



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:27 AM UTC

PDB ID : 6X01 / pdb_00006x01
Title : Crystal structure of the GltPh V216C-A391C mutant cross-linked in outward-facing state
Authors : Chen, I.; Font, J.; Ryan, R.
Deposited on : 2020-05-15
Resolution : 3.65 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

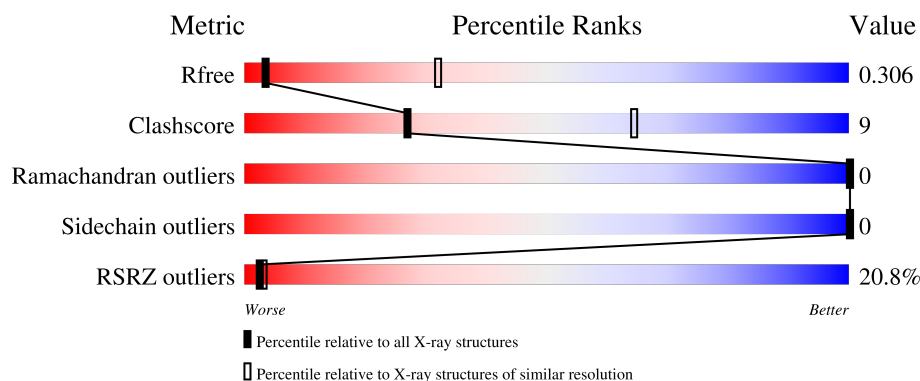
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

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	422	21% 73% 22% 5%
1	B	422	21% 76% 19% 5%
1	C	422	18% 73% 22% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ASP	A	501	-	-	X	-
2	ASP	C	501	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8862 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	400	Total	C	N	O	S	0	0	0
			2943	1938	468	519	18			
1	B	400	Total	C	N	O	S	0	0	0
			2943	1938	468	519	18			
1	C	400	Total	C	N	O	S	0	0	0
			2943	1938	468	519	18			

There are 24 discrepancies between the modelled and reference sequences:

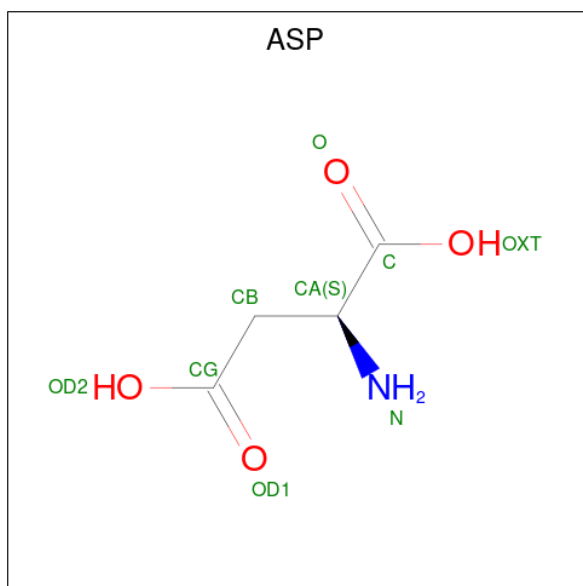
Chain	Residue	Modelled	Actual	Comment	Reference
A	216	CYS	VAL	engineered mutation	UNP O59010
A	321	SER	CYS	engineered mutation	UNP O59010
A	391	CYS	ALA	engineered mutation	UNP O59010
A	418	THR	-	expression tag	UNP O59010
A	419	LEU	-	expression tag	UNP O59010
A	420	VAL	-	expression tag	UNP O59010
A	421	PRO	-	expression tag	UNP O59010
A	422	ARG	-	expression tag	UNP O59010
B	216	CYS	VAL	engineered mutation	UNP O59010
B	321	SER	CYS	engineered mutation	UNP O59010
B	391	CYS	ALA	engineered mutation	UNP O59010
B	418	THR	-	expression tag	UNP O59010
B	419	LEU	-	expression tag	UNP O59010
B	420	VAL	-	expression tag	UNP O59010
B	421	PRO	-	expression tag	UNP O59010
B	422	ARG	-	expression tag	UNP O59010
C	216	CYS	VAL	engineered mutation	UNP O59010
C	321	SER	CYS	engineered mutation	UNP O59010
C	391	CYS	ALA	engineered mutation	UNP O59010
C	418	THR	-	expression tag	UNP O59010
C	419	LEU	-	expression tag	UNP O59010
C	420	VAL	-	expression tag	UNP O59010
C	421	PRO	-	expression tag	UNP O59010

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Chain	Residue	Modelled	Actual	Comment	Reference
C	422	ARG	-	expression tag	UNP O59010

