



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 05:13 AM GMT

PDB ID : 3D6K
Title : The crystal structure of a putative aminotransferase from *Corynebacterium diphtheriae*
Authors : Tan, K.; Zhang, R.; Duggan, E.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2008-05-19
Resolution : 2.00 Å(reported)

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

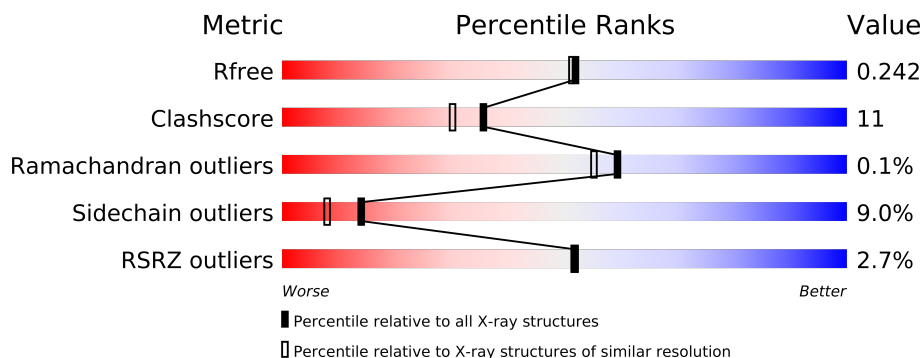
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	422	
1	B	422	
1	C	422	
1	D	422	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	EDO	C	422	-	X
4	EDO	D	422	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13332 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	Se	0	0	0
			3118	1983	527	594	4	10			
1	B	409	Total	C	N	O	S	Se	0	0	0
			3147	2002	532	599	4	10			
1	C	413	Total	C	N	O	S	Se	0	0	0
			3176	2018	539	605	4	10			
1	D	412	Total	C	N	O	S	Se	0	0	0
			3168	2014	538	602	4	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q6NJY4
A	-1	ASN	-	expression tag	UNP Q6NJY4
A	0	ALA	-	expression tag	UNP Q6NJY4
B	-2	SER	-	expression tag	UNP Q6NJY4
B	-1	ASN	-	expression tag	UNP Q6NJY4
B	0	ALA	-	expression tag	UNP Q6NJY4
C	-2	SER	-	expression tag	UNP Q6NJY4
C	-1	ASN	-	expression tag	UNP Q6NJY4
C	0	ALA	-	expression tag	UNP Q6NJY4
D	-2	SER	-	expression tag	UNP Q6NJY4
D	-1	ASN	-	expression tag	UNP Q6NJY4
D	0	ALA	-	expression tag	UNP Q6NJY4

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is water.

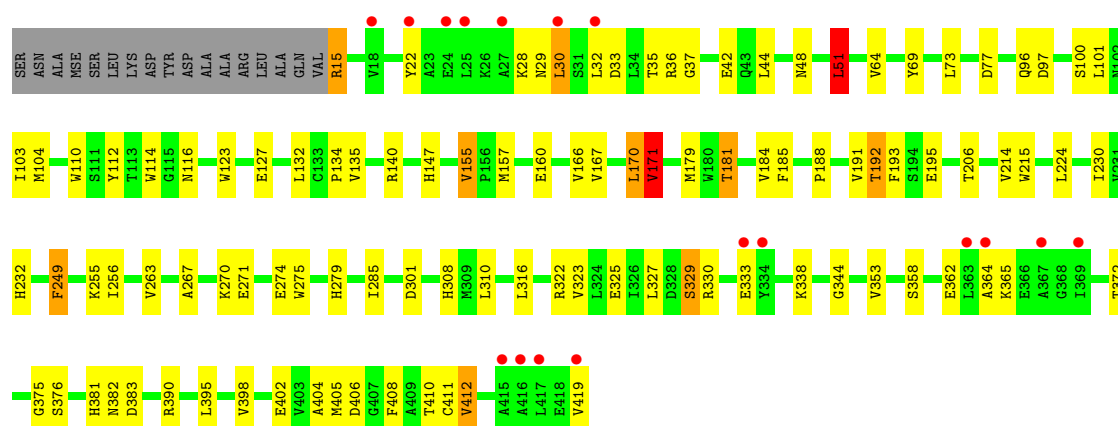
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	211	Total	O	0	0
			211	211		
5	B	182	Total	O	0	0
			182	182		
5	C	164	Total	O	0	0
			164	164		
5	D	126	Total	O	0	0
			126	126		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

