



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:40 PM UTC

PDB ID : 6WZB / pdb_00006wzb
Title : Crystal structure of the GltPh V216C-G388C mutant cross-linked with divalent mercury
Authors : Chen, I.; Font, J.; Ryan, R.
Deposited on : 2020-05-13
Resolution : 3.45 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

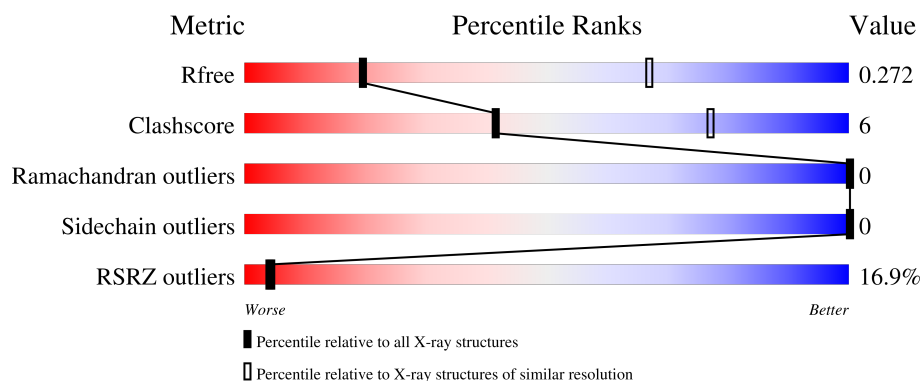
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	15% 83% 14% .
1	B	422	13% 81% 17% .
1	C	422	21% 81% 16% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9144 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	411	Total	C	N	O	S	0	0	0
			3034	2000	479	537	18			
1	B	411	Total	C	N	O	S	0	0	0
			3038	2002	480	538	18			
1	C	411	Total	C	N	O	S	0	0	0
			3036	2001	481	536	18			

There are 24 discrepancies between the modelled and reference sequences:

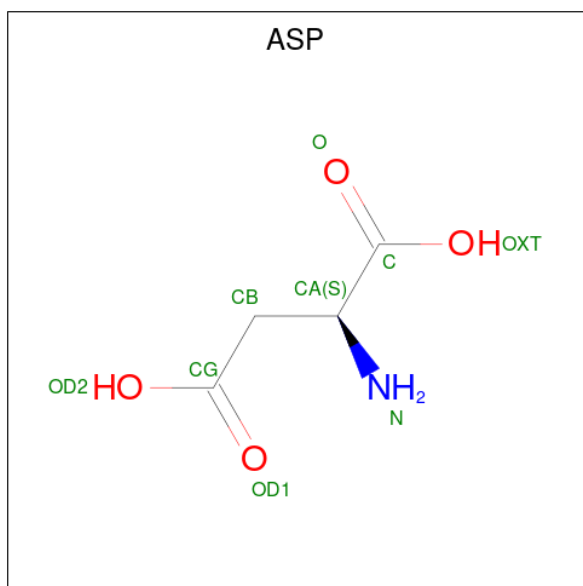
Chain	Residue	Modelled	Actual	Comment	Reference
A	216	CYS	VAL	engineered mutation	UNP O59010
A	321	SER	CYS	engineered mutation	UNP O59010
A	388	CYS	GLY	engineered mutation	UNP O59010
A	418	THR	-	expression tag	UNP O59010
A	419	LEU	-	expression tag	UNP O59010
A	420	VAL	-	expression tag	UNP O59010
A	421	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	388	CYS	GLY	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	388	CYS	GLY	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		