- Molecule 2 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



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

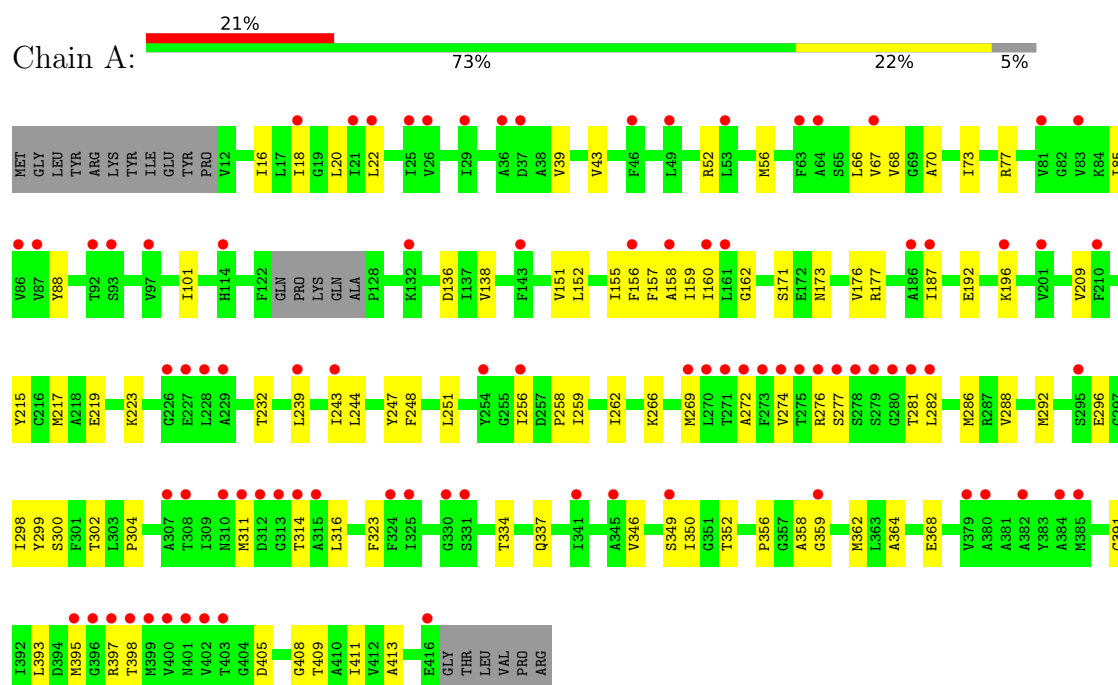
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

