



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:23 PM GMT

PDB ID : 4A21
Title : STRUCTURE OF MYCOBACTERIUM TUBERCULOSIS FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE BOUND TO SULFATE
Authors : Coincon, M.; De La Paz Santangelo, M.; Gest, P.M.; Guerin, M.E.; Pham, H.; Ryan, G.; Puckett, S.E.; Spencer, J.S.; Gonzalez-Juarrero, M.; Daher, R.; Lenaerts, A.J.; Schnappinger, D.; Therisod, M.; Ehrt, S.; Jackson, M.; Sygusch, J.
Deposited on : 2011-09-21
Resolution : 2.35 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>

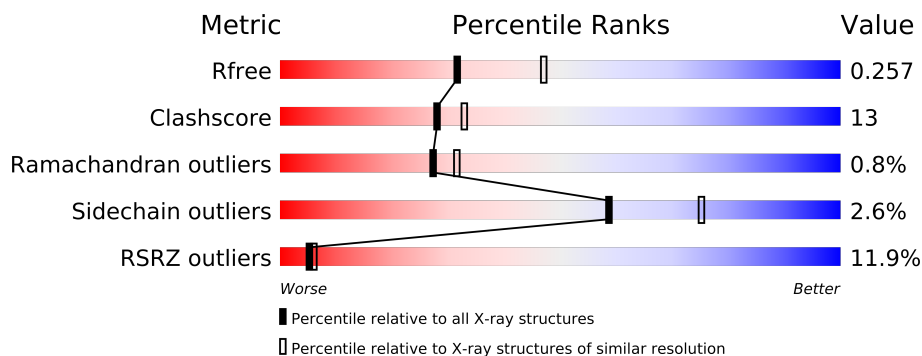
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.35 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	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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	344	
1	B	344	
1	C	344	
1	D	344	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	NA	A	1347	-	X

2 Entry composition

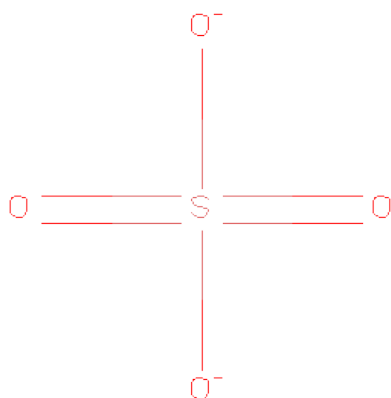
There are 4 unique types of molecules in this entry. The entry contains 19522 atoms, of which 9296 are hydrogens and 0 are deuterium.

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 FRUCTOSE-BISPHOSPHATEALDOLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	314	Total	C	H	N	O	S	0	0	0
			4671	1488	2325	395	453	10			
1	B	314	Total	C	H	N	O	S	0	0	0
			4671	1488	2325	395	453	10			
1	C	314	Total	C	H	N	O	S	0	0	0
			4669	1488	2323	395	453	10			
1	D	314	Total	C	H	N	O	S	0	0	0
			4669	1488	2323	395	453	10			

- 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	A	1	Total	O	S	0	0
			5	4	1		

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

- 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		

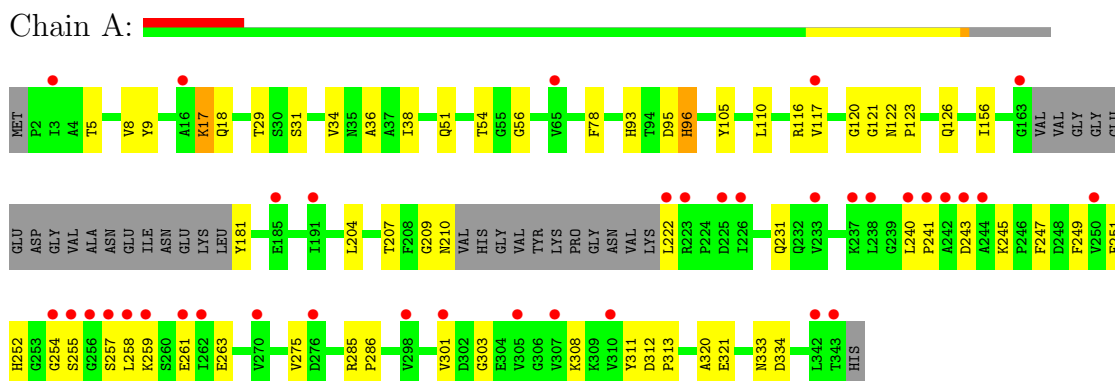
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	215	Total	O	0	0
			215	215		
4	B	205	Total	O	0	0
			205	205		
4	C	185	Total	O	0	0
			185	185		
4	D	195	Total	O	0	0
			195	195		

