	0.43
1:C:152:LEU:HD12	1:C:155:ILE:HD12	2.00	0.43
1:C:30:LEU:O	1:C:35:TYR:HB2	2.19	0.43
1:A:138:VAL:O	1:C:52:ARG:NH2	2.37	0.43
1:B:108:ASN:HB3	1:B:111:ALA:HB2	2.00	0.43
1:B:49:LEU:HD23	1:B:204:TYR:CZ	2.54	0.43
1:A:83:VAL:O	1:A:87:VAL:HG23	2.19	0.43
1:C:265:ALA:HA	1:C:288:VAL:HG11	2.01	0.43
1:A:299:TYR:CD1	1:A:299:TYR:C	2.96	0.42
1:A:352:THR:HG21	1:A:359:GLY:HA2	2.00	0.42
1:B:108:ASN:HA	1:B:109:PRO:HD3	1.84	0.42
1:B:152:LEU:HB2	1:B:153:PRO:HD3	2.01	0.42
1:B:276:ARG:HG2	1:B:395:MET:HA	2.01	0.42
1:B:303:LEU:HB2	1:B:304:PRO:HD3	2.01	0.42
1:C:79:GLY:O	1:C:83:VAL:HG23	2.20	0.42
1:A:298:ILE:HD13	1:A:413:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ARG:NH2	1:C:138:VAL:O	2.52	0.42
1:C:205:ALA:N	1:C:206:PRO:HD2	2.34	0.42
1:B:235:VAL:HG21	1:B:393:LEU:HD22	2.02	0.42
1:C:337:GLN:O	1:C:340:THR:HG22	2.20	0.42
1:B:159:ILE:HD11	1:B:301:PHE:CD2	2.55	0.42
1:B:156:PHE:O	1:B:160:ILE:HG12	2.19	0.42
1:B:195:TYR:O	1:B:198:VAL:HG22	2.20	0.42
1:B:333:LEU:HD22	1:B:341:ILE:HD11	2.02	0.42
1:A:367:LEU:O	1:A:370:VAL:HG23	2.19	0.41
1:B:79:GLY:O	1:B:83:VAL:HG23	2.20	0.41
1:A:228:LEU:O	1:A:231:VAL:HG12	2.20	0.41
1:A:88:TYR:CD1	1:A:88:TYR:C	2.98	0.41
1:C:276:ARG:HG2	1:C:395:MET:HA	2.02	0.41
1:A:13:LEU:O	1:A:17:LEU:HD23	2.21	0.41
1:B:94:ALA:HA	1:B:346:VAL:HG21	2.02	0.41
1:B:205:ALA:N	1:B:206:PRO:HD2	2.36	0.41
1:C:391:ALA:O	1:C:395:MET:HG3	2.20	0.41
1:A:246:VAL:O	1:A:250:LEU:HB2	2.20	0.41
1:C:159:ILE:HD11	1:C:301:PHE:HD2	1.86	0.41
1:B:186:ALA:O	1:C:183:LEU:HD13	2.20	0.41
1:A:236:TYR:HD1	1:A:239:LEU:HD12	1.86	0.41
1:B:317:TYR:HE1	1:B:393:LEU:HD13	1.86	0.41
1:C:325:ILE:HG21	1:C:379:VAL:HG13	2.03	0.41
1:A:394:ASP:OD1	1:A:397:ARG:NH2	2.53	0.41
1:C:83:VAL:O	1:C:87:VAL:HG23	2.21	0.41
1:C:104:ALA:HB1	1:C:323:PHE:HB3	2.02	0.41
1:C:277:SER:HB2	1:C:356:PRO:HD3	2.01	0.41
1:A:327:ASN:HD22	1:A:327:ASN:HA	1.65	0.40
1:B:337:GLN:O	1:B:340:THR:HG22	2.21	0.40
1:C:282:LEU:HD12	1:C:282:LEU:HA	1.95	0.40
1:C:287:ARG:O	1:C:291:GLU:HG2	2.21	0.40
1:A:61:ILE:HD11	1:A:195:TYR:CE1	2.56	0.40
1:C:161:LEU:O	1:C:165:ILE:HG12	2.20	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	406/420 (97%)	385 (95%)	20 (5%)	1 (0%)	43	71
1	B	406/420 (97%)	386 (95%)	19 (5%)	1 (0%)	43	71
1	C	406/420 (97%)	385 (95%)	20 (5%)	1 (0%)	43	71