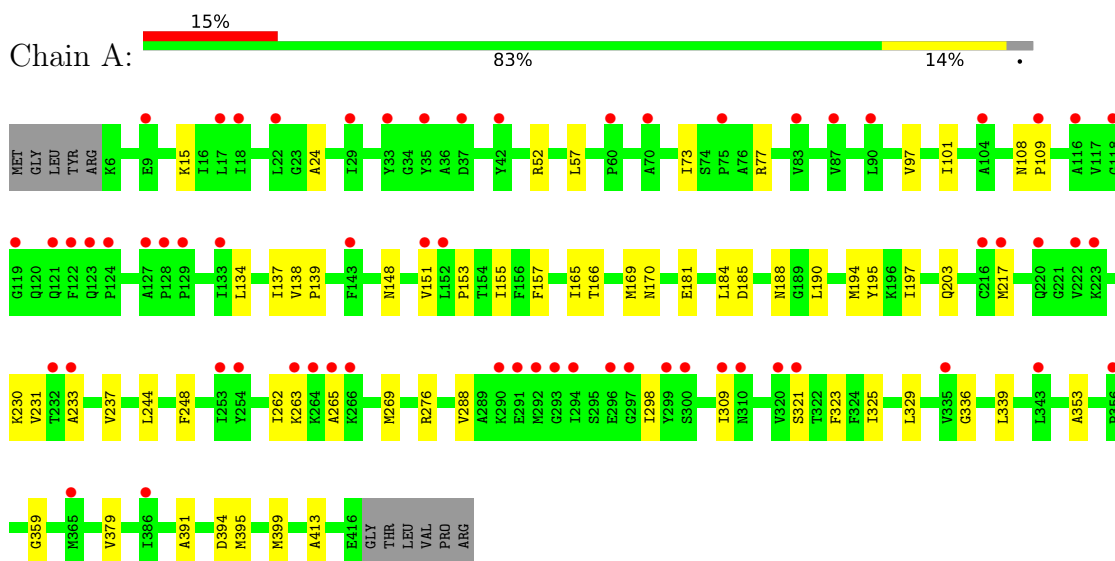
- Molecule 4 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Hg 1	0	0
4	B	1	Total 1	Hg 1	0	0
4	C	1	Total 1	Hg 1	0	0

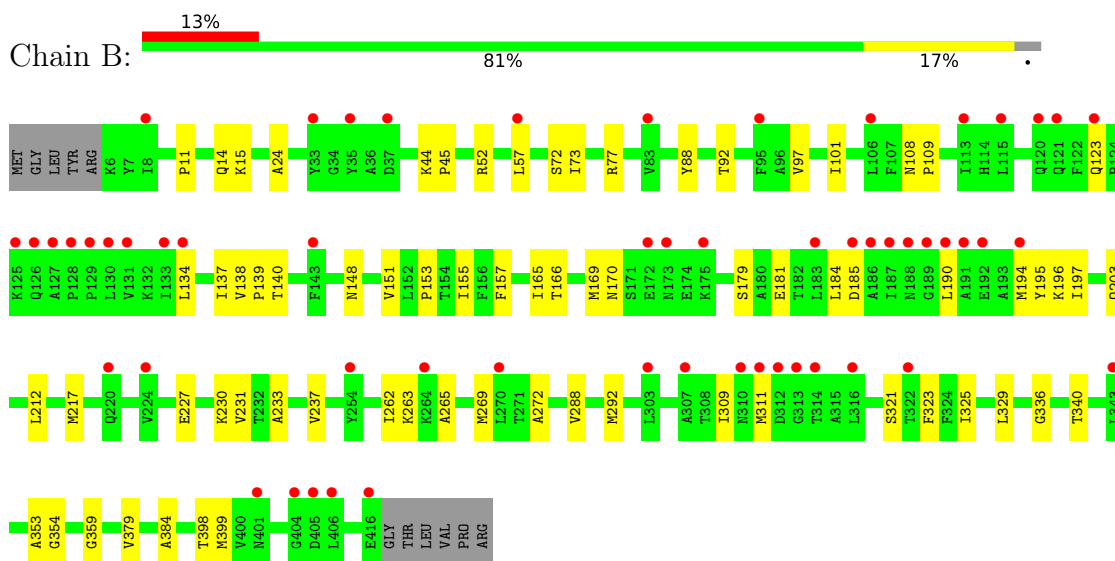
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

