



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:22 PM GMT

PDB ID : 4A22
Title : STRUCTURE OF MYCOBACTERIUM TUBERCULOSIS FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE BOUND TO N-(4-HYDROXYBUTYL)-GLYCOLOYDHYDROXAMICACID BIS-PHOSPHATE
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Deposited on : 2011-09-21
Resolution : 1.90 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>

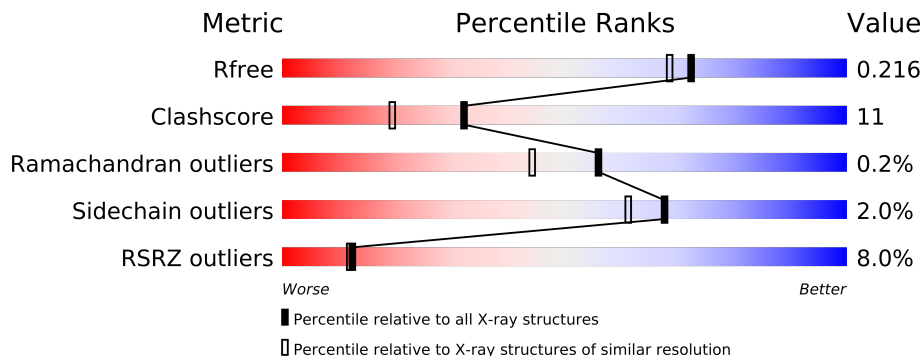
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.90 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	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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	1346	-	X
4	ZN	B	1345	-	X
5	SO4	B	1347	-	X

2 Entry composition i

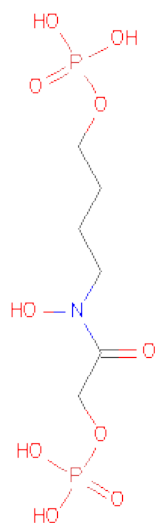
There are 6 unique types of molecules in this entry. The entry contains 20736 atoms, of which 9796 are hydrogens and 0 are deuterium.

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	329	Total	C	H	N	O	S	0	0	0
			4894	1557	2442	415	470	10			
1	B	329	Total	C	H	N	O	S	0	0	0
			4894	1557	2442	415	470	10			
1	C	329	Total	C	H	N	O	S	0	0	0
			4897	1557	2445	415	470	10			
1	D	329	Total	C	H	N	O	S	0	0	0
			4897	1557	2445	415	470	10			

- Molecule 2 is 4-{HYDROXY[(PHOSPHONOOXY)ACETYL]AMINO}BUTYLDIHYDROGEN PHOSPHATE (three-letter code: TD4) (formula: $C_6H_{15}NO_{10}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			30	6	11	1	10	2		
2	B	1	Total	C	H	N	O	P	0	0
			30	6	11	1	10	2		

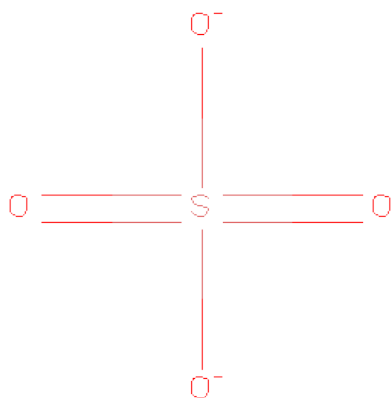
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

- Molecule 6 is water.

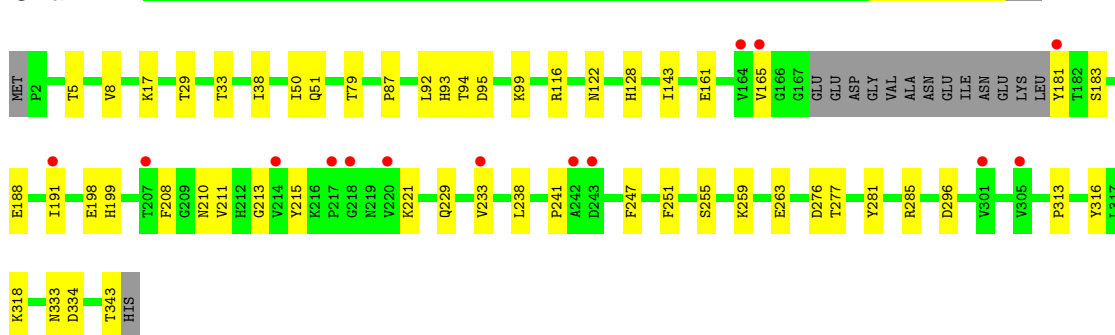
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	279	Total	O	0	0
			279	279		
6	B	253	Total	O	0	0
			253	253		
6	C	218	Total	O	0	0
			218	218		
6	D	296	Total	O	0	0
			296	296		

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.