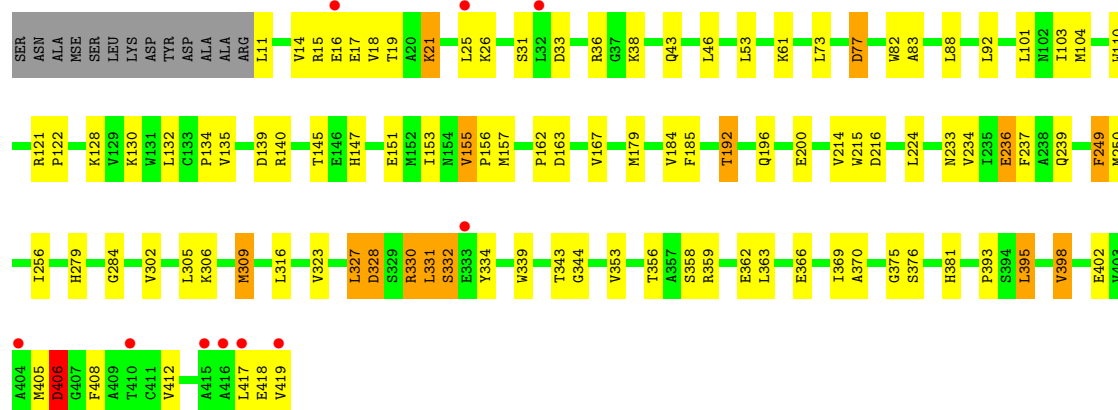
• Molecule 1: Putative aminotransferase

Chain A:



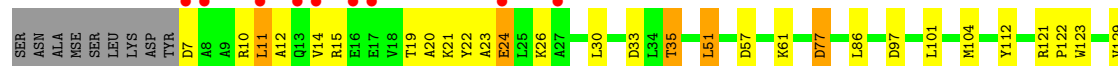
• Molecule 1: Putative aminotransferase

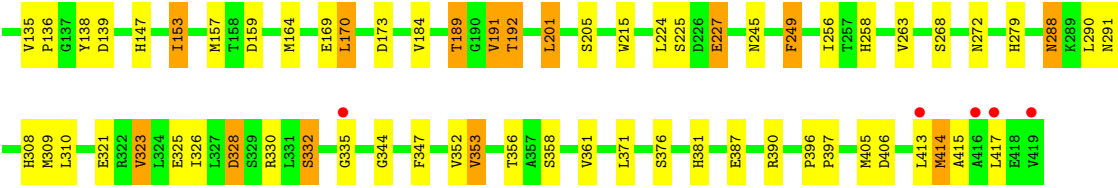
Chain B:



• Molecule 1: Putative aminotransferase

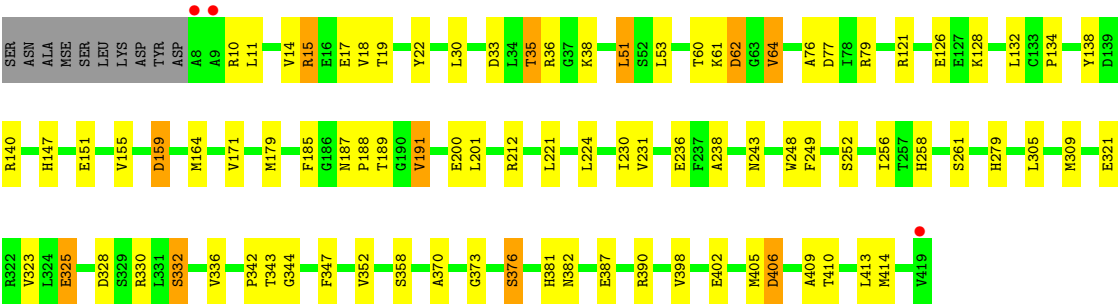
Chain C:





● Molecule 1: Putative aminotransferase

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.25Å 56.08Å 173.59Å 90.00° 102.47° 90.00°	Depositor
Resolution (Å)	42.68 – 2.00 42.68 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.4 (42.68-2.00) 90.4 (42.68-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.241 0.192 , 0.242	Depositor DCC
R_{free} test set	5228 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.1	EDS
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 103049 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13332	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: CL, EDO, SO4

