



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 8, 2021 – 10:17 AM EST

PDB ID : 6X01
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17
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)	:	2.17

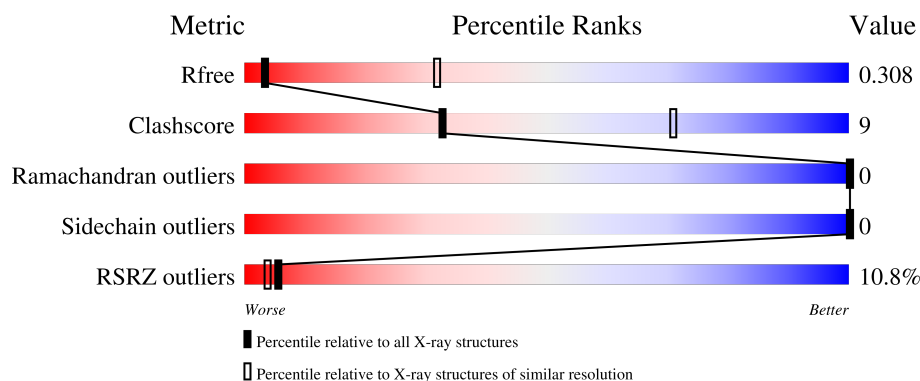
1 Overall quality at a glance

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}	130704	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

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 $\leq 5\%$. 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	
1	B	422	
1	C	422	

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:

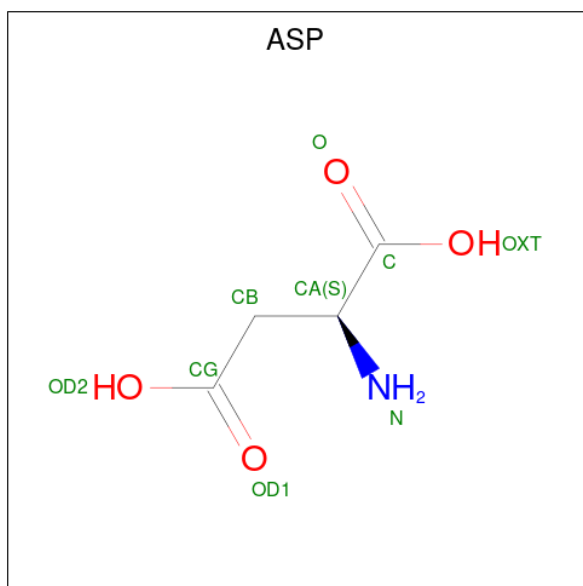
Chain	Residue	Modelled	Actual	Comment	Reference
A	216	CYS	VAL	engineered mutation	UNP O59010
A	321	SER	CYS	engineered mutation	UNP O59010
A	391	CYS	ALA	engineered mutation	UNP O59010
A	418	THR	-	expression tag	UNP O59010
A	419	LEU	-	expression tag	UNP O59010
A	420	VAL	-	expression tag	UNP O59010
A	421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

Continued on next page...

Continued from previous page...

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

- Molecule 2 is ASPARTIC ACID (three-letter code: 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		

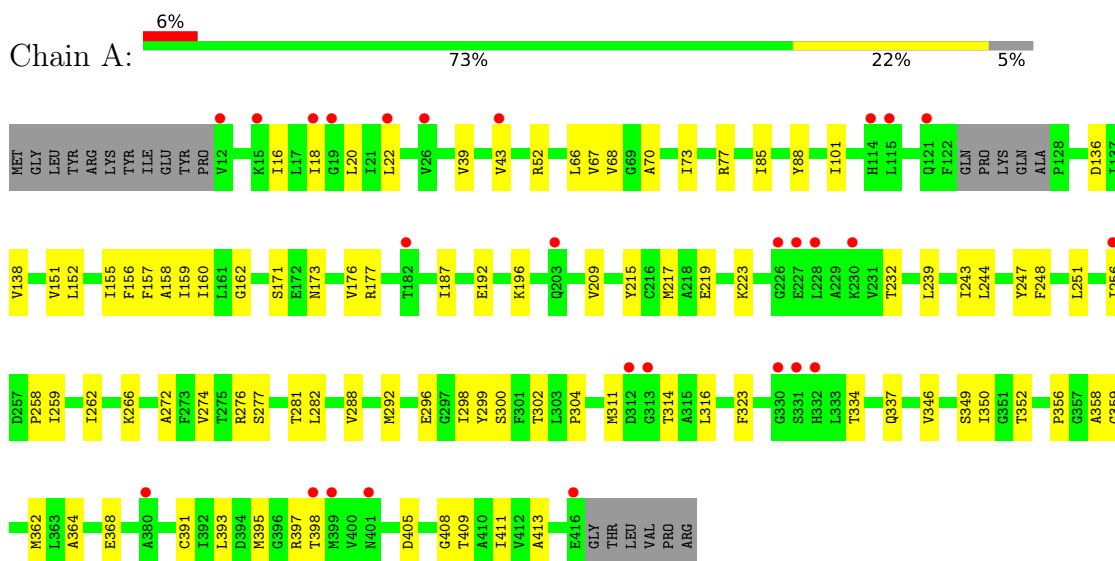
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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		