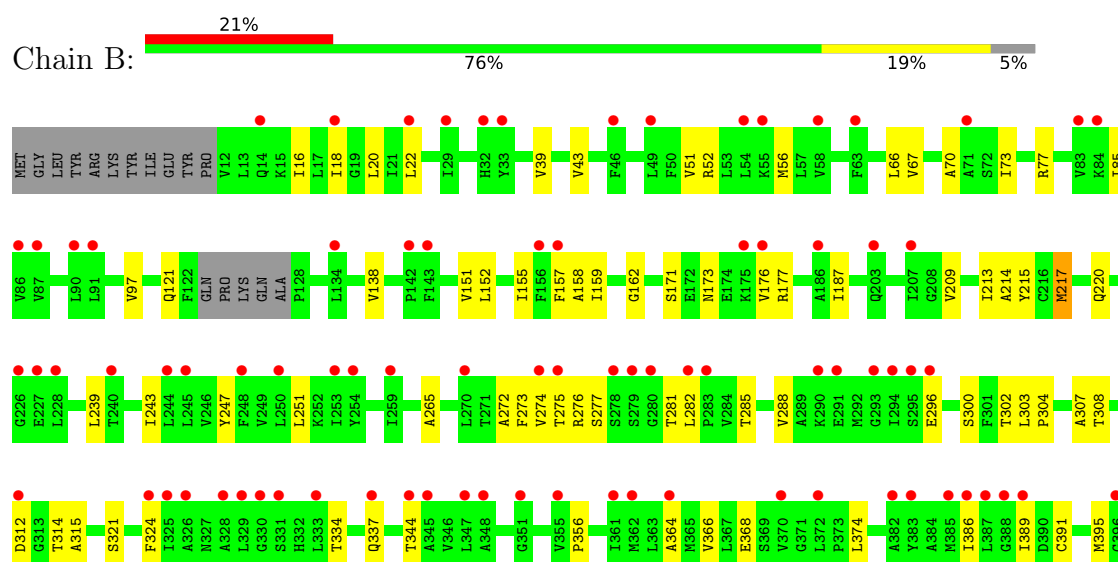
3 Residue-property plots

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

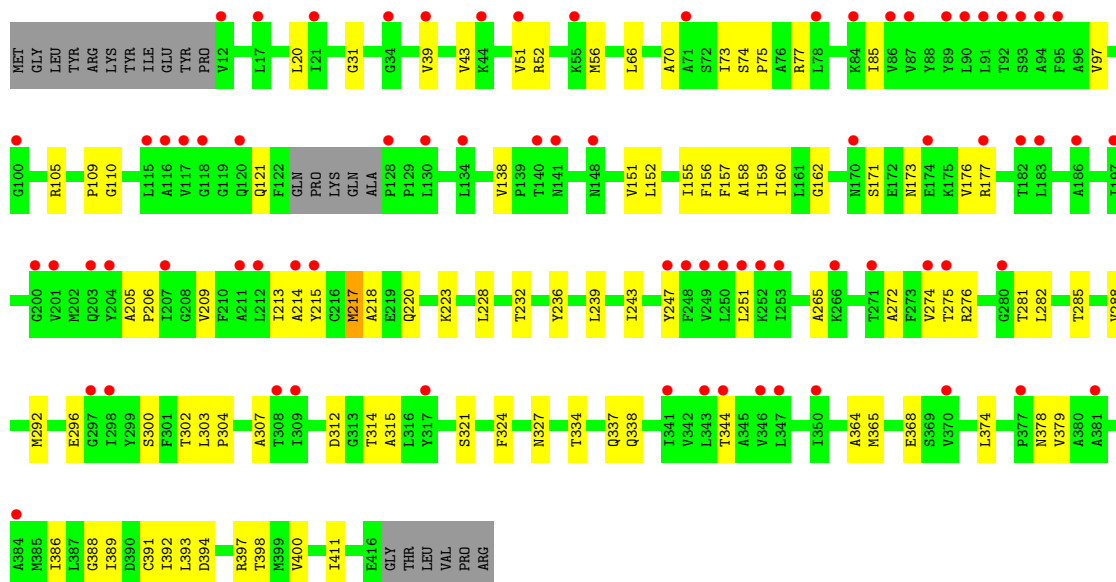
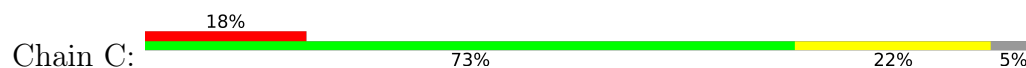


• Molecule 1: Glutamate transporter homolog





● 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	113.98Å 113.98Å 321.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.84 – 3.65 44.84 – 3.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.84-3.65) 99.7 (44.84-3.65)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.66Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.272 , 0.309 0.275 , 0.306	Depositor DCC
R_{free} test set	1231 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	155.4	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 98.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.078 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8862	wwPDB-VP
Average B, all atoms (Å ²)	176.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

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	0.14	0/2991	0.32	0/4070
1	B	0.19	0/2991	0.38	2/4070 (0.0%)
1	C	0.16	0/2991	0.39	2/4070 (0.0%)
All	All	0.16	0/8973	0.36	4/12210 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	217	MET	N-CA-C	-9.39	101.72	113.55
1	B	217	MET	N-CA-C	-6.33	105.21	113.12
1	B	214	ALA	N-CA-C	-6.29	104.51	111.36
1	C	214	ALA	N-CA-C	-5.61	105.31	111.82

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	2943	0	3147	64	0
1	B	2943	0	3147	50	0
1	C	2943	0	3147	62	0
2	A	9	0	3	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	9	0	3	3	0
2	C	9	0	3	5	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
All	All	8862	0	9450	169	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 9.