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	0.67	0/3188	0.76	3/4322 (0.1%)
1	B	0.79	4/3217 (0.1%)	0.76	0/4362
1	C	0.76	3/3246 (0.1%)	0.74	4/4401 (0.1%)
1	D	0.64	0/3238	0.70	0/4390
All	All	0.72	7/12889 (0.1%)	0.74	7/17475 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	406	ASP	C-N	7.62	1.46	1.33
1	C	415	ALA	C-O	5.92	1.34	1.23
1	C	24	GLU	CD-OE2	5.56	1.31	1.25
1	B	16	GLU	C-O	5.40	1.33	1.23
1	B	16	GLU	CD-OE1	5.26	1.31	1.25
1	B	21	LYS	CE-NZ	5.17	1.61	1.49
1	C	328	ASP	CG-OD1	5.06	1.36	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	VAL	CG1-CB-CG2	5.97	120.45	110.90
1	C	22	TYR	O-C-N	5.21	131.03	122.70
1	C	328	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	383	ASP	CB-CG-OD1	5.06	122.86	118.30
1	C	173	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	51	LEU	CA-CB-CG	5.03	126.88	115.30
1	C	328	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3118	0	3026	59	0
1	B	3147	0	3059	89	0
1	C	3176	0	3086	59	0
1	D	3168	0	3082	66	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	4	0	6	1	0
4	D	4	0	6	1	0
5	A	211	0	0	3	0
5	B	182	0	0	5	0
5	C	164	0	0	1	0
5	D	126	0	0	0	0
All	All	13332	0	12277	262	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (262) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:104:MSE:HE2	1:B:214:VAL:CG1	1.50	1.39
1:B:104:MSE:HE3	1:B:250:MSE:HG3	1.21	1.18
1:A:15:ARG:HB3	1:A:15:ARG:NH2	1.59	1.15
1:B:104:MSE:HE2	1:B:214:VAL:HG11	1.16	1.12
1:D:22:TYR:HB2	1:D:414:MSE:HE3	1.30	1.12
1:D:256:ILE:HG23	1:D:309:MSE:HE1	1.23	1.09
1:B:104:MSE:HE1	1:B:216:ASP:HB2	1.17	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:33:ASP:HB3	1:B:370:ALA:HB3	1.37	1.07
5:B:511:HOH:O	1:D:382:ASN:HB2	1.61	0.99
1:B:104:MSE:CE	1:B:214:VAL:CG1	2.40	0.99
1:B:185:PHE:H	1:B:192:THR:HG22	1.29	0.97
1:B:309:MSE:HE2	1:B:309:MSE:HA	1.45	0.96
1:D:33:ASP:HB3	1:D:370:ALA:HB3	1.45	0.96
1:D:22:TYR:CB	1:D:414:MSE:HE3	1.96	0.96
1:B:134:PRO:HB3	1:B:157:MSE:HE3	1.45	0.96
1:B:33:ASP:CB	1:B:370:ALA:HB3	1.96	0.95
1:D:11:LEU:O	1:D:15:ARG:HG2	1.68	0.93
1:C:189:THR:HG23	1:C:191:VAL:HG13	1.51	0.93
1:C:256:ILE:HG23	1:C:309:MSE:HE1	1.51	0.92
1:A:184:VAL:HA	1:A:192:THR:HB	1.54	0.89
1:C:256:ILE:HG23	1:C:309:MSE:CE	2.03	0.88
1:C:11:LEU:O	1:C:14:VAL:HG12	1.71	0.88
1:A:147:HIS:NE2	1:B:279:HIS:HD2	1.72	0.87
1:A:15:ARG:HH21	1:A:15:ARG:HB3	1.40	0.87
1:C:326:ILE:O	1:C:330:ARG:HB3	1.74	0.86
1:B:104:MSE:HE1	1:B:216:ASP:CB	2.05	0.86
1:C:279:HIS:HD2	1:D:147:HIS:NE2	1.74	0.85
1:B:104:MSE:HE3	1:B:250:MSE:CG	2.06	0.85
1:B:157:MSE:CE	1:B:162:PRO:HA	2.07	0.84
1:B:104:MSE:HE2	1:B:214:VAL:HG12	1.58	0.83