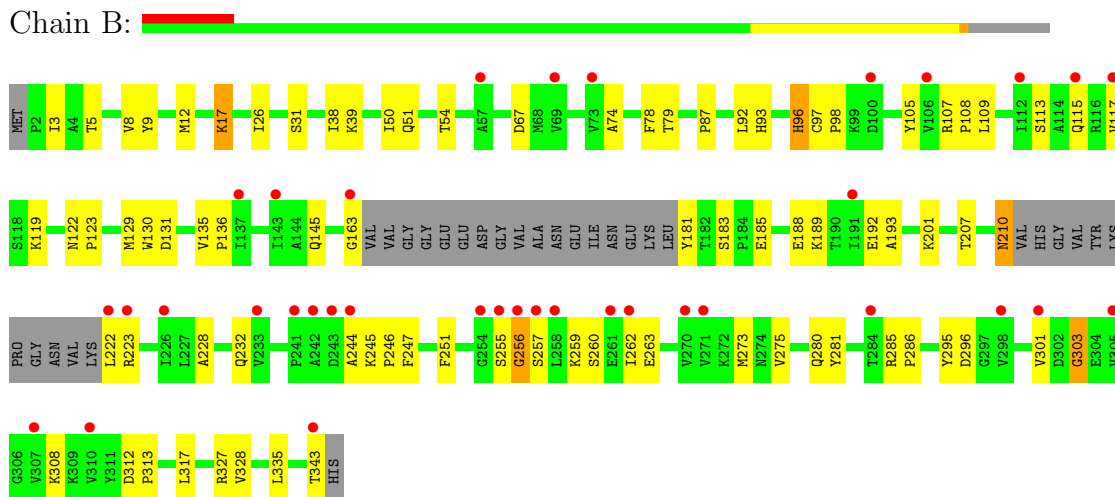
3 Residue-property plots

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.

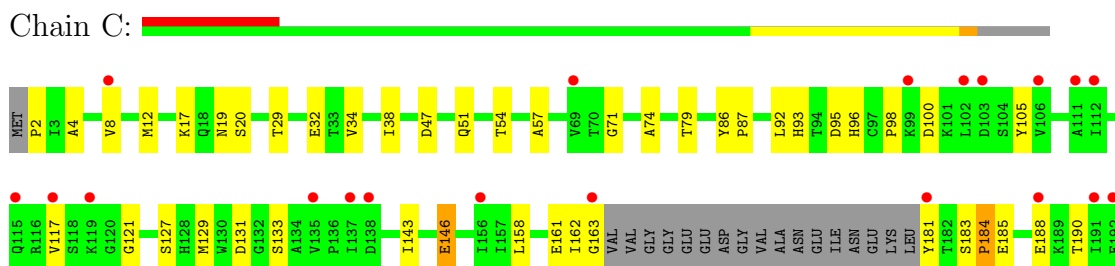
• Molecule 1: FRUCTOSE-BISPHOSPHATEALDOLASE

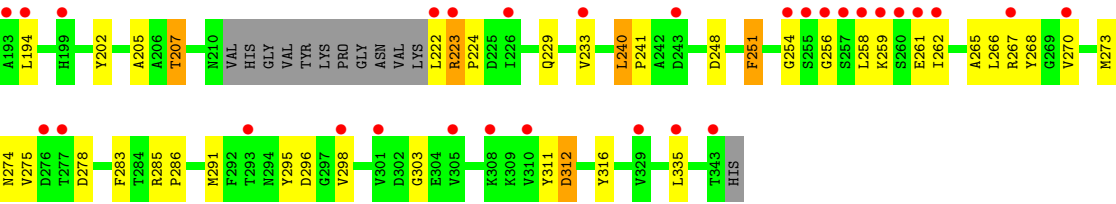


• Molecule 1: FRUCTOSE-BISPHOSPHATEALDOLASE



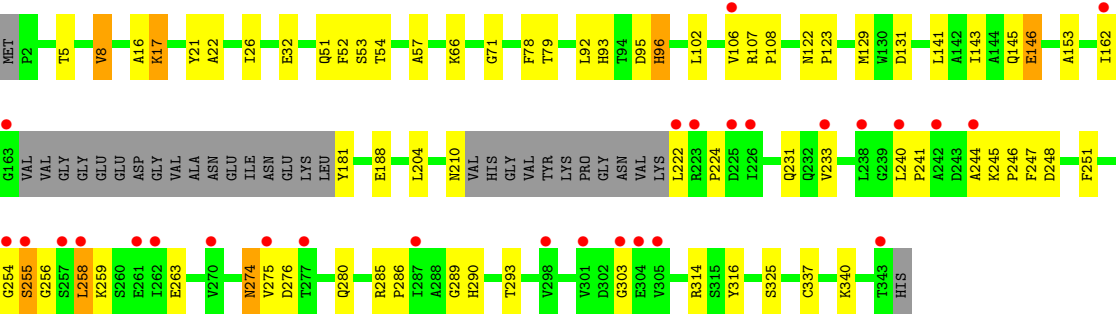
• Molecule 1: FRUCTOSE-BISPHOSPHATEALDOLASE





● Molecule 1: FRUCTOSE-BISPHOSPHATEALDOLASE

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	336.94Å 43.23Å 103.02Å 90.00° 99.57° 90.00°	Depositor
Resolution (Å)	42.87 – 2.35 42.87 – 2.35	Depositor EDS
% Data completeness (in resolution range)	91.2 (42.87-2.35) 99.1 (42.87-2.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.34Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.211 , 0.261 0.215 , 0.257	Depositor DCC
R_{free} test set	4631 reflections (7.52%)	DCC
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 31.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 61593 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19522	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	0.36	0/2391	0.51	0/3236
1	B	0.36	0/2391	0.52	0/3236
1	C	0.33	0/2391	0.48	0/3236
1	D	0.35	0/2391	0.50	0/3236
All	All	0.35	0/9564	0.50	0/12944

There are no bond length outliers.