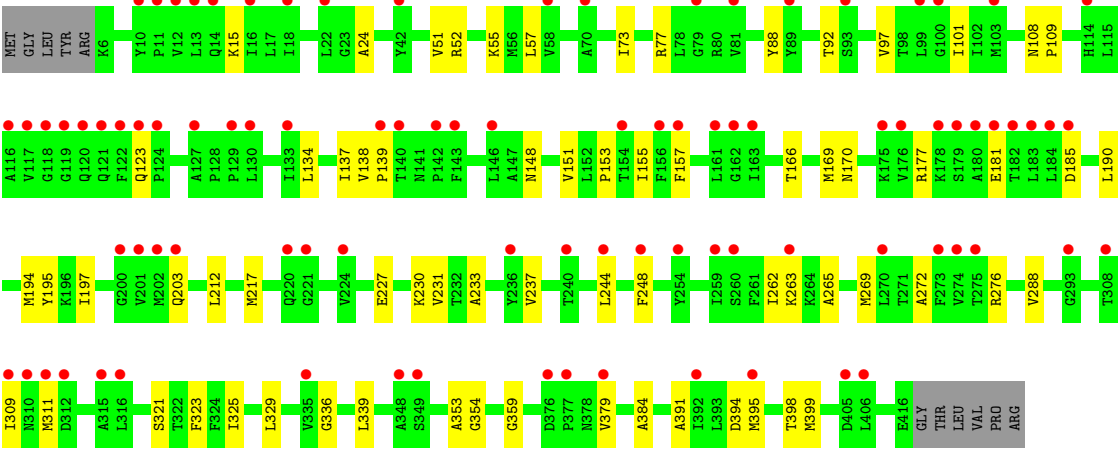
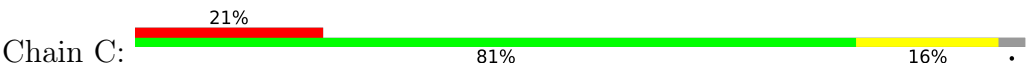
- Molecule 1: Glutamate transporter homolog



- Molecule 1: Glutamate transporter homolog



- Molecule 1: Glutamate transporter homolog



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	112.11Å 204.57Å 207.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.31 – 3.45 49.31 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.31-3.45) 99.9 (49.31-3.45)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.233 , 0.268 0.238 , 0.272	Depositor DCC
R_{free} test set	1555 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	113.1	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.005 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.025 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9144	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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, HG

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	0/3087	0.37	0/4205
1	B	0.14	0/3091	0.37	0/4210
1	C	0.15	0/3089	0.38	0/4207
All	All	0.14	0/9267	0.37	0/12622

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 [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	3034	0	3233	39	0
1	B	3038	0	3239	46	0
1	C	3036	0	3238	43	0
2	A	9	0	3	1	0
2	B	9	0	3	1	0
2	C	9	0	3	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
All	All	9144	0	9719	120	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 6.