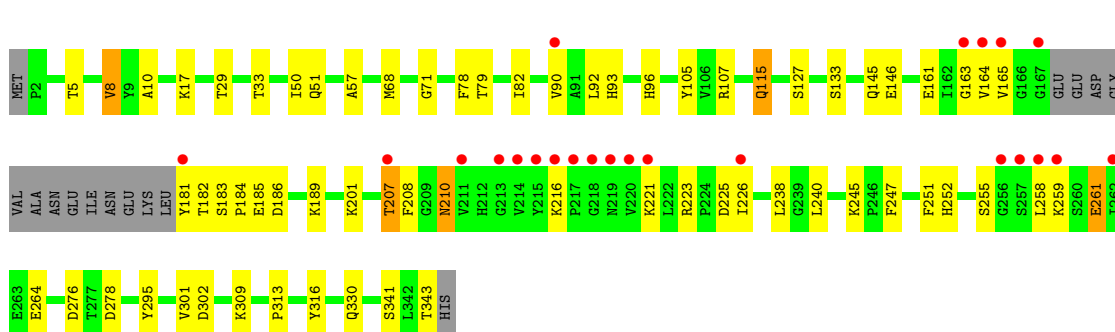
• Molecule 1: FRUCTOSE-BISPHOSPHATEALDOLASE

Chain A:



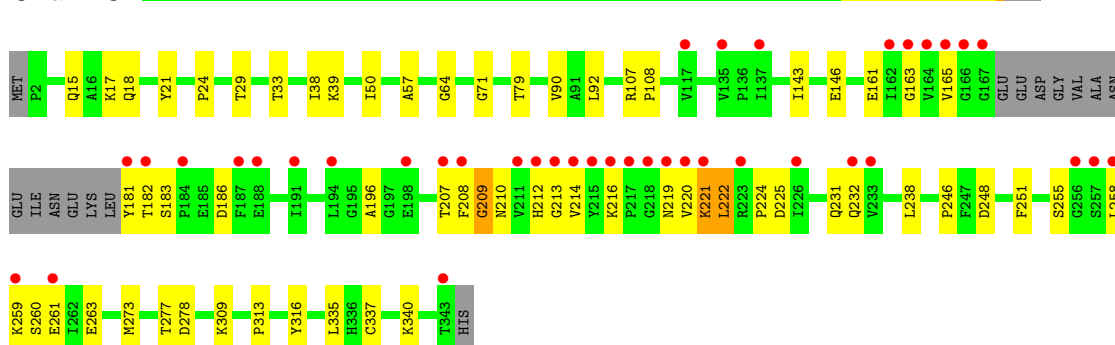
• Molecule 1: FRUCTOSE-BISPHOSPHATEALDOLASE

Chain B:



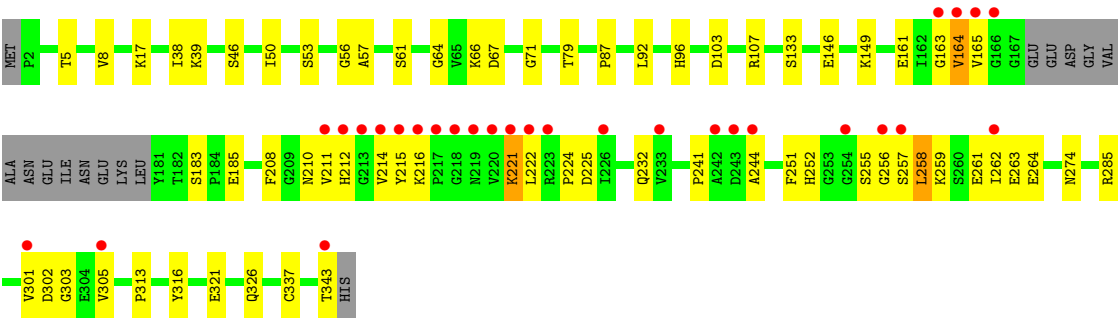
• Molecule 1: FRUCTOSE-BISPHOSPHATEALDOLASE

Chain C:



● 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	335.39Å 42.98Å 102.60Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	45.41 – 1.90 46.70 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.41-1.90) 99.3 (46.70-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.90Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.179 , 0.221 0.178 , 0.216	Depositor DCC
R_{free} test set	8855 reflections (7.75%)	DCC
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 38.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 114280 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20736	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 4.05% 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, ZN, SO4, TD4

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	0.44	0/2501	0.58	0/3387
1	B	0.43	0/2501	0.56	0/3387
1	C	0.37	0/2501	0.56	0/3387
1	D	0.44	0/2501	0.59	0/3387
All	All	0.42	0/10004	0.57	0/13548

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	2452	2442	0	38	0
1	B	2452	2442	0	68	1
1	C	2452	2445	0	53	0
1	D	2452	2445	0	62	0
2	A	19	11	0	4	0
2	B	19	11	0	4	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	10	0	0	3	0
5	B	10	0	0	3	0
5	C	10	0	0	3	0
5	D	10	0	0	4	0
6	A	279	0	0	9	0
6	B	253	0	0	13	0
6	C	218	0	0	7	0
6	D	296	0	0	23	1
All	All	10940	9796	0	224	1