There are no bond angle outliers.

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	2346	2325	0	52	0
1	B	2346	2325	0	65	0
1	C	2346	2323	0	66	0
1	D	2346	2323	0	60	0
2	A	10	0	0	2	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
4	A	215	0	0	21	1
4	B	205	0	0	22	1
4	C	185	0	0	22	1
4	D	195	0	0	14	0
All	All	10226	9296	0	237	2

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 13.

All (237) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:258:LEU:HB3	4:A:2170:HOH:O	1.57	1.03
1:B:257:SER:HA	4:B:2161:HOH:O	1.58	1.03
1:A:181:TYR:CZ	4:A:2138:HOH:O	2.22	0.92
1:C:267:ARG:HA	4:C:2033:HOH:O	1.71	0.89
1:C:163:GLY:HA3	1:C:207:THR:OG1	1.85	0.77
1:C:259:LYS:HE3	4:C:2139:HOH:O	1.84	0.75
1:B:87:PRO:O	1:B:343:THR:HG22	1.89	0.72
1:A:181:TYR:CE2	4:A:2138:HOH:O	2.42	0.70
1:D:255:SER:HB2	2:D:1345:SO4:O3	1.92	0.70
1:D:224:PRO:HG2	4:D:2146:HOH:O	1.91	0.69
1:C:278:ASP:O	4:C:2148:HOH:O	2.10	0.69
1:D:17:LYS:HE2	1:D:245:LYS:O	1.93	0.69
1:A:51:GLN:HA	1:A:93:HIS:O	1.92	0.68
1:C:254:GLY:HA2	4:C:2134:HOH:O	1.94	0.67
1:A:303:GLY:O	4:A:2195:HOH:O	2.12	0.66
1:D:222:LEU:N	4:D:2104:HOH:O	2.28	0.66
1:D:96:HIS:O	4:D:2045:HOH:O	2.13	0.66
1:C:184:PRO:O	4:C:2113:HOH:O	2.14	0.65
2:A:1345:SO4:O4	4:A:2215:HOH:O	2.14	0.64
1:B:79:THR:HG22	1:B:92:LEU:HD22	1.80	0.64
1:D:181:TYR:N	4:D:2100:HOH:O	2.30	0.64
1:B:210:ASN:OD1	1:B:210:ASN:N	2.31	0.64
1:C:185:GLU:HA	4:C:2113:HOH:O	1.99	0.62
1:C:129:MET:HE3	1:C:131:ASP:HB2	1.81	0.62
1:D:259:LYS:O	1:D:263:GLU:HG2	1.99	0.62
1:C:181:TYR:CZ	1:C:223:ARG:HG3	2.34	0.62
1:B:327:ARG:HB2	4:B:2194:HOH:O	2.00	0.62
1:B:145:GLN:NE2	1:B:193:ALA:O	2.33	0.62
1:A:120:GLY:N	4:A:2105:HOH:O	2.33	0.62
1:D:240:LEU:HB3	1:D:241:PRO:HD2	1.81	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:254:GLY:CA	4:C:2134:HOH:O	2.47	0.61
1:B:222:LEU:N	4:B:2128:HOH:O	2.33	0.61
1:B:201:LYS:O	4:B:2125:HOH:O	2.16	0.60
1:B:301:VAL:HG11	4:B:2182:HOH:O	2.01	0.60
1:B:232:GLN:HB2	4:B:2152:HOH:O	2.01	0.60
1:C:265:ALA:HB2	1:C:270:VAL:HG22	1.83	0.60
1:B:26:ILE:HD13	1:B:328:VAL:HG23	1.84	0.60
1:B:257:SER:C	4:B:2160:HOH:O	2.41	0.59
1:A:18:GLN:HG3	4:A:2020:HOH:O	2.02	0.59
1:D:5:THR:OG1	1:D:8:VAL:HG11	2.02	0.59
1:C:266:LEU:C	4:C:2033:HOH:O	2.41	0.59
1:B:295:TYR:CE2	1:B:296:ASP:HB3	2.38	0.59
1:B:181:TYR:CZ	1:B:223:ARG:HG3	2.39	0.58
1:C:133:SER:HB2	1:C:163:GLY:C	2.24	0.57
1:B:96:HIS:HE1	4:B:2071:HOH:O	1.86	0.57
1:C:29:THR:HG22	1:D:314:ARG:HD3	1.86	0.57
1:C:222:LEU:O	1:C:223:ARG:HG2	2.03	0.57
1:D:274:ASN:HD21	1:D:274:ASN:N	2.01	0.57
1:B:255:SER:C	4:B:2158:HOH:O	2.42	0.56
1:B:17:LYS:HE2	1:B:245:LYS:HB3	1.87	0.56
1:C:163:GLY:CA	1:C:207:THR:OG1	2.54	0.56
1:D:181:TYR:N	4:D:2101:HOH:O	2.38	0.56