1:B:104:MSE:CE	1:B:216:ASP:HB2	2.07	0.83
1:D:256:ILE:HG23	1:D:309:MSE:CE	2.07	0.83
1:C:330:ARG:NH1	1:C:406:ASP:OD2	2.11	0.82
1:D:22:TYR:HB2	1:D:414:MSE:CE	2.10	0.81
1:D:330:ARG:HG2	1:D:409:ALA:CB	2.11	0.81
1:A:33:ASP:OD1	1:A:35:THR:HB	1.79	0.81
1:A:279:HIS:HD2	1:B:147:HIS:NE2	1.79	0.80
1:B:132:LEU:HB2	1:B:179:MSE:HG3	1.66	0.78
1:D:33:ASP:CB	1:D:370:ALA:HB3	2.14	0.77
1:C:33:ASP:OD1	1:C:35:THR:HB	1.83	0.77
1:B:104:MSE:CE	1:B:250:MSE:HG3	2.10	0.76
1:B:157:MSE:HE2	1:B:162:PRO:HA	1.67	0.76
1:C:153:ILE:HD11	1:C:170:LEU:HD21	1.69	0.75
1:A:15:ARG:CZ	1:A:15:ARG:HB3	2.17	0.75
1:B:157:MSE:HE1	1:B:162:PRO:CA	2.16	0.75
1:B:309:MSE:CE	1:B:309:MSE:HA	2.16	0.74
1:D:347:PHE:CD1	1:D:390:ARG:HD3	2.23	0.74
1:B:406:ASP:HB2	5:B:489:HOH:O	1.88	0.73
1:B:353:VAL:O	1:B:356:THR:HB	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:15:ARG:CB	1:A:15:ARG:NH2	2.45	0.73
1:A:15:ARG:CZ	1:A:15:ARG:CB	2.66	0.73
1:B:359:ARG:NH2	1:B:362:GLU:OE1	2.23	0.72
1:C:184:VAL:HA	1:C:192:THR:HB	1.70	0.72
1:D:330:ARG:HG2	1:D:409:ALA:HB1	1.70	0.72
1:B:157:MSE:HE2	1:B:157:MSE:HA	1.71	0.72
1:D:321:GLU:O	1:D:325:GLU:HG2	1.90	0.71
1:C:157:MSE:HE3	1:C:189:THR:HG21	1.74	0.69
1:C:147:HIS:NE2	1:D:279:HIS:HD2	1.90	0.69
1:B:104:MSE:CE	1:B:214:VAL:HG12	2.19	0.67
1:A:147:HIS:NE2	1:B:279:HIS:CD2	2.60	0.67
1:B:184:VAL:HA	1:B:192:THR:HB	1.77	0.66
1:C:330:ARG:HG3	1:C:330:ARG:O	1.97	0.65
1:B:134:PRO:HB3	1:B:157:MSE:CE	2.23	0.65
1:D:159:ASP:OD2	1:D:159:ASP:N	2.29	0.65
1:A:28:LYS:HB3	1:A:30:LEU:HD13	1.79	0.64
1:B:17:GLU:O	1:B:21:LYS:HB2	1.97	0.64
1:B:139:ASP:HB3	1:B:376:SER:O	1.98	0.64
1:D:330:ARG:CG	1:D:409:ALA:HB1	2.28	0.63
1:A:181:THR:HG22	1:A:215:TRP:HA	1.81	0.63
1:D:330:ARG:HH12	1:D:406:ASP:HA	1.62	0.63
1:A:255:LYS:HE2	5:B:555:HOH:O	1.97	0.63
1:A:322:ARG:HD3	1:A:402:GLU:OE2	1.98	0.62
1:B:104:MSE:CE	1:B:214:VAL:HG11	2.10	0.62
1:C:279:HIS:CD2	1:D:147:HIS:NE2	2.63	0.62
1:D:238:ALA:HB1	1:D:243:ASN:O	1.99	0.62
1:A:192:THR:HG23	5:A:581:HOH:O	1.98	0.62
1:D:230:ILE:HD12	1:D:231:VAL:N	2.14	0.62
1:D:330:ARG:HH12	1:D:406:ASP:CA	2.12	0.62
1:D:330:ARG:NH2	1:D:410:THR:OG1	2.33	0.62
1:D:230:ILE:HD12	1:D:231:VAL:H	1.66	0.61
1:C:15:ARG:HD2	1:C:417:LEU:HD22	1.82	0.61
1:D:19:THR:HA	1:D:414:MSE:HE1	1.83	0.61
1:C:347:PHE:CD1	1:C:390:ARG:HD3	2.35	0.61
1:B:331:LEU:HD21	1:B:412:VAL:HG11	1.83	0.60
1:A:166:VAL:HG12	1:A:170:LEU:HD22	1.82	0.60
1:A:69:TYR:HB2	1:B:38:LYS:HD2	1.83	0.60
1:A:112:TYR:HA	1:A:123:TRP:HB2	1.84	0.60
1:A:157:MSE:HE1	1:A:191:VAL:HG11	1.82	0.60
1:B:33:ASP:HB2	1:B:370:ALA:HB3	1.82	0.60
1:A:375:GLY:O	1:A:381:HIS:HA	2.02	0.59