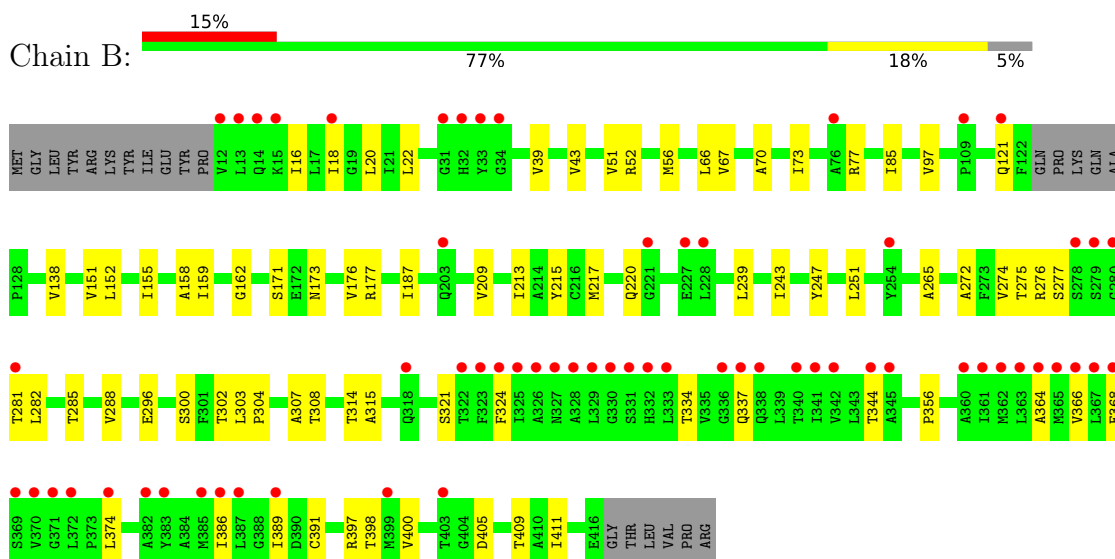
3 Residue-property plots [i](#)

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.

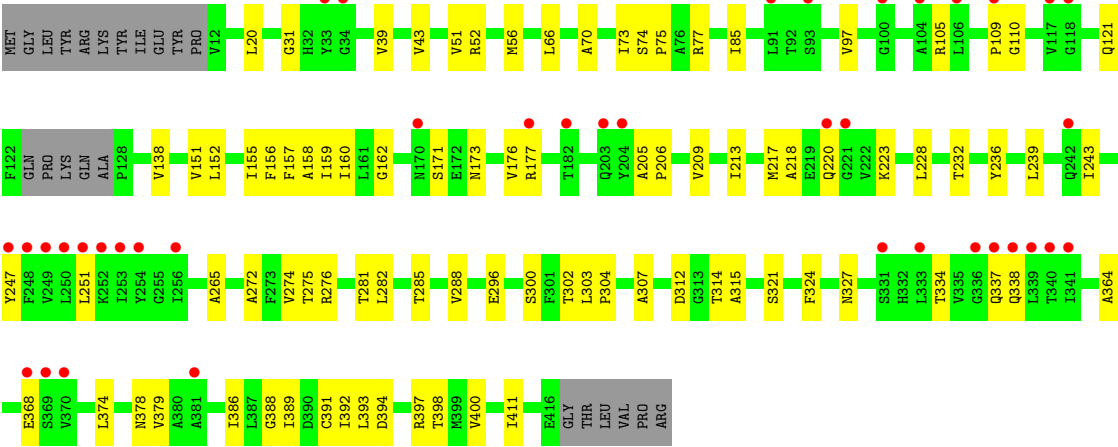
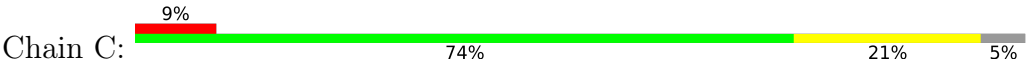
• Molecule 1: Glutamate transporter homolog