1:D:79:THR:HG22	1:D:92:LEU:HD22	1.86	0.56
1:C:254:GLY:C	4:C:2134:HOH:O	2.44	0.55
1:B:260:SER:HB3	4:B:2163:HOH:O	2.04	0.55
1:C:261:GLU:HG2	4:C:2141:HOH:O	2.05	0.55
1:A:121:GLY:N	4:A:2105:HOH:O	2.39	0.55
1:B:17:LYS:HE3	1:B:247:PHE:O	2.07	0.55
1:B:260:SER:CB	4:B:2163:HOH:O	2.54	0.55
1:A:258:LEU:HB2	1:A:261:GLU:CD	2.28	0.54
1:B:343:THR:HG23	4:B:2067:HOH:O	2.07	0.54
1:D:107:ARG:HB2	1:D:108:PRO:HD3	1.90	0.54
1:D:122:ASN:HB3	4:D:2006:HOH:O	2.08	0.54
1:A:54:THR:HG23	1:A:105:TYR:CD2	2.42	0.54
1:A:34:VAL:O	1:A:38:ILE:HG13	2.07	0.54
1:B:343:THR:C	4:B:2204:HOH:O	2.46	0.53
1:D:325:SER:HB2	4:D:2168:HOH:O	2.08	0.53
1:D:53:SER:HA	1:D:95:ASP:HB3	1.90	0.53
1:D:52:PHE:HA	4:D:2031:HOH:O	2.07	0.53
1:A:259:LYS:HE3	1:A:334:ASP:OD1	2.09	0.53
1:C:51:GLN:HA	1:C:93:HIS:O	2.08	0.53
1:C:258:LEU:HB2	1:C:261:GLU:HG3	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:129:MET:HE3	1:B:131:ASP:HB2	1.91	0.52
1:B:257:SER:CA	4:B:2160:HOH:O	2.57	0.52
1:A:116:ARG:O	4:A:2105:HOH:O	2.19	0.52
1:B:107:ARG:N	1:B:108:PRO:CD	2.73	0.52
1:B:38:ILE:HG13	1:B:50:ILE:HD12	1.90	0.52
1:C:143:ILE:O	1:C:146:GLU:HG3	2.10	0.52
1:D:17:LYS:CE	1:D:245:LYS:O	2.58	0.52
1:B:259:LYS:O	1:B:263:GLU:HG2	2.10	0.52
1:D:289:GLY:O	1:D:293:THR:HG21	2.08	0.52
1:D:54:THR:HG21	4:D:2045:HOH:O	2.09	0.52
1:A:96:HIS:HE1	4:A:2086:HOH:O	1.93	0.52
1:D:274:ASN:ND2	1:D:274:ASN:N	2.57	0.52
1:D:290:HIS:CG	1:D:316:TYR:HB3	2.45	0.52
1:D:258:LEU:N	1:D:258:LEU:HD21	2.24	0.51
1:A:311:TYR:CE1	1:B:281:TYR:HB2	2.45	0.51
1:A:308:LYS:HD3	4:B:2085:HOH:O	2.09	0.51
1:D:143:ILE:O	1:D:146:GLU:HG3	2.09	0.51
1:A:243:ASP:CB	4:A:2164:HOH:O	2.58	0.51
1:B:256:GLY:N	4:B:2159:HOH:O	2.43	0.51
1:D:276:ASP:O	1:D:280:GLN:HG3	2.11	0.51
1:C:312:ASP:OD1	1:C:312:ASP:C	2.50	0.51
1:C:251:PHE:HB2	1:C:270:VAL:HG12	1.93	0.51
1:A:17:LYS:HE2	1:A:245:LYS:HB3	1.91	0.51
1:A:110:LEU:HD21	1:A:156:ILE:HD13	1.92	0.50
1:D:153:ALA:HB1	4:D:2095:HOH:O	2.10	0.50
1:D:141:LEU:O	1:D:145:GLN:HG3	2.11	0.50
1:B:185:GLU:OE2	1:B:189:LYS:HE2	2.12	0.50
1:D:66:LYS:HD3	4:D:2051:HOH:O	2.11	0.50
1:C:273:MET:HE3	1:C:335:LEU:HD22	1.94	0.49
1:D:255:SER:CB	2:D:1345:SO4:O3	2.59	0.49
1:C:240:LEU:HB3	1:C:241:PRO:HD2	1.93	0.49
1:C:273:MET:CE	1:C:335:LEU:HD22	2.42	0.49
1:D:244:ALA:O	1:D:246:PRO:HD3	2.13	0.49
1:C:2:PRO:HB2	4:C:2001:HOH:O	2.12	0.49
1:B:39:LYS:HG2	4:B:2031:HOH:O	2.11	0.49
1:D:26:ILE:HD11	1:D:275:VAL:HG23	1.94	0.49
1:B:5:THR:OG1	1:B:8:VAL:HG11	2.13	0.49
1:A:255:SER:HB2	2:A:1344:SO4:O4	2.12	0.49
1:A:78:PHE:CE1	1:B:74:ALA:HB2	2.47	0.49
1:B:9:TYR:O	1:B:12:MET:HB2	2.12	0.49
1:C:262:ILE:O	1:C:266:LEU:HG	2.13	0.49
1:C:267:ARG:CA	4:C:2033:HOH:O	2.44	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:162:ILE:CD1	1:D:204:LEU:HD12	2.43	0.49