All (120) 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:262:ILE:HG23	1:A:269:MET:HE1	1.76	0.68
1:C:262:ILE:HG23	1:C:269:MET:HE1	1.75	0.67
1:B:262:ILE:HG23	1:B:269:MET:HE1	1.76	0.67
1:B:166:THR:HA	1:B:169:MET:HE2	1.77	0.67
1:B:329:LEU:HD21	1:B:379:VAL:HG22	1.78	0.65
1:B:194:MET:HA	1:B:197:ILE:HD12	1.79	0.65
1:A:194:MET:HA	1:A:197:ILE:HD12	1.79	0.64
1:A:329:LEU:HD21	1:A:379:VAL:HG22	1.79	0.64
1:C:194:MET:HA	1:C:197:ILE:HD12	1.79	0.64
1:C:329:LEU:HD21	1:C:379:VAL:HG22	1.82	0.61
1:C:166:THR:HA	1:C:169:MET:HE2	1.83	0.60
1:A:166:THR:HA	1:A:169:MET:HE2	1.84	0.59
1:C:148:ASN:O	1:C:148:ASN:ND2	2.37	0.57
1:A:148:ASN:O	1:A:148:ASN:ND2	2.37	0.57
1:A:109:PRO:HB2	1:A:231:VAL:HG22	1.87	0.57
1:C:109:PRO:HB2	1:C:231:VAL:HG22	1.87	0.56
1:B:109:PRO:HB2	1:B:231:VAL:HG22	1.86	0.56
1:B:148:ASN:ND2	1:B:148:ASN:O	2.39	0.56
1:B:15:LYS:NZ	1:B:203:GLN:OE1	2.41	0.53
1:C:77:ARG:NH2	1:C:170:ASN:OD1	2.41	0.53
1:A:359:GLY:N	2:A:501:ASP:OD2	2.40	0.53
1:B:359:GLY:N	2:B:501:ASP:OD1	2.40	0.52
1:A:151:VAL:O	1:A:155:ILE:HG12	2.09	0.52
1:C:151:VAL:O	1:C:155:ILE:HG12	2.10	0.52
1:C:73:ILE:HD11	1:C:309:ILE:HD13	1.92	0.52
1:A:73:ILE:HD11	1:A:309:ILE:HD13	1.93	0.51
1:C:15:LYS:NZ	1:C:203:GLN:OE1	2.43	0.51
1:A:138:VAL:O	1:C:52:ARG:NH2	2.43	0.51
1:B:195:TYR:CE2	1:B:353:ALA:HB2	2.46	0.51
1:A:134:LEU:O	1:A:137:ILE:HG12	2.11	0.51
1:C:195:TYR:CE2	1:C:353:ALA:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LYS:NZ	1:A:203:GLN:OE1	2.44	0.50
1:A:195:TYR:CE2	1:A:353:ALA:HB2	2.47	0.49
1:B:195:TYR:CZ	1:B:353:ALA:HB2	2.47	0.49
1:A:24:ALA:HA	1:A:217:MET:HG3	1.94	0.49
1:B:134:LEU:O	1:B:137:ILE:HG12	2.12	0.49
1:B:265:ALA:HA	1:B:288:VAL:HG11	1.94	0.49
1:A:195:TYR:CZ	1:A:353:ALA:HB2	2.48	0.49
1:C:97:VAL:O	1:C:101:ILE:HG12	2.13	0.49
1:A:194:MET:HE1	1:B:157:PHE:HE1	1.78	0.48
1:A:52:ARG:NH2	1:B:138:VAL:O	2.45	0.48
1:B:24:ALA:HA	1:B:217:MET:HG3	1.94	0.48
1:C:134:LEU:O	1:C:137:ILE:HG12	2.12	0.48
1:C:265:ALA:HA	1:C:288:VAL:HG11	1.96	0.48