All	All	1218/1260 (97%)	1156 (95%)	59 (5%)	3 (0%)	43	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	10	TYR
1	C	224	VAL
1	A	10	TYR

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	316/328 (96%)	279 (88%)	37 (12%)	5	20
1	B	316/328 (96%)	285 (90%)	31 (10%)	7	27
1	C	316/328 (96%)	286 (90%)	30 (10%)	8	29
All	All	948/984 (96%)	850 (90%)	98 (10%)	7	24

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	13	LEU
1	A	37	ASP
1	A	72	SER
1	A	73	ILE
1	A	74	SER
1	A	98	THR
1	A	106	LEU
1	A	115	LEU
1	A	121	GLN
1	A	148	ASN
1	A	152	LEU
1	A	171	SER
1	A	172	GLU
1	A	197	ILE
1	A	198	VAL
1	A	222	VAL
1	A	241	LEU
1	A	250	LEU
1	A	259	ILE
1	A	278	SER
1	A	288	VAL
1	A	292	MET
1	A	296	GLU
1	A	300	SER
1	A	308	THR
1	A	329	LEU
1	A	333	LEU
1	A	334	THR
1	A	340	THR
1	A	347	LEU
1	A	355	VAL
1	A	370	VAL
1	A	372	LEU
1	A	378	ASN
1	A	392	ILE
1	A	398	THR
1	B	9	GLU
1	B	13	LEU
1	B	78	LEU
1	B	98	THR
1	B	106	LEU
1	B	121	GLN

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Mol	Chain	Res	Type
1	B	131	VAL
1	B	148	ASN
1	B	152	LEU
1	B	182	THR
1	B	197	ILE
1	B	213	ILE
1	B	222	VAL
1	B	224	VAL
1	B	241	LEU
1	B	275	THR
1	B	288	VAL
1	B	296	GLU
1	B	300	SER
1	B	308	THR
1	B	309	ILE
1	B	329	LEU
1	B	334	THR
1	B	340	THR
1	B	347	LEU
1	B	355	VAL
1	B	368	GLU
1	B	370	VAL
1	B	372	LEU
1	B	392	ILE
1	B	398	THR
1	C	13	LEU
1	C	17	LEU
1	C	30	LEU
1	C	72	SER
1	C	106	LEU
1	C	148	ASN
1	C	152	LEU
1	C	165	ILE
1	C	197	ILE
1	C	198	VAL
1	C	213	ILE
1	C	222	VAL
1	C	236	TYR
1	C	278	SER
1	C	288	VAL
1	C	298	ILE
1	C	308	THR

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Mol	Chain	Res	Type
1	C	309	ILE
1	C	320	VAL
1	C	329	LEU
1	C	333	LEU
1	C	334	THR
1	C	340	THR
1	C	355	VAL
1	C	368	GLU
1	C	370	VAL
1	C	372	LEU
1	C	392	ILE
1	C	398	THR
1	C	402	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	GLN
1	A	327	ASN
1	A	337	GLN
1	A	338	GLN
1	B	203	GLN
1	B	220	GLN
1	B	327	ASN
1	C	203	GLN
1	C	220	GLN
1	C	327	ASN
1	C	338	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ASP	A	503	-	7,8,8	1.18	1 (14%)	6,10,10	1.40	1 (16%)
3	ASP	B	503	-	7,8,8	1.19	1 (14%)	6,10,10	1.21	1 (16%)
3	ASP	C	503	-	7,8,8	1.13	1 (14%)	6,10,10	1.25	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ASP	A	503	-	-	2/8/8/8	-
3	ASP	B	503	-	-	4/8/8/8	-