4:C:2039:HOH:O	1:D:32:GLU:HG3	2.12	0.48
1:C:32:GLU:HB2	4:C:2041:HOH:O	2.13	0.48
1:B:303:GLY:N	4:B:2180:HOH:O	2.46	0.48
4:A:2180:HOH:O	1:B:308:LYS:HG2	2.13	0.48
1:A:333:ASN:HB3	4:A:2209:HOH:O	2.13	0.48
1:A:17:LYS:HE3	1:A:247:PHE:O	2.12	0.48
1:A:286:PRO:HG2	1:A:320:ALA:HA	1.95	0.48
1:A:308:LYS:CD	4:B:2085:HOH:O	2.62	0.48
1:C:12:MET:HE1	1:C:47:ASP:HB3	1.96	0.48
1:C:283:PHE:O	1:C:286:PRO:HD2	2.14	0.48
1:C:161:GLU:HG3	1:C:205:ALA:HB1	1.96	0.48
1:A:117:VAL:C	4:A:2105:HOH:O	2.53	0.47
1:B:223:ARG:NE	4:B:2150:HOH:O	2.48	0.47
1:B:67:ASP:HA	4:B:2052:HOH:O	2.15	0.47
1:D:17:LYS:HD3	1:D:248:ASP:OD1	2.15	0.47
1:C:188:GLU:HG3	4:C:2113:HOH:O	2.15	0.47
1:B:113:SER:O	1:B:117:VAL:HG21	2.15	0.47
1:A:252:HIS:HB3	4:A:2087:HOH:O	2.14	0.47
1:D:240:LEU:HD13	1:D:240:LEU:N	2.29	0.47
1:D:244:ALA:C	1:D:246:PRO:HD3	2.34	0.47
1:B:295:TYR:CG	1:B:296:ASP:N	2.83	0.46
1:C:190:THR:HG21	1:C:194:LEU:HD13	1.97	0.46
1:D:254:GLY:O	1:D:256:GLY:N	2.48	0.46
1:C:4:ALA:HB2	1:C:8:VAL:HG21	1.97	0.46
1:B:3:ILE:HD12	1:B:79:THR:HG23	1.97	0.46
1:C:57:ALA:O	1:C:71:GLY:HA3	2.16	0.46
1:A:122:ASN:HB3	1:A:123:PRO:HD2	1.97	0.46
1:D:122:ASN:HB3	1:D:123:PRO:HD2	1.97	0.46
1:A:95:ASP:OD1	1:A:96:HIS:CD2	2.68	0.46
1:B:273:MET:CE	1:B:335:LEU:HD22	2.46	0.46
1:D:21:TYR:CE2	1:D:340:LYS:HD3	2.51	0.46
1:D:102:LEU:HD21	1:D:106:VAL:HB	1.98	0.46
1:C:267:ARG:NE	4:C:2143:HOH:O	2.48	0.46
1:A:312:ASP:C	1:A:312:ASP:OD1	2.51	0.46
1:C:262:ILE:HD11	1:C:273:MET:HE2	1.98	0.46
1:A:9:TYR:CD2	1:A:126:GLN:HB3	2.51	0.46
1:A:31:SER:HB2	1:A:78:PHE:CZ	2.51	0.46
1:D:51:GLN:HA	1:D:93:HIS:O	2.16	0.45
1:D:16:ALA:HB2	1:D:21:TYR:O	2.17	0.45
1:B:31:SER:HB2	1:B:78:PHE:CZ	2.50	0.45
1:D:17:LYS:HE3	1:D:247:PHE:O	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:295:TYR:CG	1:C:296:ASP:N	2.84	0.45
1:A:122:ASN:HB3	4:A:2005:HOH:O	2.15	0.45
1:C:54:THR:HG23	1:C:105:TYR:CD2	2.51	0.45
1:A:240:LEU:HB3	1:A:241:PRO:HD2	1.99	0.45
1:B:135:VAL:HB	1:B:136:PRO:HD2	1.98	0.45
1:C:254:GLY:HA3	1:C:274:ASN:O	2.17	0.45
4:A:2180:HOH:O	1:B:308:LYS:CG	2.65	0.45
1:A:259:LYS:O	1:A:263:GLU:HG2	2.17	0.44
1:D:95:ASP:O	1:D:96:HIS:C	2.55	0.44
1:A:29:THR:HG23	1:A:56:GLY:HA3	1.99	0.44
1:A:313:PRO:HD2	1:B:280:GLN:HG2	1.98	0.44
1:C:274:ASN:HB3	4:C:2035:HOH:O	2.18	0.44
1:B:163:GLY:C	1:B:207:THR:HG22	2.38	0.44
1:D:240:LEU:HB3	1:D:241:PRO:CD	2.46	0.44
1:A:243:ASP:HB3	4:A:2164:HOH:O	2.18	0.44
1:A:117:VAL:HA	4:A:2105:HOH:O	2.17	0.43
1:C:17:LYS:HD3	1:C:248:ASP:OD1	2.17	0.43
1:C:117:VAL:HA	1:C:121:GLY:O	2.18	0.43
1:D:303:GLY:C	4:D:2158:HOH:O	2.56	0.43
1:D:245:LYS:N	4:D:2137:HOH:O	2.38	0.43
1:D:244:ALA:HA	4:D:2135:HOH:O	2.17	0.43