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1344:TD4:C06	5:B:1347:SO4:O2	1.78	1.28
1:A:259:LYS:NZ	1:A:334:ASP:OD1	1.69	1.26
1:D:261:GLU:OE2	6:D:2220:HOH:O	1.72	1.05
1:C:216:LYS:NZ	1:D:303:GLY:O	1.96	0.97
1:C:232:GLN:NE2	6:C:2141:HOH:O	1.98	0.96
1:B:146:GLU:OE2	6:B:2138:HOH:O	1.86	0.94
1:A:181:TYR:HH	1:A:221:LYS:HE3	1.33	0.92
1:D:146:GLU:OE1	6:D:2156:HOH:O	1.87	0.92
1:C:216:LYS:HD3	1:D:305:VAL:HG11	1.54	0.89
1:D:225:ASP:OD2	6:D:2207:HOH:O	1.93	0.86
1:D:262:ILE:HD13	1:D:263:GLU:N	1.90	0.86
1:A:318:LYS:NZ	6:A:2253:HOH:O	2.08	0.85
1:A:259:LYS:HZ3	1:A:334:ASP:CG	1.79	0.85
1:C:309:LYS:NZ	6:C:2187:HOH:O	2.09	0.84
1:B:5:THR:HG1	1:B:8:VAL:HG11	1.45	0.82
1:D:255:SER:OG	5:D:1344:SO4:O3	1.97	0.81
1:B:163:GLY:HA3	1:B:207:THR:CG2	2.12	0.80
1:A:181:TYR:N	6:A:2167:HOH:O	2.15	0.79
1:B:223:ARG:NH1	6:B:2181:HOH:O	2.18	0.77
1:D:61:SER:HG	1:D:67:ASP:H	1.33	0.77
5:C:1345:SO4:O3	6:C:2060:HOH:O	2.03	0.77
1:A:87:PRO:O	1:A:343:THR:HG22	1.86	0.76
6:C:2180:HOH:O	1:D:216:LYS:NZ	2.20	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:326:GLN:NE2	6:D:2267:HOH:O	2.14	0.74
1:C:207:THR:O	1:C:207:THR:HG21	1.87	0.74
1:D:208:PHE:CE2	1:D:222:LEU:HD12	2.22	0.74
1:D:258:LEU:HB2	1:D:261:GLU:CD	2.06	0.74
1:B:107:ARG:NE	6:B:2093:HOH:O	2.06	0.74
5:D:1345:SO4:O2	6:D:2291:HOH:O	2.06	0.73
1:A:181:TYR:OH	1:A:221:LYS:HG3	1.90	0.72
1:D:259:LYS:O	1:D:262:ILE:HG13	1.89	0.71
1:B:163:GLY:HA3	1:B:207:THR:HG23	1.73	0.70
1:A:122:ASN:ND2	6:A:2142:HOH:O	2.16	0.70
1:B:341:SER:OG	1:B:343:THR:HG23	1.92	0.69
1:D:257:SER:HA	6:D:2220:HOH:O	1.93	0.69
1:A:296:ASP:OD1	6:A:2213:HOH:O	2.10	0.69
1:C:182:THR:N	1:C:207:THR:CG2	2.57	0.68
2:A:1344:TD4:O09	5:A:1350:SO4:O3	0.68	0.67
5:D:1344:SO4:O2	6:D:2198:HOH:O	2.11	0.67
1:D:5:THR:OG1	1:D:8:VAL:HG11	1.94	0.67
1:B:115:GLN:OE1	6:B:2112:HOH:O	2.12	0.67
1:C:259:LYS:O	1:C:263:GLU:HG2	1.94	0.66
1:B:238:LEU:CB	1:B:240:LEU:HD11	2.25	0.66
1:B:330:GLN:OE1	6:B:2245:HOH:O	2.12	0.66
1:C:207:THR:O	1:C:207:THR:CG2	2.43	0.66
1:D:208:PHE:CD2	1:D:222:LEU:HD12	2.31	0.65
1:B:309:LYS:HD2	6:B:2224:HOH:O	1.97	0.65
1:C:17:LYS:HD3	1:C:248:ASP:OD1	1.96	0.65
1:D:46:SER:HG	1:D:337:CYS:HG	1.43	0.65
1:A:181:TYR:HH	1:A:221:LYS:CE	2.08	0.65
1:B:238:LEU:HB2	1:B:240:LEU:HD11	1.80	0.64
1:B:163:GLY:HA3	1:B:207:THR:HG22	1.79	0.64
1:D:224:PRO:HB2	1:D:264:GLU:HG2	1.80	0.64
1:B:163:GLY:C	1:B:164:VAL:HG21	2.19	0.63
2:A:1344:TD4:O09	6:A:2069:HOH:O	2.15	0.63