1:A:37:GLY:O	1:A:255:LYS:NZ	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:271:GLU:HG3	5:A:588:HOH:O	2.02	0.59
1:A:181:THR:CG2	1:A:215:TRP:HA	2.33	0.59
1:C:12:ALA:O	1:C:15:ARG:HB2	2.03	0.59
1:C:164:MSE:HE1	1:C:201:LEU:HD13	1.84	0.58
1:B:192:THR:HG23	5:B:599:HOH:O	2.04	0.58
1:B:224:LEU:HG	1:B:344:GLY:HA2	1.86	0.58
1:A:270:LYS:O	1:A:274:GLU:HG3	2.03	0.58
1:C:224:LEU:HG	1:C:344:GLY:HA2	1.85	0.57
1:B:21:LYS:HE2	1:B:330:ARG:NH1	2.20	0.57
1:A:181:THR:HG22	1:A:214:VAL:O	2.04	0.57
1:D:212:ARG:HG3	1:D:248:TRP:CZ2	2.40	0.57
1:B:157:MSE:HE1	1:B:162:PRO:HA	1.79	0.57
1:D:330:ARG:HG2	1:D:409:ALA:HB3	1.86	0.57
1:A:185:PHE:H	1:A:192:THR:HG22	1.70	0.56
1:B:157:MSE:CE	1:B:162:PRO:CA	2.75	0.56
1:B:128:LYS:HD3	1:B:151:GLU:OE1	2.05	0.56
1:B:14:VAL:O	1:B:18:VAL:HG13	2.06	0.56
1:C:164:MSE:CE	1:C:201:LEU:HD13	2.36	0.56
1:C:328:ASP:O	1:C:332:SER:HB2	2.06	0.56
1:C:309:MSE:HE2	1:C:309:MSE:HA	1.89	0.55
1:C:189:THR:HG23	1:C:191:VAL:H	1.71	0.55
1:A:188:PRO:HB3	1:A:390:ARG:HG3	1.89	0.55
1:C:21:LYS:HD2	1:C:330:ARG:NH2	2.21	0.54
1:C:20:ALA:O	1:C:21:LYS:C	2.45	0.54
1:C:353:VAL:HG23	1:C:356:THR:OG1	2.08	0.54
1:B:121:ARG:HB2	1:B:122:PRO:HD2	1.90	0.54
1:D:132:LEU:HB2	1:D:179:MSE:HG3	1.90	0.54
1:D:330:ARG:NH1	1:D:406:ASP:HA	2.22	0.54
1:B:15:ARG:HG2	1:B:417:LEU:HD22	1.90	0.53
1:A:167:VAL:O	1:A:171:VAL:HB	2.09	0.53
1:B:323:VAL:HG22	1:B:405:MSE:HG3	1.91	0.53
1:D:61:LYS:HG3	1:D:62:ASP:OD1	2.10	0.52
1:B:323:VAL:HG21	1:B:393:PRO:HB3	1.92	0.52
1:D:35:THR:HG22	1:D:36:ARG:HG3	1.92	0.52
1:B:25:LEU:HD11	1:B:369:ILE:HD11	1.92	0.52
1:C:11:LEU:O	1:C:14:VAL:CG1	2.53	0.51
1:C:288:ASN:ND2	1:C:291:ASN:H	2.07	0.51
1:B:398:VAL:O	1:B:402:GLU:HG3	2.09	0.51
1:D:323:VAL:HG22	1:D:405:MSE:HG3	1.91	0.51
1:D:134:PRO:HA	1:D:155:VAL:O	2.09	0.51
1:B:104:MSE:HE2	1:B:214:VAL:HG13	1.74	0.51
1:D:18:VAL:O	1:D:414:MSE:HE1	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:414:MSE:HA	1:C:414:MSE:HE2	1.93	0.50
1:B:302:VAL:HG22	1:B:306:LYS:HD2	1.93	0.50
1:B:157:MSE:HE1	1:B:162:PRO:CG	2.41	0.50
1:B:302:VAL:HG12	5:B:545:HOH:O	2.11	0.50
1:A:101:LEU:HD23	1:B:284:GLY:HA2	1.93	0.50
1:A:325:GLU:O	1:A:329:SER:HB3	2.12	0.49
1:C:288:ASN:C	1:C:288:ASN:HD22	2.14	0.49
1:B:216:ASP:HA	1:B:250:MSE:HB2	1.93	0.49
1:A:48:ASN:HA	1:A:51:LEU:HD22	1.94	0.49
1:B:157:MSE:HE1	1:B:162:PRO:HG3	1.95	0.49
1:C:308:HIS:HD2	1:C:309:MSE:CE	2.26	0.49
1:A:181:THR:HG21	1:A:215:TRP:CE3	2.47	0.49
1:C:169:GLU:HA	1:C:169:GLU:OE1	2.13	0.49
1:A:256:ILE:O	1:A:308:HIS:HE1	1.96	0.49
1:C:215:TRP:HB3	1:C:249:PHE:HA	1.94	0.49
1:D:398:VAL:O	1:D:402:GLU:HG3	2.13	0.48
1:C:7:ASP:OD2	1:C:335:GLY:HA3	2.13	0.48