1:C:285:ARG:HB3	1:C:286:PRO:HD3	2.01	0.43
1:B:122:ASN:HB3	1:B:123:PRO:HD2	2.00	0.43
1:B:51:GLN:HA	1:B:93:HIS:O	2.19	0.43
1:A:285:ARG:N	1:A:286:PRO:HD2	2.33	0.43
1:D:188:GLU:HG3	1:D:233:VAL:CG1	2.49	0.43
1:A:204:LEU:O	1:A:249:PHE:HA	2.19	0.43
1:C:98:PRO:HB2	1:C:100:ASP:OD1	2.19	0.43
1:D:285:ARG:N	1:D:286:PRO:HD2	2.33	0.43
1:B:312:ASP:OD1	1:B:312:ASP:C	2.58	0.42
1:B:313:PRO:O	1:B:317:LEU:HG	2.19	0.42
1:C:185:GLU:CA	4:C:2113:HOH:O	2.64	0.42
1:C:298:VAL:HA	1:C:311:TYR:HB3	2.00	0.42
1:D:210:ASN:HB3	1:D:222:LEU:HD22	2.02	0.42
1:C:185:GLU:O	1:C:188:GLU:HB2	2.20	0.42
1:B:228:ALA:O	1:B:232:GLN:HG3	2.19	0.42
4:A:2180:HOH:O	1:B:308:LYS:HE3	2.19	0.42
1:C:183:SER:C	1:C:185:GLU:H	2.23	0.42
1:C:223:ARG:N	1:C:224:PRO:HD3	2.34	0.42
1:A:231:GLN:NE2	1:A:249:PHE:CE2	2.87	0.42
1:B:244:ALA:O	1:B:246:PRO:HD3	2.20	0.42
1:C:19:ASN:O	1:C:20:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:5:THR:N	1:A:8:VAL:CG1	2.82	0.42
1:B:285:ARG:HB3	1:B:286:PRO:HD3	2.02	0.42
1:C:229:GLN:O	1:C:233:VAL:HG21	2.20	0.42
1:C:158:LEU:O	1:C:202:TYR:HB2	2.19	0.42
1:A:36:ALA:HB3	1:A:321:GLU:HG3	2.01	0.41
1:D:17:LYS:O	1:D:245:LYS:HE3	2.21	0.41
1:B:115:GLN:O	1:B:119:LYS:HG2	2.20	0.41
1:C:74:ALA:HB2	1:D:78:PHE:CD1	2.56	0.41
1:C:79:THR:HG22	1:C:92:LEU:HD22	2.02	0.41
1:D:290:HIS:CD2	1:D:316:TYR:HB3	2.53	0.41
1:B:54:THR:HG23	1:B:105:TYR:CD2	2.55	0.41
1:D:57:ALA:O	1:D:71:GLY:HA3	2.20	0.41
1:A:254:GLY:C	1:A:257:SER:HG	2.23	0.41
1:A:181:TYR:CD1	1:A:181:TYR:N	2.89	0.41
1:B:343:THR:HA	4:B:2067:HOH:O	2.20	0.41
1:B:109:LEU:HD21	1:B:109:LEU:HA	1.85	0.41
1:D:231:GLN:HA	1:D:231:GLN:OE1	2.20	0.41
1:B:201:LYS:HB3	1:B:201:LYS:HE2	1.70	0.41
1:B:188:GLU:O	1:B:192:GLU:HG3	2.21	0.41
1:C:268:TYR:N	1:C:268:TYR:CD1	2.87	0.41
1:C:86:TYR:HA	1:C:87:PRO:HD3	1.92	0.41
1:B:107:ARG:HB2	1:B:108:PRO:HD3	2.02	0.41
1:B:257:SER:HB2	1:B:262:ILE:HD12	2.01	0.41
1:C:266:LEU:O	4:C:2033:HOH:O	2.22	0.41
1:A:78:PHE:CD1	1:B:74:ALA:HB2	2.56	0.41
1:C:291:MET:HE2	1:C:316:TYR:CE2	2.56	0.41
1:C:34:VAL:O	1:C:38:ILE:HG13	2.21	0.41
1:D:129:MET:HE3	1:D:131:ASP:HB2	2.03	0.41
1:C:32:GLU:OE1	1:D:32:GLU:OE1	2.39	0.41
1:C:162:ILE:HA	4:C:2099:HOH:O	2.20	0.41
1:D:22:ALA:O	1:D:337:CYS:HB3	2.20	0.41
1:B:97:CYS:HA	1:B:98:PRO:HD2	1.98	0.41
1:A:209:GLY:C	1:A:222:LEU:HD21	2.42	0.40
1:A:117:VAL:CA	4:A:2105:HOH:O	2.69	0.40
1:A:222:LEU:HD13	1:A:261:GLU:OE1	2.20	0.40
1:A:285:ARG:HB3	1:A:286:PRO:HD3	2.02	0.40
1:C:303:GLY:N	4:C:2159:HOH:O	2.45	0.40
1:A:210:ASN:HA	1:A:222:LEU:HD22	2.04	0.40
1:C:267:ARG:N	4:C:2033:HOH:O	2.52	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:2126:HOH:O	4:A:2211:HOH:O[1_545]	2.17	0.03
4:B:2180:HOH:O	4:C:2159:HOH:O[1_565]	2.17	0.03