• 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	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) 99.8 (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 0.272 , 0.308	Depositor DCC
R_{free} test set	1227 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 , 119.1	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	0.85	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	0.26	0/2991	0.43	0/4070
1	B	0.26	0/2991	0.41	0/4070
1	C	0.26	0/2991	0.42	0/4070
All	All	0.26	0/8973	0.42	0/12210

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	2943	0	3147	60	0
1	B	2943	0	3147	47	0
1	C	2943	0	3147	59	0
2	A	9	0	3	4	0
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	160	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 (160) 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:276:ARG:NH1	1:C:391:CYS:SG	2.52	0.82
1:C:398:THR:HG1	2:C:501:ASP:N	1.79	0.81
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: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: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: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:A:358:ALA:HB1	1:A:362:MET:HE1	1.78	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
1:A:70:ALA:HB3	1:A:162:GLY:HA3	1.82	0.61
1:B:398:THR:HG1	2:B:501:ASP:N	1.97	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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:A:352:THR:HA	1:A:362:MET:CE	2.43	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:247:TYR:OH	1:C:312:ASP:OD2	2.26	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:215:TYR:C	1:A:217:MET:H	2.17	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:277:SER:HB2	1:A:356:PRO:HD3	1.95	0.47
1:A:157:PHE:HA	1:C:56:MET:HE3	1.97	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:20:LEU:HD12	1:C:213:ILE:HG12	1.97	0.46
1:A:352:THR:HA	1:A:362:MET:HE2	1.98	0.46
1:B:56:MET:HE3	1:C:157:PHE:HA	1.98	0.45
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
1:C:105:ARG:HD2	1:C:338:GLN:NE2	2.30	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:405:ASP:O	1:A:409:THR:OG1	2.23	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: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
1:C:173:ASN:HB3	1:C:176:VAL:HG22	2.01	0.41
1:B:215:TYR:C	1:B:217:MET:H	2.24	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: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

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. There are no such sidechains identified.

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 monosaccharides 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	B	501	-	2,8,8	0.36	0	1,10,10	0.09	0
2	ASP	A	501	-	2,8,8	0.32	0	1,10,10	0.21	0
2	ASP	C	501	-	2,8,8	0.35	0	1,10,10	0.02	0

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	B	501	-	-	0/2/8/8	-
2	ASP	A	501	-	-	0/2/8/8	-
2	ASP	C	501	-	-	0/2/8/8	-