1:A:29:THR:H	1:A:33:THR:HG1	1.47	0.62
1:D:183:SER:OG	1:D:185:GLU:HG2	2.00	0.62
1:B:17:LYS:HE3	1:B:247:PHE:O	2.00	0.62
1:A:116:ARG:HD2	6:A:2129:HOH:O	2.00	0.61
1:C:181:TYR:HA	1:C:207:THR:HG21	1.83	0.61
1:C:182:THR:N	1:C:207:THR:HG23	2.17	0.60
1:C:79:THR:HG22	1:C:92:LEU:HD22	1.84	0.60
1:D:241:PRO:O	1:D:244:ALA:CB	2.50	0.59
5:C:1345:SO4:O3	6:C:2218:HOH:O	2.16	0.59
1:B:182:THR:HG1	1:B:207:THR:H	1.51	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:182:THR:HG1	1:C:207:THR:HG23	1.66	0.59
1:D:255:SER:CB	5:D:1344:SO4:O3	2.52	0.57
1:C:196:ALA:HB3	1:C:238:LEU:HD12	1.86	0.57
1:D:258:LEU:N	6:D:2220:HOH:O	2.29	0.57
1:D:262:ILE:HD13	1:D:263:GLU:CA	2.35	0.57
1:D:53:SER:HG	1:D:56:GLY:H	1.53	0.57
1:B:181:TYR:CB	1:B:223:ARG:NH2	2.68	0.56
1:C:163:GLY:HA3	1:C:207:THR:HB	1.87	0.56
1:B:255:SER:OG	2:B:1344:TD4:O19	2.24	0.56
1:B:181:TYR:CB	1:B:223:ARG:HH21	2.18	0.56
1:C:222:LEU:HD12	1:C:261:GLU:HB3	1.87	0.56
1:D:244:ALA:HA	6:D:2217:HOH:O	2.06	0.55
1:C:15:GLN:NE2	6:C:2014:HOH:O	2.38	0.55
1:B:276:ASP:HB2	2:B:1344:TD4:H03	1.89	0.55
1:D:241:PRO:O	1:D:244:ALA:HB1	2.07	0.55
1:D:87:PRO:O	1:D:343:THR:HG21	2.07	0.55
1:B:133:SER:HB2	1:B:163:GLY:O	2.08	0.54
1:C:255:SER:HG	1:C:278:ASP:H	1.55	0.54
1:A:333:ASN:ND2	6:A:2268:HOH:O	2.40	0.54
1:D:96:HIS:HE1	6:D:2098:HOH:O	1.91	0.54
1:C:181:TYR:HA	1:C:207:THR:CG2	2.38	0.54
1:B:295:TYR:HH	1:D:285:ARG:HH12	1.54	0.53
1:B:185:GLU:OE1	1:B:189:LYS:HE3	2.07	0.53
1:B:276:ASP:HB3	5:B:1346:SO4:O4	2.09	0.53
1:A:255:SER:OG	2:A:1344:TD4:O19	2.26	0.53
1:A:79:THR:HG22	1:A:92:LEU:HD22	1.90	0.53
1:B:182:THR:HG1	1:B:207:THR:HG21	1.74	0.53
1:A:188:GLU:HG2	1:A:233:VAL:CG1	2.39	0.52
1:D:301:VAL:HG11	1:D:302:ASP:N	2.23	0.52
1:C:209:GLY:HA3	1:C:222:LEU:HA	1.90	0.52
1:B:164:VAL:H	1:B:207:THR:HG22	1.75	0.52
1:B:182:THR:HG1	1:B:207:THR:CG2	2.22	0.52
1:B:223:ARG:NH1	1:B:226:ILE:HD12	2.24	0.52
1:D:232:GLN:HG2	6:D:2210:HOH:O	2.10	0.52
1:B:68:MET:HB3	1:B:105:TYR:CD1	2.45	0.52
1:A:213:GLY:HA2	1:A:277:THR:HG1	1.75	0.51
1:D:252:HIS:CE1	1:D:274:ASN:ND2	2.78	0.51
1:A:191:ILE:HD12	1:A:238:LEU:HD12	1.93	0.50
1:B:79:THR:HG22	1:B:92:LEU:HD22	1.91	0.50
1:C:216:LYS:HD3	1:D:305:VAL:CG1	2.36	0.50
1:D:244:ALA:HA	6:D:2212:HOH:O	2.12	0.50
2:B:1344:TD4:O07	5:B:1347:SO4:O2	0.52	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:29:THR:H	1:C:33:THR:HG1	1.58	0.50
1:A:313:PRO:HA	1:A:316:TYR:CE1	2.47	0.50
1:B:78:PHE:CE2	1:B:82:ILE:HG13	2.46	0.49