1:A:279:HIS:CD2	1:B:147:HIS:NE2	2.71	0.48
1:A:224:LEU:HG	1:A:344:GLY:HA2	1.94	0.48
1:D:342:PRO:HG3	1:D:347:PHE:O	2.14	0.48
1:C:376:SER:HA	1:C:381:HIS:CD2	2.49	0.48
1:C:101:LEU:HA	1:C:104:MSE:HE3	1.95	0.48
1:C:225:SER:OG	1:C:227:GLU:HG3	2.14	0.48
1:D:328:ASP:O	1:D:332:SER:HB2	2.13	0.47
1:D:164:MSE:HE2	1:D:200:GLU:HB3	1.96	0.47
1:A:132:LEU:HB2	1:A:179:MSE:HB2	1.96	0.47
1:B:305:LEU:O	1:B:309:MSE:HG2	2.14	0.47
1:B:334:TYR:N	1:B:334:TYR:CD1	2.83	0.47
1:B:83:ALA:HB1	1:B:88:LEU:O	2.15	0.47
1:C:139:ASP:HB3	1:C:376:SER:O	2.15	0.47
1:D:376:SER:HA	1:D:381:HIS:CD2	2.51	0.46
1:A:15:ARG:HH21	1:A:15:ARG:CB	2.19	0.46
1:C:112:TYR:HA	1:C:123:TRP:HB2	1.98	0.46
1:D:11:LEU:HA	1:D:14:VAL:HG12	1.98	0.46
1:B:77:ASP:N	1:B:77:ASP:OD1	2.48	0.46
1:C:121:ARG:HB2	1:C:122:PRO:HD2	1.96	0.46
1:B:157:MSE:HE1	1:B:162:PRO:N	2.30	0.46
1:B:38:LYS:HB2	1:B:395:LEU:HD12	1.97	0.46
1:C:290:LEU:HD12	1:D:261:SER:HB2	1.97	0.46
1:D:18:VAL:HG12	1:D:414:MSE:HE2	1.97	0.46
1:A:408:PHE:O	1:A:412:VAL:HG12	2.16	0.46
1:D:347:PHE:CE1	1:D:390:ARG:HD3	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:138:TYR:CZ	1:D:140:ARG:HB2	2.51	0.46
1:C:352:VAL:HG22	1:C:387:GLU:O	2.16	0.46
1:B:328:ASP:O	1:B:332:SER:HB2	2.16	0.45
1:A:116:ASN:HA	1:A:275:TRP:CE2	2.50	0.45
1:D:185:PHE:HE1	1:D:343:THR:CG2	2.28	0.45
1:A:110:TRP:CD1	1:A:114:TRP:HZ3	2.34	0.45
1:A:134:PRO:HA	1:A:155:VAL:O	2.17	0.45
1:C:330:ARG:CG	1:C:330:ARG:O	2.64	0.45
1:A:327:LEU:HD21	1:A:405:MSE:HE1	1.98	0.45
1:C:157:MSE:HE1	5:C:498:HOH:O	2.15	0.45
1:A:323:VAL:HG22	1:A:405:MSE:HG3	1.98	0.45
1:C:164:MSE:SE	1:C:201:LEU:HD13	2.68	0.44
1:A:330:ARG:NH1	1:A:410:THR:OG1	2.50	0.44
1:B:26:LYS:NZ	1:B:366:GLU:O	2.51	0.44
1:D:14:VAL:HA	1:D:17:GLU:HG2	1.98	0.44
1:D:138:TYR:CE1	4:D:422:EDO:H21	2.52	0.44
1:A:101:LEU:HD21	1:A:140:ARG:HB3	2.00	0.44
1:D:164:MSE:HE1	1:D:201:LEU:HD23	1.98	0.44
1:B:130:LYS:HD3	1:B:153:ILE:HD11	1.98	0.44
1:D:121:ARG:NH2	1:D:126:GLU:OE1	2.51	0.44
1:B:234:VAL:HA	1:B:237:PHE:HB2	1.99	0.44
1:D:224:LEU:HG	1:D:344:GLY:HA2	1.99	0.44
1:C:245:ASN:HB3	1:C:272:ASN:OD1	2.18	0.44
1:D:10:ARG:O	1:D:14:VAL:HG12	2.18	0.43
1:A:32:LEU:HD13	1:A:404:ALA:HB2	2.00	0.43
1:D:352:VAL:HG22	1:D:387:GLU:O	2.19	0.43
1:C:77:ASP:OD1	1:C:77:ASP:N	2.51	0.43
1:D:51:LEU:HD13	1:D:258:HIS:NE2	2.32	0.43
1:C:189:THR:CG2	1:C:191:VAL:HG13	2.36	0.43
1:C:361:VAL:HA	1:C:371:LEU:HD12	2.00	0.43
1:B:233:ASN:ND2	1:B:236:GLU:HB3	2.33	0.43
1:B:110:TRP:CE3	1:B:279:HIS:HB2	2.53	0.43
1:C:321:GLU:O	1:C:325:GLU:HG2	2.19	0.43
1:A:36:ARG:O	5:A:607:HOH:O	2.21	0.43
1:C:309:MSE:HE2	1:C:309:MSE:CA	2.49	0.43
1:A:195:GLU:HB2	1:A:232:HIS:CE1	2.53	0.43