1:C:195:TYR:CZ	1:C:353:ALA:HB2	2.49	0.48
1:A:190:LEU:O	1:A:194:MET:HG2	2.14	0.48
1:B:97:VAL:O	1:B:101:ILE:HG12	2.14	0.48
1:B:52:ARG:NH2	1:C:138:VAL:O	2.47	0.48
1:B:190:LEU:O	1:B:194:MET:HG2	2.14	0.48
1:A:97:VAL:O	1:A:101:ILE:HG12	2.13	0.47
1:A:181:GLU:O	1:A:185:ASP:HB2	2.14	0.47
1:A:233:ALA:O	1:A:237:VAL:HG22	2.15	0.47
1:B:151:VAL:O	1:B:155:ILE:HG12	2.15	0.47
1:C:24:ALA:HA	1:C:217:MET:HG3	1.96	0.47
1:B:194:MET:HE1	1:C:157:PHE:HE1	1.78	0.47
1:C:57:LEU:HD22	1:C:194:MET:HE3	1.97	0.46
1:C:181:GLU:O	1:C:185:ASP:HB2	2.15	0.46
1:C:212:LEU:HD22	1:C:384:ALA:HB1	1.98	0.46
1:C:233:ALA:O	1:C:237:VAL:HG22	2.16	0.45
1:A:269:MET:HB3	1:A:399:MET:HE3	1.96	0.45
1:B:77:ARG:NH2	1:B:170:ASN:OD1	2.49	0.45
1:B:108:ASN:H	1:B:230:LYS:HZ1	1.64	0.45
1:C:359:GLY:N	2:C:501:ASP:OD2	2.46	0.45
1:A:165:ILE:HG21	1:A:184:LEU:HB2	1.98	0.45
1:B:263:LYS:HA	1:B:263:LYS:HD2	1.77	0.45
1:C:321:SER:O	1:C:325:ILE:HG12	2.17	0.45
1:B:165:ILE:HG21	1:B:184:LEU:HB2	2.00	0.44
1:B:311:MET:HE1	1:B:354:GLY:N	2.31	0.44
1:A:157:PHE:HE1	1:C:194:MET:HE1	1.81	0.44
1:A:139:PRO:HB3	1:A:153:PRO:HB3	2.00	0.44
1:B:73:ILE:HD11	1:B:309:ILE:HD13	1.99	0.44
1:B:139:PRO:HB3	1:B:153:PRO:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ALA:O	1:B:237:VAL:HG22	2.18	0.44
1:C:272:ALA:HB1	1:C:398:THR:HG22	2.00	0.44
1:A:77:ARG:NH2	1:A:170:ASN:OD1	2.48	0.44
1:A:263:LYS:HA	1:A:263:LYS:HD2	1.75	0.44
1:A:276:ARG:HB3	1:A:394:ASP:OD2	2.17	0.44
1:B:272:ALA:HB1	1:B:398:THR:HG22	1.99	0.44
1:A:57:LEU:HD22	1:A:194:MET:HE3	1.99	0.43
1:C:101:ILE:HD12	1:C:323:PHE:HE1	1.83	0.43
1:C:88:TYR:CZ	1:C:92:THR:HG21	2.53	0.43
1:B:181:GLU:O	1:B:185:ASP:HB2	2.19	0.43
1:C:276:ARG:HB3	1:C:394:ASP:OD2	2.19	0.43
1:B:227:GLU:O	1:B:231:VAL:HG23	2.19	0.43
1:C:263:LYS:HA	1:C:263:LYS:HD2	1.78	0.43
1:A:101:ILE:HD12	1:A:323:PHE:HE1	1.84	0.42
1:A:244:LEU:O	1:A:248:PHE:HB2	2.19	0.42
1:A:321:SER:O	1:A:325:ILE:HG12	2.19	0.42
1:A:265:ALA:HA	1:A:288:VAL:HG11	2.00	0.42
1:A:188:ASN:O	1:B:179:SER:HB3	2.19	0.42
1:A:336:GLY:HA2	1:A:339:LEU:HG	2.01	0.42