3	ASP	C	503	-	-	4/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	ASP	OXT-C	-2.30	1.23	1.30
3	B	503	ASP	OXT-C	-2.27	1.23	1.30
3	C	503	ASP	OXT-C	-2.14	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	ASP	OXT-C-O	-2.86	117.60	124.08
3	C	503	ASP	OXT-C-O	-2.58	118.23	124.08
3	B	503	ASP	OXT-C-O	-2.35	118.75	124.08

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	ASP	C-CA-CB-CG
3	B	503	ASP	N-CA-CB-CG
3	B	503	ASP	C-CA-CB-CG
3	C	503	ASP	C-CA-CB-CG
3	C	503	ASP	OXT-C-CA-N
3	A	503	ASP	N-CA-CB-CG
3	C	503	ASP	N-CA-CB-CG
3	C	503	ASP	O-C-CA-N
3	B	503	ASP	O-C-CA-N
3	B	503	ASP	OXT-C-CA-N

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	ASP	5	0
3	B	503	ASP	2	0
3	C	503	ASP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	408/420 (97%)	0.56	48 (11%) 9 10	86, 125, 174, 190	0
1	B	408/420 (97%)	0.67	51 (12%) 8 9	92, 142, 206, 228	0
1	C	408/420 (97%)	0.94	78 (19%) 3 4	94, 142, 199, 223	0
All	All	1224/1260 (97%)	0.72	177 (14%) 6 7	86, 137, 196, 228	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	91	LEU	15.0
1	C	90	LEU	13.4
1	C	93	SER	12.2
1	A	329	LEU	10.7
1	B	12	VAL	9.8
1	C	94	ALA	9.1
1	C	350	ILE	8.4
1	C	95	PHE	8.4
1	C	308	THR	8.3
1	C	309	ILE	8.0
1	C	89	TYR	8.0
1	B	33	TYR	7.3
1	B	125	LYS	7.2
1	C	347	LEU	7.1
1	C	315	ALA	7.1
1	C	87	VAL	7.0
1	B	226	GLY	6.8
1	B	87	VAL	6.4
1	C	346	VAL	6.4
1	B	227	GLU	6.3
1	A	331	SER	6.2
1	B	90	LEU	6.0
1	C	186	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	117	VAL	5.9
1	C	351	GLY	5.9
1	C	343	LEU	5.8
1	B	228	LEU	5.6
1	A	414	LYS	5.6
1	A	378	ASN	5.5
1	C	86	VAL	5.5
1	C	203	GLN	5.4
1	C	92	THR	5.3
1	C	199	ASN	5.3
1	A	118	GLY	5.2
1	C	187	ILE	5.1
1	B	253	ILE	5.0
1	C	200	GLY	5.0
1	B	254	TYR	4.9
1	B	203	GLN	4.8
1	B	383	TYR	4.7
1	B	124	PRO	4.6
1	A	256	ILE	4.6
1	B	91	LEU	4.5
1	C	174	GLU	4.5
1	A	377	PRO	4.4
1	B	324	PHE	4.4
1	A	224	VAL	4.3
1	B	259	ILE	4.3
1	C	182	THR	4.2
1	C	249	VAL	4.0
1	B	325	ILE	4.0
1	B	32	HIS	3.9
1	C	34	GLY	3.9
1	C	98	THR	3.7
1	A	330	GLY	3.7
1	A	379	VAL	3.6
1	A	328	ALA	3.6
1	A	254	TYR	3.5
1	B	51	VAL	3.4
1	C	313	GLY	3.4
1	A	36	ALA	3.4
1	C	96	ALA	3.4
1	A	245	LEU	3.4
1	B	29	ILE	3.4
1	C	312	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	237	VAL	3.3
1	A	415	THR	3.3
1	C	242	GLN	3.3
1	A	115	LEU	3.3
1	B	199	ASN	3.3
1	C	204	TYR	3.2
1	C	140	THR	3.2