1:B:196:GLN:O	1:B:200:GLU:HG3	2.18	0.43
1:D:188:PRO:HB3	1:D:390:ARG:HG3	2.00	0.43
1:B:256:ILE:HG23	1:B:309:MSE:CE	2.49	0.42
1:B:82:TRP:HH2	1:B:256:ILE:CD1	2.32	0.42
1:D:256:ILE:HG12	1:D:309:MSE:SE	2.69	0.42
1:A:193:PHE:CD2	1:A:193:PHE:N	2.86	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:157:MSE:CE	1:A:191:VAL:HG11	2.48	0.42
1:D:128:LYS:HD3	1:D:151:GLU:OE1	2.19	0.42
1:B:43:GLN:O	1:B:46:LEU:HB2	2.19	0.42
1:D:60:THR:OG1	1:D:64:VAL:HG13	2.20	0.42
1:C:138:TYR:CE1	4:C:422:EDO:H21	2.54	0.42
1:D:62:ASP:N	1:D:62:ASP:OD1	2.33	0.42
1:B:128:LYS:HE3	1:B:128:LYS:HB2	1.73	0.42
1:B:101:LEU:HD21	1:B:140:ARG:HB3	2.02	0.42
1:D:187:ASN:HA	1:D:188:PRO:HA	1.78	0.42
1:C:135:VAL:HA	1:C:136:PRO:C	2.40	0.42
1:D:76:ALA:HA	1:D:79:ARG:HH11	1.84	0.42
1:C:51:LEU:HD13	1:C:258:HIS:NE2	2.35	0.42
1:A:100:SER:O	1:A:104:MSE:HG3	2.19	0.42
1:A:364:ALA:HA	1:A:411:CYS:SG	2.60	0.42
1:B:327:LEU:HB3	1:B:339:TRP:CZ2	2.55	0.42
1:A:249:PHE:HB3	1:A:267:ALA:HB3	2.02	0.42
1:D:138:TYR:CE1	1:D:140:ARG:HB2	2.54	0.42
1:D:309:MSE:HE2	1:D:309:MSE:N	2.35	0.41
1:C:308:HIS:CD2	1:C:309:MSE:CE	3.03	0.41
1:B:36:ARG:HD2	1:B:395:LEU:HD13	2.01	0.41
1:A:22:TYR:HA	1:A:410:THR:HG21	2.03	0.41
1:D:305:LEU:HD12	1:D:309:MSE:HE3	2.02	0.41
1:C:323:VAL:HB	1:C:405:MSE:HG3	2.01	0.41
1:D:189:THR:OG1	1:D:191:VAL:HG13	2.20	0.41
1:B:155:VAL:HA	1:B:156:PRO:HD3	1.87	0.41
1:C:20:ALA:O	1:C:23:ALA:HB3	2.19	0.41
1:B:408:PHE:O	1:B:412:VAL:HG12	2.20	0.41
1:B:43:GLN:HA	1:B:46:LEU:HD13	2.03	0.41
1:B:375:GLY:O	1:B:381:HIS:HA	2.21	0.41
1:B:134:PRO:HA	1:B:155:VAL:O	2.20	0.41
1:C:20:ALA:O	1:C:24:GLU:N	2.49	0.41
1:B:418:GLU:O	1:B:419:VAL:C	2.58	0.41
1:B:327:LEU:HD13	1:B:405:MSE:HE2	2.02	0.41
1:A:285:ILE:HG12	1:B:140:ARG:CZ	2.51	0.41
1:C:396:PRO:HA	1:C:397:PRO:HD3	1.91	0.41
1:B:163:ASP:O	1:B:167:VAL:HG23	2.21	0.41
1:B:215:TRP:HB3	1:B:249:PHE:HA	2.04	0.40
1:A:376:SER:HA	1:A:381:HIS:CD2	2.57	0.40
1:B:417:LEU:C	1:B:419:VAL:H	2.25	0.40
1:A:171:VAL:HG13	1:A:206:THR:HA	2.02	0.40
1:A:96:GLN:HB2	1:A:103:ILE:HD11	2.04	0.40
1:D:18:VAL:HG12	1:D:414:MSE:CE	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:103:ILE:HG21	1:B:250:MSE:HE1	2.02	0.40
1:A:181:THR:HG1	1:A:193:PHE:HE1	1.69	0.40
1:D:373:GLY:O	1:D:376:SER:HB3	2.22	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	403/422 (96%)	389 (96%)	13 (3%)	1 (0%)	56	51
1	B	407/422 (96%)	388 (95%)	19 (5%)	0	100	100
1	C	411/422 (97%)	395 (96%)	15 (4%)	1 (0%)	56	51
1	D	410/422 (97%)	394 (96%)	16 (4%)	0	100	100
All	All	1631/1688 (97%)	1566 (96%)	63 (4%)	2 (0%)	59	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	ASP
1	C	97	ASP