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	308/344 (90%)	297 (96%)	10 (3%)	1 (0%)	50	62
1	B	308/344 (90%)	293 (95%)	12 (4%)	3 (1%)	22	24
1	C	308/344 (90%)	290 (94%)	14 (4%)	4 (1%)	18	17
1	D	308/344 (90%)	296 (96%)	10 (3%)	2 (1%)	33	39
All	All	1232/1376 (90%)	1176 (96%)	46 (4%)	10 (1%)	27	31

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	255	SER
1	A	96	HIS
1	C	96	HIS
1	D	96	HIS
1	B	303	GLY
1	B	96	HIS
1	C	184	PRO
1	B	256	GLY
1	C	256	GLY
1	C	223	ARG

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	242/266 (91%)	237 (98%)	5 (2%)	66	82
1	B	242/266 (91%)	236 (98%)	6 (2%)	60	76
1	C	242/266 (91%)	234 (97%)	8 (3%)	50	65
1	D	242/266 (91%)	236 (98%)	6 (2%)	60	76
All	All	968/1064 (91%)	943 (97%)	25 (3%)	59	75

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	207	THR
1	A	251	PHE
1	A	275	VAL
1	A	301	VAL
1	B	17	LYS
1	B	130	TRP
1	B	183	SER
1	B	210	ASN
1	B	251	PHE
1	B	275	VAL
1	C	95	ASP
1	C	127	SER
1	C	146	GLU
1	C	207	THR
1	C	240	LEU
1	C	251	PHE
1	C	275	VAL
1	C	312	ASP
1	D	8	VAL
1	D	17	LYS
1	D	146	GLU
1	D	251	PHE
1	D	258	LEU
1	D	274	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	B	122	ASN

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Mol	Chain	Res	Type
1	C	252	HIS
1	D	326	GLN