All (169) 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:398:THR:HG1	2:A:501:ASP:N	1.72	0.87
1:C:398:THR:HG1	2:C:501:ASP:N	1.78	0.82
1:C:276:ARG:NH1	1:C:391:CYS:SG	2.52	0.82
1:A:66:LEU:HD21	1:A:159:ILE:HG13	1.60	0.81
1:B:155:ILE:HD11	1:B:304:PRO:HB2	1.65	0.79
1:B:66:LEU:HD21	1:B:159:ILE:HG13	1.64	0.78
1:A:209:VAL:HG22	1:A:274:VAL:HG11	1.65	0.76
1:C:155:ILE:HD11	1:C:304:PRO:HB2	1.66	0.76
1:C:236:TYR:OH	1:C:392:ILE:HG22	1.85	0.76
1:C:66:LEU:HD21	1:C:159:ILE:HG13	1.68	0.75
1:A:85:ILE:HG12	1:A:302:THR:HG23	1.69	0.74
1:C:314:THR:HA	1:C:397:ARG:HD2	1.71	0.73
1:A:314:THR:HA	1:A:397:ARG:HD2	1.70	0.72
1:A:282:LEU:HD21	1:A:304:PRO:HA	1.74	0.70
1:B:398:THR:HG1	2:B:501:ASP:N	1.92	0.68
1:A:334:THR:HG22	1:A:337:GLN:HG2	1.75	0.68
1:C:171:SER:O	1:C:177:ARG:NH1	2.28	0.67
1:B:314:THR:HA	1:B:397:ARG:HD2	1.77	0.66
1:A:272:ALA:HB2	1:A:281:THR:HG21	1.78	0.66
1:A:352:THR:HA	1:A:362:MET:HE3	1.76	0.65
1:C:105:ARG:HD2	1:C:338:GLN:HE22	1.60	0.65
1:B:171:SER:O	1:B:177:ARG:NH1	2.29	0.65
1:B:56:MET:HE3	1:C:157:PHE:HD1	1.62	0.65
1:B:276:ARG:O	2:B:501:ASP:N	2.30	0.64
1:A:171:SER:O	1:A:177:ARG:NH1	2.29	0.64
1:C:85:ILE:HG12	1:C:302:THR:HG23	1.79	0.64
1:C:398:THR:OG1	2:C:501:ASP:N	2.31	0.63
1:C:276:ARG:O	2:C:501:ASP:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ALA:HB3	1:A:162:GLY:HA3	1.82	0.61
1:A:157:PHE:HD1	1:C:56:MET:HE3	1.65	0.61
1:A:56:MET:HE3	1:B:157:PHE:HD1	1.64	0.61
1:A:398:THR:OG1	2:A:501:ASP:N	2.32	0.61
1:A:66:LEU:HD22	1:A:158:ALA:HB3	1.83	0.59
1:A:151:VAL:HG23	1:A:152:LEU:HD12	1.83	0.59
1:A:232:THR:HA	1:A:393:LEU:HD21	1.85	0.59
1:B:85:ILE:HG12	1:B:302:THR:HG23	1.84	0.59
1:A:358:ALA:HB1	1:A:362:MET:HE1	1.84	0.59
1:B:285:THR:HG22	1:B:303:LEU:HD13	1.85	0.58
1:B:52:ARG:NH2	1:C:138:VAL:O	2.36	0.58
1:C:321:SER:HB2	1:C:386:ILE:HD13	1.85	0.58
1:B:251:LEU:HD23	1:B:411:ILE:HD11	1.87	0.57
1:C:121:GLN:HB2	1:C:374:LEU:HB3	1.86	0.57
1:B:66:LEU:HD22	1:B:158:ALA:HB3	1.87	0.57
1:B:276:ARG:NH1	1:B:391:CYS:SG	2.78	0.57
1:A:243:ILE:HA	1:A:247:TYR:CD1	2.39	0.57
1:A:346:VAL:O	1:A:350:ILE:HG12	2.07	0.55
1:A:52:ARG:NH2	1:B:138:VAL:O	2.39	0.55
1:B:121:GLN:HB2	1:B:374:LEU:HB3	1.88	0.55
1:C:66:LEU:HD22	1:C:158:ALA:HB3	1.88	0.55
1:C:285:THR:HG22	1:C:303:LEU:HD13	1.87	0.55
1:A:405:ASP:O	1:A:409:THR:OG1	2.23	0.55
1:C:213:ILE:O	1:C:217:MET:HG2	2.06	0.55
1:C:272:ALA:HB2	1:C:281:THR:HG21	1.89	0.55
1:A:288:VAL:O	1:A:292:MET:HG2	2.07	0.54
1:C:324:PHE:HD2	1:C:386:ILE:HD11	1.73	0.54
1:C:213:ILE:O	1:C:217:MET:CG	2.55	0.54
1:B:398:THR:OG1	2:B:501:ASP:N	2.41	0.54
1:B:70:ALA:HB3	1:B:162:GLY:HA3	1.90	0.54
1:B:251:LEU:HA	1:B:411:ILE:HD11	1.91	0.53
1:B:282:LEU:HD13	1:B:307:ALA:HB2	1.90	0.53