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.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	ASP	3	0
2	A	501	ASP	4	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%)	0.34	27 (6%) 17 11	96, 140, 198, 236	0
1	B	400/422 (94%)	0.61	64 (16%) 1 1	124, 194, 247, 266	0
1	C	400/422 (94%)	0.24	39 (9%) 7 5	133, 187, 240, 268	0
All	All	1200/1266 (94%)	0.40	130 (10%) 5 4	96, 175, 238, 268	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	370	VAL	7.0
1	B	382	ALA	6.3
1	B	337	GLN	5.9
1	B	383	TYR	5.9
1	C	370	VAL	5.8
1	B	323	PHE	5.8
1	C	252	LYS	5.7
1	B	109	PRO	5.7
1	B	325	ILE	5.3
1	A	227	GLU	5.3
1	B	386	ILE	5.2
1	B	324	PHE	5.0
1	B	331	SER	5.0
1	B	32	HIS	4.9
1	C	341	ILE	4.9
1	B	33	TYR	4.9
1	B	374	LEU	4.8
1	B	228	LEU	4.8
1	B	372	LEU	4.7
1	B	340	THR	4.4
1	C	251	LEU	4.4
1	A	114	HIS	4.3
1	B	344	THR	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	416	GLU	4.2
1	C	337	GLN	4.2
1	C	247	TYR	4.1
1	C	106	LEU	4.0
1	B	385	MET	4.0
1	B	329	LEU	3.9
1	B	363	LEU	3.9
1	C	254	TYR	3.9
1	B	365	MET	3.9
1	C	249	VAL	3.8
1	A	332	HIS	3.8
1	B	333	LEU	3.8
1	B	341	ILE	3.8
1	A	182	THR	3.7
1	A	331	SER	3.7
1	C	170	ASN	3.7
1	B	338	GLN	3.7
1	C	340	THR	3.7
1	C	118	GLY	3.6
1	B	322	THR	3.6
1	B	31	GLY	3.6
1	B	12	VAL	3.5
1	C	34	GLY	3.5
1	B	227	GLU	3.5
1	C	182	THR	3.5
1	B	360	ALA	3.3
1	C	253	ILE	3.2
1	C	369	SER	3.2
1	C	117	VAL	3.2
1	B	318	GLN	3.2
1	A	330	GLY	3.2
1	B	364	ALA	3.1
1	B	361	ILE	3.1
1	B	389	ILE	3.1
1	A	22	LEU	3.1
1	C	203	GLN	3.0
1	B	367	LEU	3.0
1	B	326	ALA	3.0
1	A	26	VAL	3.0
1	C	333	LEU	2.9
1	B	332	HIS	2.9
1	C	336	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	220	GLN	2.8
1	C	177	ARG	2.8
1	B	368	GLU	2.8
1	A	226	GLY	2.8
1	B	328	ALA	2.8
1	B	330	GLY	2.8
1	A	18	ILE	2.8
1	B	342	VAL	2.8
1	B	362	MET	2.8
1	B	327	ASN	2.8
1	A	228	LEU	2.8
1	A	12	VAL	2.8
1	C	221	GLY	2.8
1	B	34	GLY	2.7
1	A	401	ASN	2.7
1	C	100	GLY	2.7
1	B	13	LEU	2.6
1	B	387	LEU	2.6
1	C	109	PRO	2.6
1	C	250	LEU	2.6
1	B	254	TYR	2.6
1	C	381	ALA	2.6
1	B	279	SER	2.6
1	B	345	ALA	2.6
1	C	248	PHE	2.6
1	C	256	ILE	2.6
1	B	121	GLN	2.6
1	A	15	LYS	2.5
1	A	312	ASP	2.4
1	B	280	GLY	2.4
1	B	278	SER	2.4
1	A	203	GLN	2.4
1	A	398	THR	2.4
1	B	371	GLY	2.4
1	A	115	LEU	2.4
1	B	366	VAL	2.4
1	C	368	GLU	2.4
1	A	399	MET	2.4
1	A	380	ALA	2.4
1	C	338	GLN	2.3
1	B	336	GLY	2.3
1	C	204	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	331	SER	2.3
1	A	256	ILE	2.3
1	B	14	GLN	2.2
1	B	203	GLN	2.2
1	C	104	ALA	2.2
1	B	76	ALA	2.2
1	A	43	VAL	2.2
1	C	33	TYR	2.2
1	A	121	GLN	2.2
1	C	242	GLN	2.2
1	C	339	LEU	2.2
1	B	18	ILE	2.2
1	B	399	MET	2.1
1	C	91	LEU	2.1
1	B	369	SER	2.1
1	A	19	GLY	2.1
1	B	15	LYS	2.1
1	B	221	GLY	2.1
1	B	281	THR	2.1
1	C	93	SER	2.0
1	B	403	THR	2.0
1	A	313	GLY	2.0
1	A	230	LYS	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](#)

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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
-----	------	-------	-----	-------	------	-----	-----------------------------	-------

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ASP	B	501	9/9	0.76	0.32	158,168,194,204	0
2	ASP	A	501	9/9	0.83	0.41	104,121,156,156	0
3	NA	B	503	1/1	0.88	0.15	151,151,151,151	0
3	NA	A	503	1/1	0.90	0.20	76,76,76,76	0
2	ASP	C	501	9/9	0.94	0.10	158,162,170,188	0
3	NA	A	502	1/1	0.94	0.48	123,123,123,123	0
3	NA	B	502	1/1	0.95	0.44	152,152,152,152	0
3	NA	C	502	1/1	0.98	0.17	173,173,173,173	0
3	NA	C	503	1/1	0.98	0.17	162,162,162,162	0

6.5 Other polymers [i](#)

There are no such residues in this entry.