Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 06:00 am BST

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 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 (i) 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 (i)) were used in the production of this report:

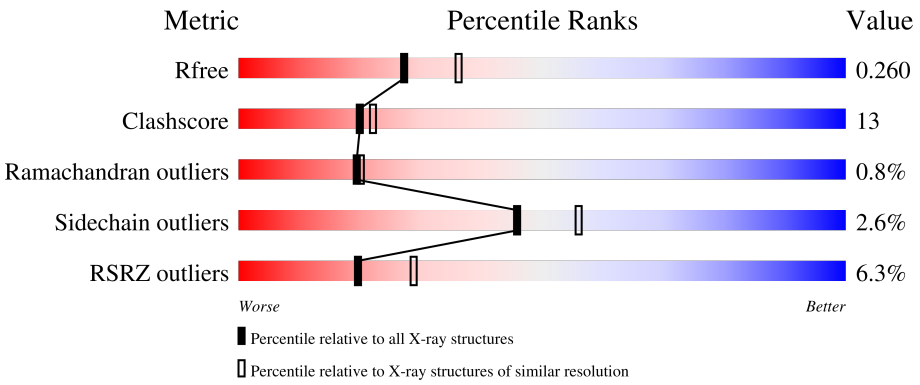
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 <=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	344	6% 74% 17% • 9%
1	B	344	5% 66% 24% • 9%
1	C	344	8% 67% 22% • 9%
1	D	344	5% 70% 19% • 9%

Validation Pipeline (wwPDB-VP) : 2.36.2

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	D	1345	-	-	X	-

2 Entry composition (i)

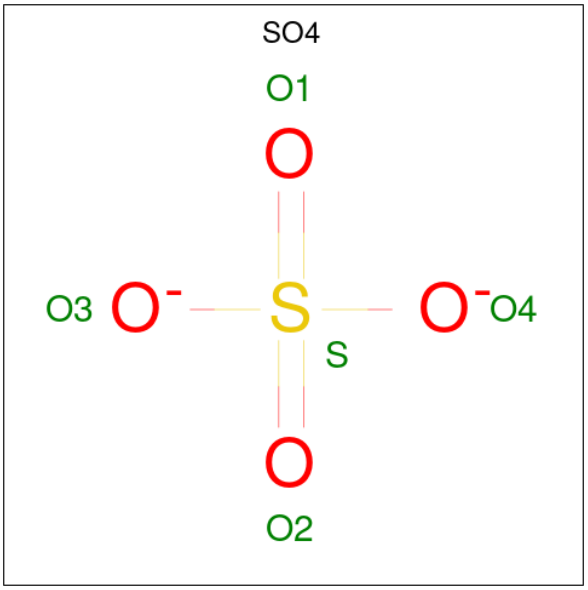
There are 4 unique types of molecules in this entry. The entry contains 19522 atoms, of which 9296 are hydrogens and 0 are deuteriums.

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 FRUCTOSE-BISPHOSPHATE ALDOLASE.

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

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Na 2 2	0	0

- Molecule 4 is water.

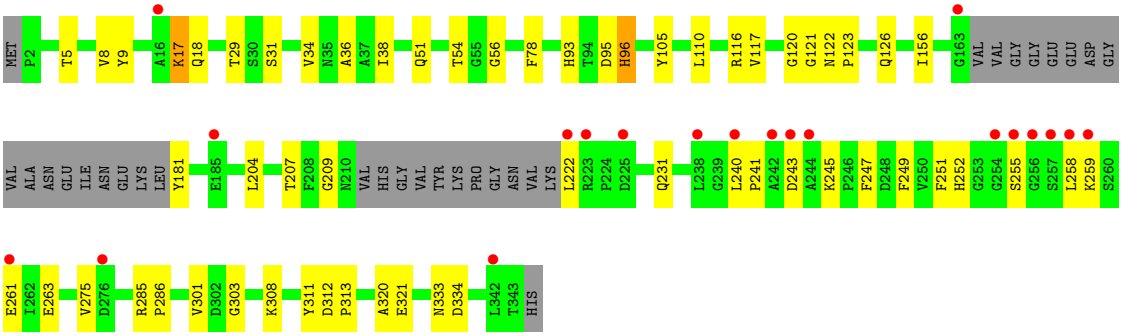
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	215	Total O 215 215	0	0
4	B	205	Total O 205 205	0	0
4	C	185	Total O 185 185	0	0
4	D	195	Total O 195 195	0	0

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.