1:A:215:TYR:C	1:A:217:MET:H	2.17	0.53
1:A:73:ILE:HB	1:A:77:ARG:HG2	1.90	0.53
1:A:251:LEU:HD23	1:A:411:ILE:HD11	1.92	0.52
1:C:251:LEU:HD23	1:C:411:ILE:HD11	1.90	0.52
1:B:209:VAL:HG13	1:B:274:VAL:HG21	1.90	0.52
1:C:209:VAL:HG13	1:C:274:VAL:HG21	1.92	0.52
1:B:247:TYR:OH	1:B:312:ASP:OD2	2.28	0.51
1:C:73:ILE:HB	1:C:77:ARG:HG2	1.93	0.51
1:B:209:VAL:HA	1:B:274:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:GLN:HG2	1:C:223:LYS:HD2	1.92	0.51
1:C:70:ALA:HB3	1:C:162:GLY:HA3	1.93	0.50
1:B:73:ILE:HB	1:B:77:ARG:HG2	1.93	0.50
1:B:173:ASN:HB3	1:B:176:VAL:HG22	1.94	0.50
1:C:265:ALA:HA	1:C:288:VAL:HG11	1.92	0.50
1:C:394:ASP:OD1	2:C:501:ASP:N	2.45	0.50
1:A:296:GLU:HA	1:A:299:TYR:CE1	2.46	0.49
1:C:232:THR:HA	1:C:393:LEU:HD21	1.93	0.49
1:A:298:ILE:HG21	1:A:413:ALA:HB2	1.94	0.49
1:B:272:ALA:HB2	1:B:281:THR:HG21	1.94	0.49
1:A:243:ILE:HA	1:A:247:TYR:HD1	1.78	0.49
1:C:282:LEU:HD13	1:C:307:ALA:HB2	1.95	0.49
1:A:173:ASN:HB3	1:A:176:VAL:HG22	1.94	0.49
1:A:155:ILE:HD11	1:A:304:PRO:HB2	1.94	0.48
1:B:265:ALA:HA	1:B:288:VAL:HG11	1.94	0.48
1:A:258:PRO:O	1:A:262:ILE:HG12	2.12	0.48
1:B:272:ALA:HB1	1:B:398:THR:HG22	1.96	0.48
1:C:209:VAL:HA	1:C:274:VAL:HG11	1.95	0.48
1:C:397:ARG:NE	2:C:501:ASP:OD2	2.45	0.48
1:A:359:GLY:N	2:A:501:ASP:OD1	2.26	0.48
1:C:220:GLN:NE2	1:C:388:GLY:O	2.47	0.48
1:A:352:THR:HA	1:A:362:MET:CE	2.43	0.47
1:B:405:ASP:O	1:B:409:THR:OG1	2.24	0.47
1:C:51:VAL:HG22	1:C:275:THR:HG23	1.96	0.47
1:A:256:ILE:HD13	1:A:411:ILE:HD13	1.95	0.47
1:A:286:MET:HE3	1:A:300:SER:HA	1.96	0.47
1:A:277:SER:HB2	1:A:356:PRO:HD3	1.95	0.47
1:A:276:ARG:O	2:A:501:ASP:N	2.48	0.47
1:C:39:VAL:HG13	1:C:43:VAL:HB	1.96	0.47
1:C:220:GLN:OE1	1:C:389:ILE:HA	2.15	0.47
1:A:68:VAL:HG12	1:A:296:GLU:OE2	2.14	0.47
1:A:248:PHE:HE1	1:A:262:ILE:HD11	1.79	0.47
1:A:391:CYS:O	1:A:395:MET:HG3	2.15	0.47
1:B:20:LEU:HD12	1:B:213:ILE:HG12	1.96	0.47
1:A:67:VAL:HG11	1:A:187:ILE:HD13	1.97	0.47
1:A:239:LEU:HD23	1:A:316:LEU:HD13	1.97	0.47
1:C:247:TYR:OH	1:C:312:ASP:OD2	2.26	0.46
1:B:215:TYR:C	1:B:217:MET:H	2.24	0.46
1:C:20:LEU:HD12	1:C:213:ILE:HG12	1.97	0.46
1:B:243:ILE:HA	1:B:247:TYR:CD1	2.50	0.45
1:C:334:THR:HG23	1:C:337:GLN:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ARG:HD2	1:C:338:GLN:NE2	2.30	0.45
1:C:344:THR:HG23	1:C:365:MET:HE2	1.98	0.45
1:B:277:SER:HB2	1:B:356:PRO:HD3	1.98	0.45
1:C:364:ALA:O	1:C:368:GLU:HG2	2.17	0.45
1:B:18:ILE:O	1:B:22:LEU:HG	2.16	0.45
1:B:51:VAL:HG22	1:B:275:THR:HG23	1.98	0.45
1:A:16:ILE:O	1:A:20:LEU:N	2.48	0.45
1:A:244:LEU:O	1:A:248:PHE:HB2	2.17	0.45
1:C:151:VAL:HG23	1:C:152:LEU:HD12	1.97	0.45
1:A:262:ILE:HD12	1:A:269:MET:HE1	1.97	0.45