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 10 ligands modelled in this entry, 2 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	1344	-	4,4,4	0.19	0	6,6,6	0.12	0
2	SO4	A	1345	-	4,4,4	0.19	0	6,6,6	0.13	0
2	SO4	B	1344	-	4,4,4	0.11	0	6,6,6	0.24	0
2	SO4	B	1345	-	4,4,4	0.16	0	6,6,6	0.19	0
2	SO4	C	1344	-	4,4,4	0.12	0	6,6,6	0.13	0
2	SO4	C	1345	-	4,4,4	0.08	0	6,6,6	0.16	0
2	SO4	D	1344	-	4,4,4	0.11	0	6,6,6	0.33	0
2	SO4	D	1345	-	4,4,4	0.21	0	6,6,6	0.29	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	1344	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1345	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1344	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1345	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1344	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1345	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1344	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1345	-	-	0/0/0/0	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	314/344 (91%)	0.86	37 (11%) 5 6	14, 27, 52, 81	0
1	B	314/344 (91%)	0.82	36 (11%) 5 7	15, 27, 49, 91	0
1	C	314/344 (91%)	1.07	50 (15%) 3 3	18, 35, 63, 99	0
1	D	314/344 (91%)	0.78	28 (8%) 10 11	15, 27, 49, 77	0
All	All	1256/1376 (91%)	0.88	151 (12%) 5 6	14, 29, 55, 99	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	GLY	7.6
1	C	256	GLY	7.0
1	C	163	GLY	6.9
1	B	257	SER	6.4
1	D	305	VAL	5.9
1	A	242	ALA	5.9
1	B	255	SER	5.7
1	A	258	LEU	5.7
1	C	257	SER	5.4
1	C	255	SER	5.0
1	B	256	GLY	5.0
1	C	254	GLY	5.0
1	C	111	ALA	4.6
1	C	305	VAL	4.5
1	C	181	TYR	4.3
1	B	258	LEU	4.2
1	A	223	ARG	4.1
1	D	255	SER	4.1
1	C	267	ARG	4.1
1	C	222	LEU	4.1
1	C	260	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	163	GLY	4.0
1	A	301	VAL	4.0
1	D	238	LEU	4.0
1	B	254	GLY	3.9
1	B	305	VAL	3.6
1	B	163	GLY	3.6
1	B	242	ALA	3.5
1	D	301	VAL	3.5
1	C	193	ALA	3.5
1	A	256	GLY	3.5
1	A	305	VAL	3.5
1	C	192	GLU	3.4
1	C	117	VAL	3.4
1	C	137	ILE	3.4
1	C	258	LEU	3.4
1	D	223	ARG	3.4
1	C	262	ILE	3.4
1	B	117	VAL	3.3
1	B	343	THR	3.3
1	D	163	GLY	3.3
1	A	243	ASP	3.3
1	A	238	LEU	3.3
1	A	222	LEU	3.2
1	D	257	SER	3.2
1	B	233	VAL	3.2
1	B	301	VAL	3.1
1	B	298	VAL	3.1
1	C	301	VAL	3.1
1	B	244	ALA	3.1
1	D	226	ILE	3.1
1	C	138	ASP	3.1
1	D	225	ASP	3.1
1	D	298	VAL	3.0
1	C	298	VAL	3.0
1	D	254	GLY	3.0
1	C	343	THR	3.0
1	C	102	LEU	3.0
1	B	137	ILE	2.9
1	C	270	VAL	2.9
1	B	226	ILE	2.9
1	A	185	GLU	2.9
1	D	258	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	304	GLU	2.8
1	B	112	ILE	2.8
1	B	270	VAL	2.8
1	A	240	LEU	2.8
1	A	226	ILE	2.8
1	C	119	LYS	2.7
1	D	222	LEU	2.7
1	D	343	THR	2.7
1	C	243	ASP	2.7
1	A	250	VAL	2.7
1	B	143	ILE	2.7
1	C	103	ASP	2.7
1	B	106	VAL	2.7
1	C	233	VAL	2.7
1	D	244	ALA	2.7
1	B	262	ILE	2.6
1	C	261	GLU	2.6
1	B	222	LEU	2.6
1	C	199	HIS	2.6
1	A	257	SER	2.6
1	A	276	ASP	2.6
1	A	270	VAL	2.6
1	C	194	LEU	2.6
1	C	191	ILE	2.6
1	A	233	VAL	2.6
1	A	244	ALA	2.6
1	D	162	ILE	2.5
1	B	307	VAL	2.5
1	A	225	ASP	2.5
1	A	3	ILE	2.5
1	D	242	ALA	2.5
1	A	262	ILE	2.5
1	D	233	VAL	2.5
1	C	115	GLN	2.4
1	D	303	GLY	2.4
1	A	255	SER	2.4
1	A	65	VAL	2.4
1	C	135	VAL	2.4
1	B	261	GLU	2.4
1	C	277	THR	2.4
1	C	335	LEU	2.4
1	C	8	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	112	ILE	2.4
1	C	310	VAL	2.4
1	D	287	ILE	2.4
1	A	298	VAL	2.3
1	A	343	THR	2.3
1	C	293	THR	2.3
1	B	223	ARG	2.3
1	C	188	GLU	2.3
1	C	308	LYS	2.3
1	B	115	GLN	2.3
1	D	262	ILE	2.3
1	A	237	LYS	2.3
1	A	259	LYS	2.2
1	A	307	VAL	2.2
1	C	156	ILE	2.2
1	A	16	ALA	2.2
1	A	241	PRO	2.2
1	C	223	ARG	2.2
1	D	261	GLU	2.2
1	B	243	ASP	2.2
1	B	73	VAL	2.2
1	C	106	VAL	2.2
1	B	191	ILE	2.1
1	B	310	VAL	2.1
1	C	226	ILE	2.1
1	A	342	LEU	2.1
1	D	277	THR	2.1
1	C	69	VAL	2.1
1	D	106	VAL	2.1
1	A	191	ILE	2.1
1	D	240	LEU	2.1
1	C	259	LYS	2.1
1	B	271	VAL	2.1
1	D	270	VAL	2.1
1	A	117	VAL	2.1
1	C	329	VAL	2.1
1	B	100	ASP	2.1
1	B	284	THR	2.1
1	C	276	ASP	2.1
1	B	57	ALA	2.1
1	A	261	GLU	2.0
1	D	275	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	241	PRO	2.0
1	B	69	VAL	2.0
1	C	99	LYS	2.0
1	A	310	VAL	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(Å ²)	Q<0.9
3	NA	A	1347	1/1	0.30	3.97	43,43,43,43	0
2	SO4	C	1345	5/5	0.19	1.66	50,50,68,80	0
3	NA	A	1346	1/1	0.18	-0.03	47,47,47,47	0
2	SO4	C	1344	5/5	0.26	-0.15	51,67,74,83	0
2	SO4	D	1344	5/5	0.16	-0.26	38,43,63,87	0
2	SO4	B	1345	5/5	0.19	-0.52	50,54,67,83	0
2	SO4	D	1345	5/5	0.20	-0.58	57,59,68,88	0
2	SO4	A	1345	5/5	0.14	-1.27	38,46,52,60	0
2	SO4	A	1344	5/5	0.10	-1.35	52,55,64,65	0
2	SO4	B	1344	5/5	0.14	-1.55	41,44,65,75	0

6.5 Other polymers ⓘ

There are no such residues in this entry.