1:B:57:LEU:HD22	1:B:194:MET:HE3	2.02	0.42
1:A:108:ASN:H	1:A:230:LYS:HZ1	1.68	0.42
1:C:108:ASN:H	1:C:230:LYS:HZ1	1.67	0.42
1:A:52:ARG:HH21	1:B:140:THR:HG23	1.85	0.42
1:C:190:LEU:O	1:C:194:MET:HG2	2.20	0.42
1:C:336:GLY:HA2	1:C:339:LEU:HG	2.01	0.42
1:B:288:VAL:O	1:B:292:MET:HG2	2.20	0.41
1:C:51:VAL:O	1:C:55:LYS:HG2	2.20	0.41
1:C:123:GLN:O	1:C:123:GLN:HG3	2.20	0.41
1:C:227:GLU:O	1:C:231:VAL:HG23	2.20	0.41
1:C:391:ALA:O	1:C:395:MET:HG3	2.20	0.41
1:A:298:ILE:HD13	1:A:413:ALA:HA	2.02	0.41
1:B:321:SER:O	1:B:325:ILE:HG12	2.19	0.41
1:B:88:TYR:CZ	1:B:92:THR:HG21	2.55	0.41
1:C:169:MET:HA	1:C:177:ARG:HG2	2.03	0.41
1:C:244:LEU:O	1:C:248:PHE:HB2	2.21	0.41
1:C:139:PRO:HB3	1:C:153:PRO:HB3	2.02	0.41
1:C:269:MET:HB3	1:C:399:MET:HE3	2.02	0.41
1:B:72:SER:OG	1:B:309:ILE:HD11	2.21	0.41
1:B:11:PRO:HG2	1:B:14:GLN:HB2	2.03	0.40
1:A:391:ALA:O	1:A:395:MET:HG3	2.22	0.40
1:B:196:LYS:HA	1:B:196:LYS:HD2	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ILE:HD12	1:B:323:PHE:HE1	1.86	0.40
1:B:44:LYS:N	1:B:45:PRO:HD2	2.36	0.40
1:C:311:MET:HE1	1:C:354:GLY:N	2.36	0.40
1:B:123:GLN:HG3	1:B:123:GLN:O	2.22	0.40
1:B:212:LEU:HD22	1:B:384:ALA:HB1	2.04	0.40
1:B:269:MET:HB3	1:B:399:MET:HE3	2.03	0.40
1:B:336:GLY:O	1:B:340:THR:OG1	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	409/422 (97%)	395 (97%)	14 (3%)	0	100	100
1	B	409/422 (97%)	396 (97%)	13 (3%)	0	100	100
1	C	409/422 (97%)	395 (97%)	14 (3%)	0	100	100
All	All	1227/1266 (97%)	1186 (97%)	41 (3%)	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	320/331 (97%)	320 (100%)	0	100	100
1	B	321/331 (97%)	321 (100%)	0	100	100
1	C	320/331 (97%)	320 (100%)	0	100	100
All	All	961/993 (97%)	961 (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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	ASN
1	A	337	GLN
1	B	148	ASN
1	B	150	GLN
1	B	199	ASN
1	B	310	ASN
1	B	337	GLN
1	C	148	ASN
1	C	150	GLN
1	C	310	ASN
1	C	337	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 [i](#)