1:B:151:VAL:HG23	1:B:152:LEU:HD12	1.97	0.45
1:B:239:LEU:HB3	1:B:400:VAL:HG21	1.99	0.45
1:B:364:ALA:O	1:B:368:GLU:HG2	2.17	0.45
1:C:239:LEU:HB3	1:C:400:VAL:HG21	1.99	0.45
1:A:156:PHE:O	1:A:160:ILE:HG12	2.17	0.44
1:C:110:GLY:O	1:C:327:ASN:HB3	2.17	0.44
1:A:364:ALA:O	1:A:368:GLU:HG2	2.17	0.44
1:A:18:ILE:O	1:A:22:LEU:HG	2.16	0.44
1:C:215:TYR:C	1:C:217:MET:H	2.25	0.44
1:B:324:PHE:HD2	1:B:386:ILE:HD11	1.82	0.44
1:A:262:ILE:HG22	1:A:266:LYS:NZ	2.33	0.44
1:C:31:GLY:HA3	1:C:218:ALA:HA	1.98	0.44
1:C:243:ILE:HA	1:C:247:TYR:CD1	2.53	0.43
1:C:97:VAL:HB	1:C:315:ALA:HB1	2.00	0.43
1:B:334:THR:HG23	1:B:337:GLN:H	1.83	0.43
1:B:16:ILE:O	1:B:20:LEU:N	2.49	0.43
1:A:66:LEU:HD11	1:A:155:ILE:HG23	2.01	0.43
1:B:39:VAL:HG13	1:B:43:VAL:HB	2.00	0.43
1:C:378:ASN:OD1	1:C:379:VAL:N	2.51	0.43
1:A:136:ASP:HA	1:C:52:ARG:NH2	2.33	0.42
1:A:302:THR:HG21	1:A:409:THR:HA	2.01	0.42
1:C:228:LEU:HB3	1:C:389:ILE:HD13	2.02	0.42
1:A:138:VAL:O	1:C:52:ARG:NH2	2.50	0.42
1:B:296:GLU:O	1:B:300:SER:HB3	2.19	0.42
1:A:259:ILE:H	1:A:259:ILE:HD12	1.84	0.42
1:B:273:PHE:CE2	1:B:395:MET:HE2	2.55	0.42
1:A:219:GLU:O	1:A:223:LYS:NZ	2.51	0.42
1:B:344:THR:HB	1:B:366:VAL:HG23	2.00	0.42
1:C:156:PHE:O	1:C:160:ILE:HG12	2.20	0.42
1:C:109:PRO:HB2	1:C:324:PHE:HB2	2.01	0.41
1:A:88:TYR:CE2	1:A:408:GLY:HA3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ASN:HB3	1:C:176:VAL:HG22	2.01	0.41
1:C:288:VAL:HG12	1:C:292:MET:HE3	2.02	0.41
1:B:321:SER:HB2	1:B:386:ILE:HD13	2.03	0.41
1:A:311:MET:HB2	1:A:349:SER:HB2	2.01	0.41
1:A:101:ILE:HG23	1:A:323:PHE:CE2	2.54	0.41
1:B:67:VAL:HG11	1:B:187:ILE:HD13	2.03	0.41
1:C:205:ALA:N	1:C:206:PRO:HD2	2.36	0.41
1:A:66:LEU:HD12	1:A:300:SER:O	2.20	0.41
1:A:192:GLU:O	1:A:196:LYS:HG2	2.21	0.41
1:B:152:LEU:HD11	1:B:308:THR:OG1	2.20	0.41
1:B:220:GLN:OE1	1:B:389:ILE:HA	2.21	0.41
1:C:213:ILE:HD12	1:C:213:ILE:HA	1.78	0.41
1:B:97:VAL:HB	1:B:315:ALA:HB1	2.02	0.41
1:A:262:ILE:O	1:A:266:LYS:HG2	2.21	0.40
1:A:262:ILE:C	1:A:266:LYS:HZ2	2.29	0.40
1:C:296:GLU:O	1:C:300:SER:HB3	2.21	0.40
1:A:39:VAL:HG13	1:A:43:VAL:HB	2.02	0.40
1:C:74:SER:OG	1:C:75:PRO:HD3	2.21	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	396/422 (94%)	379 (96%)	17 (4%)	0	100	100
1	B	396/422 (94%)	381 (96%)	15 (4%)	0	100	100
1	C	396/422 (94%)	380 (96%)	16 (4%)	0	100	100
All	All	1188/1266 (94%)	1140 (96%)	48 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	311/331 (94%)	311 (100%)	0	100	100
1	B	311/331 (94%)	311 (100%)	0	100	100
1	C	311/331 (94%)	311 (100%)	0	100	100
All	All	933/993 (94%)	933 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	ASN
1	A	188	ASN
1	A	332	HIS
1	C	141	ASN
1	C	188	ASN
1	C	338	GLN