1:D:263:GLU:HG3	6:D:2223:HOH:O	2.12	0.49
1:D:61:SER:HG	1:D:67:ASP:N	2.07	0.49
1:D:66:LYS:HE3	6:D:2066:HOH:O	2.13	0.49
1:C:183:SER:OG	1:C:186:ASP:N	2.41	0.49
1:B:301:VAL:HG11	1:B:302:ASP:N	2.28	0.49
1:D:214:VAL:HG11	1:D:215:TYR:N	2.27	0.49
1:B:258:LEU:HB2	1:B:261:GLU:HG3	1.94	0.49
1:B:29:THR:H	1:B:33:THR:HG1	1.60	0.48
1:C:107:ARG:HB2	1:C:108:PRO:HD3	1.95	0.48
1:B:5:THR:OG1	1:B:8:VAL:HG11	2.11	0.48
1:D:183:SER:HG	1:D:185:GLU:HG2	1.76	0.48
1:C:18:GLN:NE2	6:C:2021:HOH:O	2.36	0.48
1:B:107:ARG:NH2	6:B:2093:HOH:O	2.47	0.48
1:C:221:LYS:HG3	1:C:221:LYS:O	2.15	0.47
1:B:238:LEU:HB3	1:B:240:LEU:HD11	1.97	0.47
1:C:214:VAL:HG22	1:C:277:THR:CG2	2.43	0.47
1:D:210:ASN:C	1:D:211:VAL:HG21	2.35	0.47
1:B:309:LYS:HG3	6:B:2223:HOH:O	2.14	0.47
1:A:259:LYS:O	1:A:263:GLU:HG3	2.13	0.47
1:B:182:THR:HG1	1:B:207:THR:N	2.13	0.47
1:B:161:GLU:OE2	1:B:165:VAL:HG21	2.14	0.47
1:D:321:GLU:OE1	6:D:2262:HOH:O	2.21	0.47
1:A:221:LYS:O	1:A:221:LYS:HG3	2.14	0.47
1:B:10:ALA:CB	1:B:201:LYS:HE3	2.45	0.47
1:B:313:PRO:HA	1:B:316:TYR:CZ	2.50	0.47
1:D:79:THR:HG22	1:D:92:LEU:HD22	1.96	0.47
1:A:281:TYR:HH	1:A:285:ARG:HD3	1.80	0.47
1:C:222:LEU:HD13	1:C:224:PRO:HD3	1.97	0.46
1:B:17:LYS:HE2	1:B:245:LYS:CB	2.45	0.46
1:B:93:HIS:ND1	1:B:127:SER:OG	2.48	0.46
1:B:181:TYR:HB2	1:B:223:ARG:NH2	2.30	0.46
1:D:133:SER:HB2	1:D:163:GLY:C	2.36	0.46
1:A:38:ILE:HG13	1:A:50:ILE:HD12	1.97	0.46
5:A:1350:SO4:O3	6:A:2069:HOH:O	2.19	0.46
1:C:165:VAL:HG13	1:C:212:HIS:CG	2.50	0.46
1:A:229:GLN:HB2	6:A:2186:HOH:O	2.16	0.46
1:B:240:LEU:HD13	1:B:240:LEU:N	2.31	0.46
1:A:198:GLU:HG2	1:A:199:HIS:N	2.31	0.46
1:B:210:ASN:HB3	1:B:252:HIS:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:99:LYS:HE3	1:A:143:ILE:HD12	1.98	0.45
1:D:5:THR:HG1	1:D:8:VAL:H	1.64	0.45
1:D:149:LYS:CG	6:D:2061:HOH:O	2.64	0.45
1:C:313:PRO:HA	1:C:316:TYR:CE2	2.51	0.45
1:A:188:GLU:O	1:A:191:ILE:HG23	2.16	0.45
1:B:182:THR:HG21	6:B:2147:HOH:O	2.17	0.45
1:B:255:SER:HG	1:B:278:ASP:H	1.64	0.45
1:C:21:TYR:CE2	1:C:340:LYS:HD3	2.51	0.45
1:C:182:THR:H	1:C:207:THR:CG2	2.27	0.44
1:A:95:ASP:OD2	2:A:1344:TD4:H03A	2.17	0.44
1:A:198:GLU:HG2	1:A:199:HIS:ND1	2.32	0.44
1:C:255:SER:OG	5:C:1344:SO4:O4	2.35	0.44
1:D:163:GLY:CA	6:D:2166:HOH:O	2.65	0.44
1:C:64:GLY:CA	1:D:39:LYS:HD3	2.48	0.44
1:B:238:LEU:HB3	1:B:240:LEU:CD1	2.48	0.44
1:C:213:GLY:O	1:C:214:VAL:HG21	2.18	0.44
1:D:149:LYS:HG2	6:D:2061:HOH:O	2.17	0.44
1:B:259:LYS:HG2	6:B:2089:HOH:O	2.16	0.44