1	C	113	ILE	3.2
1	A	376	ASP	3.1
1	C	175	LYS	3.1
1	C	344	THR	3.1
1	B	321	CYS	3.1
1	C	298	ILE	3.1
1	B	212	LEU	3.1
1	B	411	ILE	3.1
1	B	34	GLY	3.0
1	C	354	GLY	3.0
1	A	372	LEU	3.0
1	C	406	LEU	3.0
1	C	178	LYS	3.0
1	B	250	LEU	2.9
1	C	212	LEU	2.9
1	C	181	GLU	2.9
1	C	345	ALA	2.9
1	B	372	LEU	2.9
1	B	402	VAL	2.8
1	C	109	PRO	2.8
1	B	202	MET	2.8
1	C	88	TYR	2.8
1	C	349	SER	2.8
1	C	185	ASP	2.8
1	A	255	GLY	2.7
1	A	241	LEU	2.7
1	C	305	LEU	2.7
1	A	233	ALA	2.7
1	A	12	VAL	2.7
1	B	395	MET	2.7
1	B	230	LYS	2.7
1	A	106	LEU	2.7
1	A	400	VAL	2.7
1	C	201	VAL	2.7
1	B	347	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	197	ILE	2.6
1	B	248	PHE	2.6
1	A	416	GLU	2.6
1	C	271	THR	2.6
1	B	18	ILE	2.6
1	A	231	VAL	2.6
1	B	290	LYS	2.6
1	C	371	GLY	2.6
1	B	239	LEU	2.6
1	A	380	ALA	2.6
1	C	196	LYS	2.6
1	A	313	GLY	2.6
1	B	79	GLY	2.5
1	B	175	LYS	2.5
1	A	381	ALA	2.5
1	A	37	ASP	2.5
1	B	387	LEU	2.5
1	C	97	VAL	2.5
1	C	402	VAL	2.5
1	B	314	THR	2.4
1	C	300	SER	2.4
1	C	409	THR	2.4
1	C	17	LEU	2.4
1	C	239	LEU	2.4
1	A	110	GLY	2.4
1	C	310	ASN	2.4
1	C	413	ALA	2.4
1	A	107	PHE	2.4
1	B	396	GLY	2.3
1	B	186	ALA	2.3
1	C	207	ILE	2.3
1	C	348	ALA	2.3
1	C	121	GLN	2.3
1	C	183	LEU	2.3
1	A	229	ALA	2.3
1	A	183	LEU	2.3
1	B	361	ILE	2.3
1	C	118	GLY	2.2
1	B	416	GLU	2.2
1	B	54	LEU	2.2
1	B	285	THR	2.2
1	A	342	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	296	GLU	2.2
1	B	292	MET	2.2
1	B	382	ALA	2.2
1	B	313	GLY	2.2
1	A	160	ILE	2.1
1	C	250	LEU	2.1
1	C	303	LEU	2.1
1	A	269	MET	2.1
1	C	291	GLU	2.1
1	A	285	THR	2.1
1	C	314	THR	2.1
1	A	10	TYR	2.1
1	C	265	ALA	2.1
1	A	396	GLY	2.1
1	C	198	VAL	2.1
1	A	341	ILE	2.1
1	C	353	ALA	2.1
1	B	118	GLY	2.1
1	B	86	VAL	2.1
1	A	77	ARG	2.1
1	A	156	PHE	2.1
1	A	102	ILE	2.0
1	C	318	GLN	2.0
1	A	152	LEU	2.0
1	A	325	ILE	2.0
1	A	401	ASN	2.0
1	C	119	GLY	2.0
1	C	261	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NA	B	501	1/1	0.86	0.29	119,119,119,119	0
2	NA	C	502	1/1	0.90	0.29	105,105,105,105	0
2	NA	A	501	1/1	0.91	0.22	104,104,104,104	0
2	NA	C	501	1/1	0.93	0.19	116,116,116,116	0
3	ASP	A	503	9/9	0.93	0.08	94,94,95,96	0
3	ASP	B	503	9/9	0.94	0.10	111,112,113,114	0
2	NA	B	502	1/1	0.96	0.08	104,104,104,104	0
3	ASP	C	503	9/9	0.96	0.10	107,108,110,110	0
2	NA	A	502	1/1	0.97	0.07	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.