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 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	$\# Z > 2$
2	ASP	A	501	-	7,8,8	1.15	1 (14%)	6,10,10	1.34	1 (16%)
2	ASP	B	501	-	7,8,8	1.15	1 (14%)	6,10,10	1.38	1 (16%)
2	ASP	C	501	-	7,8,8	1.16	1 (14%)	6,10,10	1.38	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
2	ASP	A	501	-	-	0/8/8/8	-
2	ASP	B	501	-	-	0/8/8/8	-
2	ASP	C	501	-	-	1/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ASP	OXT-C	-2.28	1.23	1.30
2	C	501	ASP	OXT-C	-2.25	1.23	1.30
2	A	501	ASP	OXT-C	-2.23	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	ASP	OXT-C-O	-2.76	117.82	124.08
2	B	501	ASP	OXT-C-O	-2.68	117.99	124.08
2	A	501	ASP	OXT-C-O	-2.50	118.40	124.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	ASP	OXT-C-CA-N

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ASP	4	0
2	B	501	ASP	3	0
2	C	501	ASP	5	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	400/422 (94%)	0.99	87 (21%) 2 3	96, 140, 198, 236	0
1	B	400/422 (94%)	1.02	87 (21%) 2 3	124, 194, 247, 266	0
1	C	400/422 (94%)	0.96	75 (18%) 3 4	133, 187, 240, 268	0
All	All	1200/1266 (94%)	0.99	249 (20%) 2 3	96, 175, 238, 268	0