Of 12 ligands modelled in this entry, 9 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	C	501	-	7,8,8	1.16	1 (14%)	6,10,10	1.31	1 (16%)
2	ASP	B	501	-	7,8,8	1.15	1 (14%)	6,10,10	1.25	1 (16%)
2	ASP	A	501	-	7,8,8	1.16	1 (14%)	6,10,10	1.37	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	C	501	-	-	2/8/8/8	-
2	ASP	B	501	-	-	2/8/8/8	-
2	ASP	A	501	-	-	2/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	ASP	OXT-C	-2.30	1.23	1.30
2	C	501	ASP	OXT-C	-2.29	1.23	1.30
2	B	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	A	501	ASP	OXT-C-O	-2.57	118.25	124.08
2	C	501	ASP	OXT-C-O	-2.37	118.70	124.08
2	B	501	ASP	OXT-C-O	-2.28	118.92	124.08

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	ASP	CA-CB-CG-OD1
2	B	501	ASP	CA-CB-CG-OD2

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Mol	Chain	Res	Type	Atoms
2	A	501	ASP	CA-CB-CG-OD1
2	C	501	ASP	CA-CB-CG-OD1
2	C	501	ASP	CA-CB-CG-OD2
2	A	501	ASP	CA-CB-CG-OD2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	ASP	1	0
2	B	501	ASP	1	0
2	A	501	ASP	1	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	411/422 (97%)	0.67	62 (15%) 5 5	69, 107, 151, 204	0
1	B	411/422 (97%)	0.71	56 (13%) 7 6	69, 99, 148, 198	0
1	C	411/422 (97%)	1.04	90 (21%) 2 3	74, 112, 159, 208	0
All	All	1233/1266 (97%)	0.81	208 (16%) 4 4	69, 107, 156, 208	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	128	PRO	9.9
1	C	179	SER	9.5
1	C	119	GLY	9.0
1	B	127	ALA	8.1
1	C	181	GLU	7.7
1	C	118	GLY	7.6
1	C	259	ILE	7.4
1	B	120	GLN	7.2
1	B	130	LEU	7.2
1	A	124	PRO	6.9
1	C	180	ALA	6.9
1	B	185	ASP	6.6
1	C	70	ALA	6.6
1	B	126	GLN	6.5
1	C	143	PHE	6.4
1	A	119	GLY	6.2
1	C	310	ASN	6.0
1	B	190	LEU	5.9
1	A	300	SER	5.8
1	C	14	GLN	5.7
1	C	203	GLN	5.7
1	A	118	GLY	5.7
1	C	120	GLN	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	157	PHE	5.4
1	B	106	LEU	5.4
1	B	189	GLY	5.4
1	B	192	GLU	5.4
1	C	273	PHE	5.2
1	A	121	GLN	5.2
1	A	264	LYS	5.1
1	A	37	ASP	5.1
1	B	133	ILE	4.9
1	B	310	ASN	4.8
1	B	312	ASP	4.7
1	A	42	TYR	4.7
1	C	176	VAL	4.7
1	C	175	LYS	4.7
1	A	290	LYS	4.6
1	C	18	ILE	4.5
1	A	129	PRO	4.5
1	C	11	PRO	4.5
1	A	33	TYR	4.5
1	A	253	ILE	4.4
1	A	291	GLU	4.4
1	B	405	ASP	4.3
1	B	187	ILE	4.2
1	B	194	MET	4.2
1	B	33	TYR	4.2
1	A	122	PHE	4.2
1	A	222	VAL	4.1
1	C	142	PRO	4.1
1	B	143	PHE	4.0
1	C	183	LEU	4.0
1	C	263	LYS	4.0
1	C	309	ILE	4.0
1	C	312	ASP	3.9
1	A	263	LYS	3.9
1	B	121	GLN	3.9
1	B	129	PRO	3.8
1	A	127	ALA	3.8
1	C	178	LYS	3.8
1	A	133	ILE	3.8
1	A	232	THR	3.8
1	A	254	TYR	3.7
1	B	172	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	117	VAL	3.7
1	C	254	TYR	3.7
1	B	35	TYR	3.6
1	C	201	VAL	3.6
1	C	293	GLY	3.6
1	C	202	MET	3.6
1	C	130	LEU	3.6
1	A	297	GLY	3.5
1	C	13	LEU	3.5
1	C	244	LEU	3.5
1	A	296	GLU	3.5
1	A	151	VAL	3.5
1	C	12	VAL	3.5
1	A	35	TYR	3.5
1	C	123	GLN	3.5
1	B	134	LEU	3.4
1	C	184	LEU	3.4
1	C	116	ALA	3.4
1	A	75	PRO	3.4