1:A:5:THR:HG1	1:A:8:VAL:H	1.65	0.44
1:C:273:MET:HE3	1:C:335:LEU:HD22	2.00	0.44
1:B:51:GLN:HA	1:B:93:HIS:O	2.18	0.44
1:C:231:GLN:OE1	1:C:246:PRO:HD2	2.18	0.43
1:A:211:VAL:HG13	1:A:215:TYR:CE2	2.53	0.43
1:D:313:PRO:HA	1:D:316:TYR:CE1	2.53	0.43
1:A:313:PRO:HA	1:A:316:TYR:CZ	2.53	0.43
1:C:208:PHE:O	1:C:208:PHE:CG	2.72	0.43
1:D:164:VAL:N	6:D:2140:HOH:O	2.50	0.43
1:B:182:THR:HG23	1:B:183:SER:N	2.33	0.43
1:C:182:THR:H	1:C:207:THR:HG23	1.83	0.43
1:B:258:LEU:HB2	1:B:261:GLU:CG	2.48	0.43
1:C:210:ASN:N	1:C:210:ASN:OD1	2.51	0.43
1:B:183:SER:OG	1:B:186:ASP:CG	2.56	0.43
1:B:107:ARG:CZ	6:B:2093:HOH:O	2.58	0.43
1:D:258:LEU:HB2	1:D:261:GLU:CG	2.48	0.43
1:B:57:ALA:O	1:B:71:GLY:HA3	2.19	0.43
1:C:220:VAL:O	1:C:220:VAL:HG13	2.19	0.43
1:C:38:ILE:HG13	1:C:50:ILE:HD12	2.01	0.42
1:D:103:ASP:OD1	1:D:107:ARG:NH1	2.46	0.42
1:A:161:GLU:OE2	1:A:165:VAL:HG21	2.19	0.42
1:D:161:GLU:CD	6:D:2098:HOH:O	2.58	0.42
1:C:258:LEU:HG	1:C:260:SER:H	1.83	0.42
1:B:183:SER:HA	1:B:184:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:208:PHE:CD1	1:C:208:PHE:N	2.87	0.42
1:C:143:ILE:O	1:C:146:GLU:HG2	2.19	0.42
1:D:165:VAL:HG22	1:D:212:HIS:CE1	2.54	0.42
1:D:262:ILE:CD1	1:D:263:GLU:N	2.73	0.42
1:D:164:VAL:HB	6:D:2140:HOH:O	2.20	0.42
1:B:255:SER:HB3	1:B:278:ASP:CG	2.40	0.42
1:B:17:LYS:HE2	1:B:245:LYS:HB2	2.02	0.42
1:A:51:GLN:HA	1:A:93:HIS:O	2.20	0.42
1:D:57:ALA:O	1:D:71:GLY:HA3	2.20	0.42
1:D:165:VAL:HG13	1:D:210:ASN:ND2	2.35	0.41
1:A:94:THR:HG1	1:A:128:HIS:HD1	1.69	0.41
1:C:161:GLU:HG2	1:C:163:GLY:O	2.21	0.41
1:C:39:LYS:HD3	1:D:64:GLY:HA3	2.03	0.41
1:D:38:ILE:HG13	1:D:50:ILE:HD12	2.03	0.41
1:C:216:LYS:O	1:C:219:ASN:OD1	2.38	0.41
1:B:216:LYS:NZ	6:B:2178:HOH:O	2.25	0.41
1:B:181:TYR:O	6:B:2151:HOH:O	2.21	0.41
1:D:256:GLY:HA2	6:D:2219:HOH:O	2.20	0.41
1:B:50:ILE:HD13	1:B:90:VAL:HG12	2.01	0.41
1:B:208:PHE:CD1	1:B:208:PHE:N	2.89	0.41
1:A:17:LYS:HE3	1:A:247:PHE:O	2.21	0.41
1:A:208:PHE:N	1:A:208:PHE:CD1	2.89	0.41
1:B:225:ASP:OD1	1:B:264:GLU:OE2	2.39	0.41
1:B:10:ALA:HB3	1:B:201:LYS:HE3	2.03	0.40
1:A:276:ASP:HB3	5:A:1349:SO4:O2	2.20	0.40
1:D:221:LYS:HG2	6:D:2171:HOH:O	2.20	0.40
1:C:24:PRO:HD3	1:C:337:CYS:SG	2.60	0.40
1:B:182:THR:CG2	1:B:183:SER:N	2.84	0.40
1:C:57:ALA:O	1:C:71:GLY:HA3	2.21	0.40
1:B:133:SER:CB	1:B:163:GLY:O	2.68	0.40
1:C:313:PRO:HA	1:C:316:TYR:CZ	2.56	0.40
1:C:273:MET:CE	1:C:335:LEU:HD22	2.51	0.40
1:C:50:ILE:HD13	1:C:90:VAL:HG12	2.04	0.40