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	91	LEU	13.2
1	C	90	LEU	9.4
1	B	87	VAL	9.4
1	C	87	VAL	8.2
1	A	22	LEU	7.8
1	C	249	VAL	7.6
1	B	86	VAL	7.2
1	B	18	ILE	7.1
1	C	86	VAL	6.9
1	B	90	LEU	6.6
1	B	324	PHE	6.3
1	A	21	ILE	6.0
1	A	18	ILE	6.0
1	A	227	GLU	5.9
1	C	134	LEU	5.8
1	B	361	ILE	5.8
1	B	228	LEU	5.6
1	B	382	ALA	5.5
1	C	174	GLU	5.5
1	C	346	VAL	5.4
1	B	83	VAL	5.4
1	A	26	VAL	5.2
1	A	187	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	203	GLN	5.1
1	A	25	ILE	5.0
1	A	63	PHE	5.0
1	B	325	ILE	5.0
1	A	416	GLU	5.0
1	A	49	LEU	4.9
1	C	95	PHE	4.9
1	B	370	VAL	4.9
1	A	312	ASP	4.8
1	C	117	VAL	4.7
1	B	91	LEU	4.7
1	B	385	MET	4.7
1	B	254	TYR	4.7
1	C	17	LEU	4.6
1	C	343	LEU	4.6
1	B	383	TYR	4.5
1	C	350	ILE	4.3
1	C	252	LYS	4.2
1	A	400	VAL	4.2
1	B	55	LYS	4.2
1	B	372	LEU	4.2
1	C	93	SER	4.2
1	B	227	GLU	4.2
1	A	83	VAL	4.1
1	B	291	GLU	4.1
1	A	160	ILE	4.0
1	A	114	HIS	4.0
1	A	402	VAL	4.0
1	C	204	TYR	3.9
1	C	308	THR	3.9
1	C	251	LEU	3.9
1	A	330	GLY	3.9
1	B	33	TYR	3.8
1	C	177	ARG	3.8
1	A	186	ALA	3.8
1	A	313	GLY	3.8
1	C	182	THR	3.8
1	A	331	SER	3.8
1	B	331	SER	3.8
1	C	118	GLY	3.7
1	A	314	THR	3.6
1	B	280	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	386	ILE	3.6
1	C	377	PRO	3.6
1	C	51	VAL	3.5
1	C	275	THR	3.5
1	B	402	VAL	3.5
1	A	275	THR	3.5
1	B	326	ALA	3.4
1	A	274	VAL	3.4
1	B	71	ALA	3.4
1	B	295	SER	3.4
1	A	399	MET	3.4
1	B	63	PHE	3.3
1	B	279	SER	3.3
1	A	307	ALA	3.3
1	A	396	GLY	3.3
1	C	34	GLY	3.3
1	C	247	TYR	3.3
1	A	395	MET	3.3
1	B	134	LEU	3.3
1	B	330	GLY	3.2
1	A	276	ARG	3.2
1	C	266	LYS	3.2
1	A	398	THR	3.2
1	C	94	ALA	3.2
1	A	81	VAL	3.2
1	C	186	ALA	3.2
1	C	212	LEU	3.2
1	A	87	VAL	3.1
1	B	333	LEU	3.1
1	C	120	GLN	3.1
1	A	201	VAL	3.1
1	A	64	ALA	3.1
1	A	29	ILE	3.1
1	B	54	LEU	3.1
1	C	89	TYR	3.0
1	C	250	LEU	3.0
1	B	142	PRO	3.0
1	B	312	ASP	3.0
1	A	93	SER	3.0
1	A	401	ASN	3.0
1	C	347	LEU	3.0
1	B	58	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	355	VAL	3.0
1	C	309	ILE	2.9
1	C	381	ALA	2.9
1	C	130	LEU	2.9
1	A	86	VAL	2.9
1	B	396	GLY	2.9
1	B	389	ILE	2.9
1	B	46	PHE	2.9
1	B	207	ILE	2.9
1	C	197	ILE	2.8
1	A	36	ALA	2.8
1	A	229	ALA	2.8
1	C	215	TYR	2.8
1	C	115	LEU	2.8
1	A	272	ALA	2.8
1	B	143	PHE	2.8
1	A	161	LEU	2.8
1	C	201	VAL	2.7
1	A	228	LEU	2.7
1	A	349	SER	2.7
1	A	256	ILE	2.7
1	A	239	LEU	2.7
1	A	345	ALA	2.7
1	B	290	LYS	2.7
1	C	200	GLY	2.7
1	B	259	ILE	2.7
1	C	253	ILE	2.7
1	C	341	ILE	2.7
1	C	370	VAL	2.7
1	B	414	LYS	2.6
1	B	347	LEU	2.6
1	B	32	HIS	2.6
1	B	245	LEU	2.6
1	A	324	PHE	2.6
1	C	207	ILE	2.6
1	B	244	LEU	2.6
1	A	280	GLY	2.6
1	B	226	GLY	2.6
1	A	92	THR	2.6
1	A	271	THR	2.6
1	C	21	ILE	2.6
1	A	379	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	170	ASN	2.6
1	B	157	PHE	2.6
1	C	55	LYS	2.5
1	A	53	LEU	2.5
1	A	382	ALA	2.5
1	B	293	GLY	2.5
1	B	329	LEU	2.5
1	A	270	LEU	2.5
1	B	22	LEU	2.5
1	C	183	LEU	2.5
1	A	156	PHE	2.5
1	B	156	PHE	2.5
1	B	240	THR	2.5
1	A	278	SER	2.5
1	B	253	ILE	2.5
1	C	214	ALA	2.5
1	B	275	THR	2.5
1	A	385	MET	2.5
1	B	250	LEU	2.4
1	A	279	SER	2.4
1	C	92	THR	2.4
1	B	84	LYS	2.4
1	A	243	ILE	2.4
1	A	380	ALA	2.4
1	B	248	PHE	2.4
1	A	310	ASN	2.4
1	B	400	VAL	2.4
1	A	132	LYS	2.4
1	C	44	LYS	2.4
1	B	344	THR	2.4
1	B	186	ALA	2.4
1	B	362	MET	2.4
1	B	175	LYS	2.4
1	A	67	VAL	2.4
1	B	29	ILE	2.4
1	C	274	VAL	2.4
1	A	158	ALA	2.4
1	A	226	GLY	2.3
1	B	351	GLY	2.3
1	A	403	THR	2.3
1	B	296	GLU	2.3
1	A	277	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	278	SER	2.3
1	C	280	GLY	2.3
1	B	345	ALA	2.3
1	B	337	GLN	2.3
1	C	297	GLY	2.3
1	B	399	MET	2.3
1	C	140	THR	2.3
1	A	46	PHE	2.3
1	A	254	TYR	2.3
1	A	37	ASP	2.3
1	B	270	LEU	2.2
1	C	248	PHE	2.2
1	B	282	LEU	2.2
1	B	203	GLN	2.2
1	A	295	SER	2.2
1	C	128	PRO	2.2
1	B	348	ALA	2.2
1	C	384	ALA	2.2
1	C	39	VAL	2.2
1	B	283	PRO	2.2
1	A	273	PHE	2.2
1	A	315	ALA	2.2
1	A	384	ALA	2.2
1	B	176	VAL	2.2
1	C	100	GLY	2.2
1	C	141	ASN	2.2
1	C	116	ALA	2.1
1	A	359	GLY	2.1
1	C	271	THR	2.1
1	A	311	MET	2.1
1	B	387	LEU	2.1
1	A	397	ARG	2.1
1	B	274	VAL	2.1
1	A	269	MET	2.1
1	B	328	ALA	2.1
1	C	71	ALA	2.1
1	C	211	ALA	2.1
1	A	341	ILE	2.1
1	C	148	ASN	2.1
1	B	49	LEU	2.1
1	B	388	GLY	2.1
1	A	282	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	78	LEU	2.1
1	C	317	TYR	2.1
1	A	308	THR	2.1
1	A	210	PHE	2.1
1	C	344	THR	2.0
1	A	325	ILE	2.0
1	B	294	ILE	2.0
1	B	364	ALA	2.0
1	A	281	THR	2.0
1	B	14	GLN	2.0
1	C	12	VAL	2.0
1	A	196	LYS	2.0
1	C	84	LYS	2.0
1	C	298	ILE	2.0
1	A	143	PHE	2.0
1	A	97	VAL	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	ASP	A	501	9/9	0.58	0.23	104,121,156,156	0
3	NA	A	502	1/1	0.62	0.28	123,123,123,123	0
2	ASP	B	501	9/9	0.83	0.09	158,168,194,204	0
3	NA	B	502	1/1	0.85	0.15	152,152,152,152	0
2	ASP	C	501	9/9	0.87	0.07	158,162,170,188	0
3	NA	C	503	1/1	0.88	0.18	162,162,162,162	0
3	NA	C	502	1/1	0.93	0.08	173,173,173,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	503	1/1	0.96	0.04	76,76,76,76	0
3	NA	B	503	1/1	0.96	0.04	151,151,151,151	0

6.5 Other polymers [i](#)

There are no such residues in this entry.