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	332/334 (99%)	295 (89%)	37 (11%)	9	5
1	B	335/334 (100%)	307 (92%)	28 (8%)	16	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	337/334 (101%)	305 (90%)	32 (10%)	12 7
1	D	336/334 (101%)	313 (93%)	23 (7%)	22 15
All	All	1340/1336 (100%)	1220 (91%)	120 (9%)	14 8

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	29	ASN
1	A	30	LEU
1	A	42	GLU
1	A	44	LEU
1	A	51	LEU
1	A	64	VAL
1	A	73	LEU
1	A	77	ASP
1	A	127	GLU
1	A	135	VAL
1	A	155	VAL
1	A	160	GLU
1	A	170	LEU
1	A	171	VAL
1	A	181	THR
1	A	192	THR
1	A	230	ILE
1	A	249	PHE
1	A	263	VAL
1	A	301	ASP
1	A	310	LEU
1	A	316	LEU
1	A	329	SER
1	A	333	GLU
1	A	338	LYS
1	A	353	VAL
1	A	358	SER
1	A	362	GLU
1	A	365	LYS
1	A	372	THR
1	A	382	ASN
1	A	395	LEU
1	A	398	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	406	ASP
1	A	412	VAL
1	A	419	VAL
1	B	11	LEU
1	B	19	THR
1	B	31	SER
1	B	53	LEU
1	B	61	LYS
1	B	73	LEU
1	B	77	ASP
1	B	92	LEU
1	B	135	VAL
1	B	145	THR
1	B	155	VAL
1	B	192	THR
1	B	236	GLU
1	B	239	GLN
1	B	249	PHE
1	B	309	MSE
1	B	316	LEU
1	B	327	LEU
1	B	328	ASP
1	B	330	ARG
1	B	331	LEU
1	B	332	SER
1	B	343	THR
1	B	358	SER
1	B	363	LEU
1	B	395	LEU
1	B	398	VAL
1	B	406	ASP
1	C	10	ARG
1	C	11	LEU
1	C	19	THR
1	C	26	LYS
1	C	30	LEU
1	C	35	THR
1	C	51	LEU
1	C	57	ASP
1	C	61	LYS
1	C	77	ASP
1	C	86	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	129	VAL
1	C	153	ILE
1	C	159	ASP
1	C	170	LEU
1	C	189	THR
1	C	191	VAL
1	C	192	THR
1	C	201	LEU
1	C	205	SER
1	C	227	GLU
1	C	249	PHE
1	C	263	VAL
1	C	268	SER
1	C	288	ASN
1	C	310	LEU
1	C	323	VAL
1	C	332	SER
1	C	353	VAL
1	C	358	SER
1	C	413	LEU
1	C	414	MSE
1	D	15	ARG
1	D	30	LEU
1	D	35	THR
1	D	38	LYS
1	D	51	LEU
1	D	53	LEU
1	D	62	ASP
1	D	64	VAL
1	D	77	ASP
1	D	159	ASP
1	D	171	VAL
1	D	191	VAL
1	D	221	LEU
1	D	236	GLU
1	D	249	PHE
1	D	252	SER
1	D	325	GLU
1	D	332	SER
1	D	336	VAL
1	D	358	SER
1	D	376	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	406	ASP
1	D	413	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	96	GLN
1	A	245	ASN
1	A	279	HIS
1	A	308	HIS
1	A	381	HIS
1	B	102	ASN
1	B	245	ASN
1	B	279	HIS
1	C	43	GLN
1	C	102	ASN
1	C	196	GLN
1	C	279	HIS
1	C	288	ASN
1	C	308	HIS
1	C	381	HIS
1	D	96	GLN
1	D	102	ASN
1	D	239	GLN
1	D	245	ASN
1	D	279	HIS
1	D	381	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	SO4	A	420	-	4,4,4	0.43	0	6,6,6	0.32	0
4	EDO	A	422	-	3,3,3	0.84	0	2,2,2	0.36	0
2	SO4	B	420	-	4,4,4	0.12	0	6,6,6	0.32	0
4	EDO	B	422	-	3,3,3	0.70	0	2,2,2	0.32	0
2	SO4	C	420	-	4,4,4	0.43	0	6,6,6	0.65	0
4	EDO	C	422	-	3,3,3	0.69	0	2,2,2	0.25	0
2	SO4	D	420	-	4,4,4	0.53	0	6,6,6	0.21	0
4	EDO	D	422	-	3,3,3	0.84	0	2,2,2	0.47	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	SO4	A	420	-	-	0/0/0/0	0/0/0/0
4	EDO	A	422	-	-	0/1/1/1	0/0/0/0
2	SO4	B	420	-	-	0/0/0/0	0/0/0/0
4	EDO	B	422	-	-	0/1/1/1	0/0/0/0
2	SO4	C	420	-	-	0/0/0/0	0/0/0/0
4	EDO	C	422	-	-	0/1/1/1	0/0/0/0
2	SO4	D	420	-	-	0/0/0/0	0/0/0/0
4	EDO	D	422	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	405/422 (95%)	-0.05	17 (4%) 35 34	27, 34, 48, 54	0
1	B	409/422 (96%)	-0.02	10 (2%) 56 56	27, 35, 51, 55	0
1	C	413/422 (97%)	-0.08	14 (3%) 43 43	28, 35, 47, 55	0
1	D	412/422 (97%)	-0.25	3 (0%) 84 85	28, 36, 42, 62	0
All	All	1639/1688 (97%)	-0.10	44 (2%) 52 52	27, 35, 48, 62	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	417	LEU	7.9
1	D	419	VAL	6.5
1	A	417	LEU	6.5
1	B	417	LEU	6.2
1	A	419	VAL	5.6
1	A	18	VAL	5.1
1	A	30	LEU	4.9
1	B	419	VAL	4.7
1	D	9	ALA	4.5
1	B	32	LEU	4.3
1	C	419	VAL	4.2
1	A	333	GLU	3.9
1	C	416	ALA	3.8
1	A	369	ILE	3.7
1	C	11	LEU	3.6
1	C	413	LEU	3.5
1	B	404	ALA	3.5
1	A	32	LEU	3.4
1	C	335	GLY	3.4
1	A	27	ALA	3.3
1	A	367	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	27	ALA	3.2
1	A	364	ALA	3.2
1	C	14	VAL	3.1
1	B	415	ALA	3.0
1	A	416	ALA	2.8
1	B	25	LEU	2.8
1	A	22	TYR	2.6
1	A	25	LEU	2.5
1	A	334	TYR	2.3
1	B	16	GLU	2.3
1	A	363	LEU	2.3
1	C	16	GLU	2.3
1	A	24	GLU	2.3
1	C	24	GLU	2.3
1	B	416	ALA	2.2
1	B	410	THR	2.2
1	A	415	ALA	2.2
1	D	8	ALA	2.2
1	C	8	ALA	2.1
1	C	7	ASP	2.1
1	C	17	GLU	2.1
1	C	13	GLN	2.0
1	B	333	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	EDO	D	422	4/4	0.22	6.06	27,28,29,32	0
4	EDO	C	422	4/4	0.17	3.35	38,42,43,44	0
2	SO4	C	420	5/5	0.15	1.92	24,27,29,31	5
2	SO4	A	420	5/5	0.19	1.77	25,30,31,36	5
4	EDO	A	422	4/4	0.14	0.81	25,28,29,29	0
4	EDO	B	422	4/4	0.14	0.60	37,38,38,39	0
2	SO4	B	420	5/5	0.14	0.14	41,42,45,47	5
2	SO4	D	420	5/5	0.11	0.01	37,39,39,41	5
3	CL	A	421	1/1	0.05	-0.96	36,36,36,36	0
3	CL	B	421	1/1	0.05	-1.97	43,43,43,43	0
3	CL	D	421	1/1	0.06	-2.32	42,42,42,42	0
3	CL	C	421	1/1	0.04	-3.51	39,39,39,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.