All (1) 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)
1:B:145:GLN:OE1	6:D:2285:HOH:O[1_554]	1.77	0.43

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	325/344 (94%)	323 (99%)	2 (1%)	0	100	100
1	B	325/344 (94%)	321 (99%)	3 (1%)	1 (0%)	50	37
1	C	325/344 (94%)	321 (99%)	3 (1%)	1 (0%)	50	37
1	D	325/344 (94%)	320 (98%)	5 (2%)	0	100	100
All	All	1300/1376 (94%)	1285 (99%)	13 (1%)	2 (0%)	56	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	96	HIS
1	C	209	GLY

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	253/266 (95%)	249 (98%)	4 (2%)	75	70
1	B	253/266 (95%)	246 (97%)	7 (3%)	56	45
1	C	253/266 (95%)	249 (98%)	4 (2%)	75	70
1	D	253/266 (95%)	248 (98%)	5 (2%)	68	61
All	All	1012/1064 (95%)	992 (98%)	20 (2%)	68	61

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	SER

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Mol	Chain	Res	Type
1	A	210	ASN
1	A	241	PRO
1	A	251	PHE
1	B	8	VAL
1	B	115	GLN
1	B	207	THR
1	B	210	ASN
1	B	221	LYS
1	B	251	PHE
1	B	261	GLU
1	C	221	LYS
1	C	222	LEU
1	C	225	ASP
1	C	251	PHE
1	D	17	LYS
1	D	164	VAL
1	D	221	LYS
1	D	251	PHE
1	D	258	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	19	ASN
1	A	35	ASN
1	A	89	ASN
1	A	122	ASN
1	A	294	ASN
1	A	333	ASN
1	A	336	HIS
1	B	15	GLN
1	B	35	ASN
1	B	89	ASN
1	B	122	ASN
1	B	145	GLN
1	B	294	ASN
1	C	35	ASN
1	C	51	GLN
1	C	115	GLN
1	C	212	HIS
1	C	232	GLN

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Mol	Chain	Res	Type
1	C	280	GLN
1	D	15	GLN
1	D	35	ASN
1	D	229	GLN
1	D	280	GLN
1	D	294	ASN
1	D	326	GLN
1	D	336	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 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	TD4	A	1344	3,5,4	18,18,18	2.52	7 (38%)	25,25,25	1.44	3 (12%)
5	SO4	A	1349	3,2	4,4,4	0.25	0	6,6,6	0.09	0
5	SO4	A	1350	2	4,4,4	0.21	0	6,6,6	0.08	0
2	TD4	B	1344	3,5,4	18,18,18	2.61	7 (38%)	25,25,25	1.39	3 (12%)
5	SO4	B	1346	3,2	4,4,4	0.25	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	B	1347	2	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	C	1344	3	4,4,4	0.22	0	6,6,6	0.14	0
5	SO4	C	1345	-	4,4,4	0.20	0	6,6,6	0.23	0
5	SO4	D	1344	3	4,4,4	0.25	0	6,6,6	0.15	0
5	SO4	D	1345	-	4,4,4	0.13	0	6,6,6	0.18	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	TD4	A	1344	3,5,4	-	0/19/19/19	0/0/0/0
5	SO4	A	1349	3,2	-	0/0/0/0	0/0/0/0
5	SO4	A	1350	2	-	0/0/0/0	0/0/0/0
2	TD4	B	1344	3,5,4	-	0/19/19/19	0/0/0/0
5	SO4	B	1346	3,2	-	0/0/0/0	0/0/0/0
5	SO4	B	1347	2	-	0/0/0/0	0/0/0/0
5	SO4	C	1344	3	-	0/0/0/0	0/0/0/0
5	SO4	C	1345	-	-	0/0/0/0	0/0/0/0
5	SO4	D	1344	3	-	0/0/0/0	0/0/0/0
5	SO4	D	1345	-	-	0/0/0/0	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1344	TD4	C12-N02	6.06	1.46	1.35
2	A	1344	TD4	C12-N02	5.89	1.45	1.35
2	B	1344	TD4	O15-C14	-4.95	1.39	1.43
2	A	1344	TD4	O15-C14	-4.68	1.39	1.43
2	B	1344	TD4	P08-O09	4.54	1.66	1.51
2	A	1344	TD4	P08-O09	4.37	1.65	1.51
2	A	1344	TD4	P08-O10	2.96	1.65	1.54
2	B	1344	TD4	P08-O10	2.79	1.64	1.54
2	A	1344	TD4	P16-O18	2.75	1.64	1.54
2	B	1344	TD4	P16-O18	2.70	1.64	1.54
2	B	1344	TD4	P16-O17	2.45	1.63	1.54
2	B	1344	TD4	P08-O11	-2.28	1.46	1.54
2	A	1344	TD4	P16-O17	2.26	1.63	1.54
2	A	1344	TD4	P08-O11	-2.20	1.46	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1344	TD4	O15-C14-C12	4.30	117.03	110.39
2	B	1344	TD4	C04-C03-N02	3.49	117.54	111.17
2	B	1344	TD4	O15-C14-C12	3.40	115.65	110.39
2	A	1344	TD4	C04-C03-N02	3.26	117.12	111.17
2	B	1344	TD4	O07-C06-C05	2.54	118.48	109.19
2	A	1344	TD4	O07-C06-C05	2.08	116.82	109.19