1	C	162	GLY	3.4
1	B	188	ASN	3.3
1	A	143	PHE	3.3
1	C	121	GLN	3.3
1	A	266	LYS	3.3
1	B	123	GLN	3.3
1	C	146	LEU	3.3
1	C	248	PHE	3.2
1	B	95	PHE	3.2
1	C	79	GLY	3.2
1	B	83	VAL	3.1
1	C	376	ASP	3.1
1	C	129	PRO	3.1
1	C	163	ILE	3.1
1	C	316	LEU	3.1
1	B	404	GLY	3.1
1	A	292	MET	3.1
1	C	349	SER	3.0
1	C	16	ILE	3.0
1	A	70	ALA	3.0
1	C	10	TYR	3.0
1	B	343	LEU	3.0
1	B	311	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	109	PRO	3.0
1	B	186	ALA	2.9
1	C	100	GLY	2.9
1	C	133	ILE	2.9
1	A	116	ALA	2.9
1	C	236	TYR	2.9
1	A	128	PRO	2.9
1	A	9	GLU	2.9
1	C	114	HIS	2.8
1	C	224	VAL	2.8
1	C	103	MET	2.8
1	B	175	LYS	2.8
1	C	156	PHE	2.8
1	C	308	THR	2.8
1	A	310	ASN	2.8
1	C	99	LEU	2.8
1	B	220	GLN	2.8
1	B	401	ASN	2.7
1	B	37	ASP	2.7
1	A	217	MET	2.7
1	A	293	GLY	2.7
1	C	406	LEU	2.7
1	A	18	ILE	2.6
1	C	221	GLY	2.6
1	C	274	VAL	2.6
1	B	131	VAL	2.6
1	C	81	VAL	2.6
1	C	260	SER	2.6
1	A	365	MET	2.6
1	C	240	THR	2.6
1	A	299	TYR	2.6
1	C	220	GLN	2.6
1	C	270	LEU	2.6
1	A	83	VAL	2.6
1	C	127	ALA	2.6
1	B	115	LEU	2.5
1	B	173	ASN	2.5
1	A	29	ILE	2.5
1	C	392	ILE	2.5
1	A	17	LEU	2.5
1	C	395	MET	2.5
1	B	57	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	220	GLN	2.5
1	B	224	VAL	2.5
1	A	265	ALA	2.5
1	C	122	PHE	2.5
1	B	406	LEU	2.5
1	A	386	ILE	2.5
1	C	58	VAL	2.5
1	C	335	VAL	2.5
1	C	405	ASP	2.4
1	C	379	VAL	2.4
1	A	233	ALA	2.4
1	C	185	ASP	2.4
1	A	60	PRO	2.4
1	A	216	CYS	2.4
1	B	183	LEU	2.4
1	B	8	ILE	2.4
1	A	152	LEU	2.4
1	B	307	ALA	2.4
1	A	320	VAL	2.4
1	C	200	GLY	2.3
1	C	89	TYR	2.3
1	A	87	VAL	2.3
1	B	322	THR	2.3
1	C	140	THR	2.3
1	C	311	MET	2.3
1	C	348	ALA	2.3
1	B	303	LEU	2.3
1	B	191	ALA	2.3
1	C	182	THR	2.3
1	C	42	TYR	2.3
1	C	154	THR	2.3
1	C	93	SER	2.3
1	B	313	GLY	2.2
1	C	124	PRO	2.2
1	A	90	LEU	2.2
1	C	377	PRO	2.2
1	A	321	SER	2.2
1	A	343	LEU	2.2
1	B	416	GLU	2.2
1	A	356	PRO	2.2
1	B	314	THR	2.2
1	A	123	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	113	ILE	2.2
1	B	125	LYS	2.2
1	C	315	ALA	2.2
1	C	161	LEU	2.1
1	B	264	LYS	2.1
1	A	104	ALA	2.1
1	C	139	PRO	2.1
1	C	22	LEU	2.1
1	A	294	ILE	2.1
1	B	316	LEU	2.1
1	A	223	LYS	2.0
1	A	22	LEU	2.0
1	B	270	LEU	2.0
1	A	309	ILE	2.0
1	B	254	TYR	2.0
1	C	275	THR	2.0
1	A	335	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
3	NA	C	503	1/1	0.81	0.35	113,113,113,113	0
2	ASP	C	501	9/9	0.84	0.11	109,115,122,122	0
2	ASP	B	501	9/9	0.84	0.13	85,100,104,104	0
3	NA	B	503	1/1	0.85	0.33	76,76,76,76	0
3	NA	A	503	1/1	0.86	0.33	126,126,126,126	0
2	ASP	A	501	9/9	0.91	0.08	89,100,102,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	B	502	1/1	0.96	0.07	84,84,84,84	0
3	NA	C	502	1/1	0.97	0.11	100,100,100,100	0
3	NA	A	502	1/1	0.97	0.08	101,101,101,101	0
4	HG	A	504	1/1	0.97	0.08	184,184,184,184	0
4	HG	B	504	1/1	0.98	0.04	185,185,185,185	0
4	HG	C	504	1/1	0.98	0.04	200,200,200,200	0

6.5 Other polymers [i](#)

There are no such residues in this entry.