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	329/344 (95%)	0.20	14 (4%)	34 34	11, 22, 53, 111	0
1	B	329/344 (95%)	0.26	23 (6%)	16 16	12, 24, 58, 121	0
1	C	329/344 (95%)	0.60	40 (12%)	5 4	12, 33, 84, 139	0
1	D	329/344 (95%)	0.47	29 (8%)	10 9	11, 23, 77, 146	0
All	All	1316/1376 (95%)	0.38	106 (8%)	12 11	11, 26, 70, 146	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	164	VAL	19.1
1	D	218	GLY	12.1
1	D	165	VAL	11.0
1	D	212	HIS	10.2
1	B	220	VAL	9.7
1	C	220	VAL	9.4
1	C	215	TYR	8.5
1	C	164	VAL	8.3
1	C	216	LYS	7.7
1	D	220	VAL	7.7
1	D	214	VAL	7.7
1	C	214	VAL	7.6
1	C	165	VAL	7.2
1	B	214	VAL	6.8
1	C	217	PRO	5.9
1	B	217	PRO	5.7
1	D	163	GLY	5.7
1	D	217	PRO	5.7
1	C	163	GLY	5.7
1	C	211	VAL	5.5
1	D	215	TYR	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	216	LYS	5.5
1	B	218	GLY	5.4
1	C	218	GLY	5.3
1	B	221	LYS	5.3
1	D	219	ASN	5.2
1	C	219	ASN	4.9
1	A	218	GLY	4.9
1	A	164	VAL	4.8
1	A	220	VAL	4.8
1	D	221	LYS	4.6
1	B	165	VAL	4.6
1	D	211	VAL	4.6
1	C	221	LYS	4.5
1	B	164	VAL	4.5
1	B	215	TYR	4.5
1	A	305	VAL	4.5
1	C	167	GLY	4.4
1	B	219	ASN	4.2
1	B	211	VAL	4.1
1	C	343	THR	4.0
1	D	242	ALA	4.0
1	D	216	LYS	4.0
1	A	214	VAL	3.8
1	D	213	GLY	3.8
1	C	162	ILE	3.8
1	A	165	VAL	3.6
1	D	262	ILE	3.6
1	B	163	GLY	3.6
1	C	184	PRO	3.6
1	C	137	ILE	3.5
1	A	181	TYR	3.5
1	C	181	TYR	3.5
1	C	232	GLN	3.3
1	B	181	TYR	3.1
1	C	213	GLY	3.0
1	D	254	GLY	3.0
1	D	244	ALA	3.0
1	C	207	THR	3.0
1	C	191	ILE	2.9
1	C	166	GLY	2.9
1	C	226	ILE	2.9
1	D	226	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	262	ILE	2.8
1	D	305	VAL	2.8
1	C	212	HIS	2.7
1	D	256	GLY	2.7
1	D	243	ASP	2.7
1	A	233	VAL	2.7
1	C	187	PHE	2.7
1	A	242	ALA	2.7
1	D	166	GLY	2.7
1	C	256	GLY	2.6
1	D	257	SER	2.6
1	D	343	THR	2.6
1	C	208	PHE	2.6
1	B	256	GLY	2.5
1	A	217	PRO	2.5
1	D	223	ARG	2.5
1	C	261	GLU	2.4
1	B	258	LEU	2.4
1	C	194	LEU	2.4
1	B	257	SER	2.4
1	B	226	ILE	2.4
1	C	117	VAL	2.4
1	C	188	GLU	2.3
1	A	191	ILE	2.3
1	B	207	THR	2.3
1	D	233	VAL	2.3
1	C	182	THR	2.2
1	C	258	LEU	2.2
1	A	207	THR	2.2
1	A	301	VAL	2.2
1	C	223	ARG	2.2
1	B	259	LYS	2.2
1	C	257	SER	2.1
1	D	301	VAL	2.1
1	C	135	VAL	2.1
1	D	222	LEU	2.1
1	C	233	VAL	2.1
1	C	259	LYS	2.1
1	B	90	VAL	2.1
1	C	198	GLU	2.1
1	A	243	ASP	2.1
1	B	213	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	167	GLY	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	1346	1/1	0.22	5.09	31,31,31,31	0
5	SO4	B	1347	5/5	0.13	3.09	38,44,47,48	5
4	ZN	B	1345	1/1	0.33	2.28	45,45,45,45	1
5	SO4	D	1345	5/5	0.13	1.25	34,40,56,56	0
2	TD4	B	1344	19/19	0.20	0.57	23,34,45,47	30
5	SO4	C	1345	5/5	0.12	0.36	33,35,60,62	0
5	SO4	A	1350	5/5	0.11	0.35	33,35,38,41	5
2	TD4	A	1344	19/19	0.12	-0.14	21,31,40,41	30
5	SO4	D	1344	5/5	0.17	-0.38	34,40,52,55	0
5	SO4	B	1346	5/5	0.14	-0.43	31,32,38,39	5
5	SO4	A	1349	5/5	0.10	-0.67	22,23,28,28	5
4	ZN	A	1348	1/1	0.08	-0.78	36,36,36,36	1
5	SO4	C	1344	5/5	0.11	-0.86	38,43,51,55	0
3	NA	B	1348	1/1	0.13	-0.94	46,46,46,46	0
3	NA	C	1346	1/1	0.12	-1.29	71,71,71,71	0
3	NA	A	1345	1/1	0.06	-1.33	33,33,33,33	0
3	NA	D	1346	1/1	0.12	-1.36	73,73,73,73	0
3	NA	A	1347	1/1	0.05	-3.43	25,25,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.