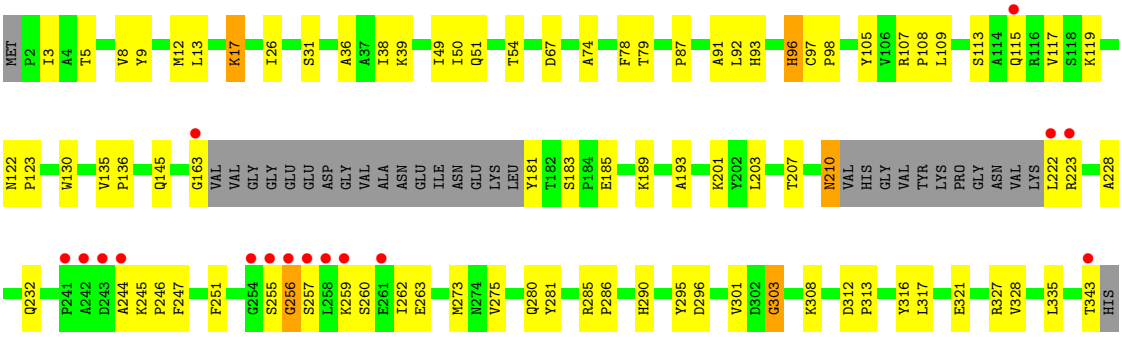
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE

Chain A:



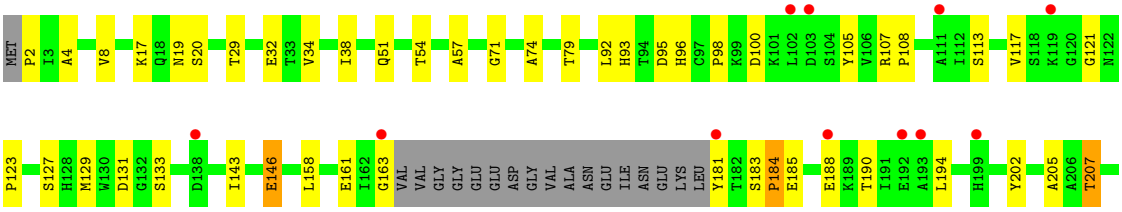
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE

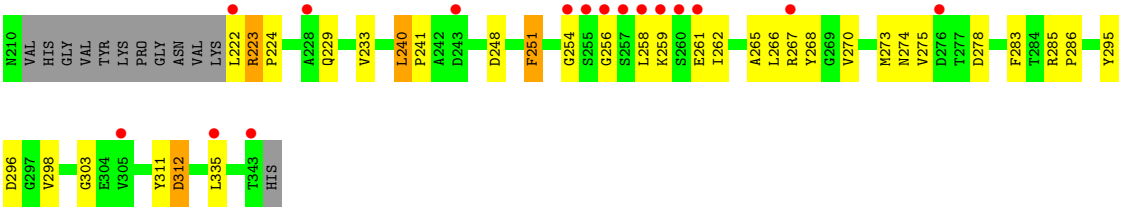
Chain B:



• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE

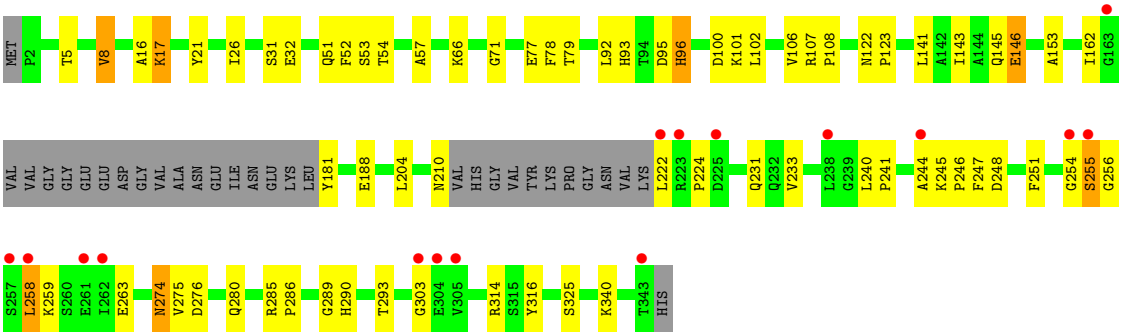
Chain C:





• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.07 (at 2.34Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.211 , 0.261 0.220 , 0.260	Depositor DCC
R_{free} test set	4629 reflections (7.52%)	wwPDB-VP
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 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, 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 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	2346	2325	2323	50	0
1	B	2346	2325	2323	66	0
1	C	2346	2323	2323	65	0
1	D	2346	2323	2323	61	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
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	215	0	0	20	1
4	B	205	0	0	22	1
4	C	185	0	0	21	1
4	D	195	0	0	14	0
All	All	10226	9296	9292	236	2

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 13.

All (236) 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:258:LEU:HB3	4:A:2170:HOH:O	1.58	1.02
1:B:257:SER:HA	4:B:2161:HOH:O	1.61	0.99
1:A:181:TYR:CZ	4:A:2138:HOH:O	2.22	0.92
1:C:267:ARG:HA	4:C:2033:HOH:O	1.68	0.92
1:C:163:GLY:HA3	1:C:207:THR:OG1	1.84	0.78
1:C:259:LYS:HE3	4:C:2139:HOH:O	1.84	0.75
1:B:87:PRO:O	1:B:343:THR:HG21	1.89	0.72
1:A:181:TYR:CE2	4:A:2138:HOH:O	2.42	0.70
1:C:278:ASP:O	4:C:2148:HOH:O	2.10	0.69
1:D:224:PRO:HG2	4:D:2146:HOH:O	1.90	0.69
1:D:255:SER:HB2	2:D:1345:SO4:O3	1.93	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	1.94	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:C:254:GLY:HA2	4:C:2134:HOH:O	1.95	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:HG21	1:B:92:LEU:HD21	1.80	0.64
1:D:181:TYR:N	4:D:2100:HOH:O	2.30	0.64
1:C:181:TYR:CZ	1:C:223:ARG:HG3	2.32	0.64
1:B:210:ASN:N	1:B:210:ASN:OD1	2.31	0.64
1:D:240:LEU:HB3	1:D:241:PRO:HD2	1.81	0.63
1:C:185:GLU:HA	4:C:2113:HOH:O	1.99	0.63
1:B:327:ARG:HB2	4:B:2194:HOH:O	2.00	0.62
1:D:259:LYS:O	1:D:263:GLU:HG2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:GLY:CA	4:C:2134:HOH:O	2.47	0.61
1:B:232:GLN:HB2	4:B:2152:HOH:O	2.00	0.61
1:B:222:LEU:N	4:B:2128:HOH:O	2.33	0.61
1:B:301:VAL:HG13	4:B:2182:HOH:O	2.00	0.60
1:C:265:ALA:HB1	1:C:270:VAL:HG21	1.82	0.60
1:B:26:ILE:HD12	1:B:328:VAL:HG22	1.83	0.60
1:B:201:LYS:O	4:B:2125:HOH:O	2.16	0.60
1:D:5:THR:OG1	1:D:8:VAL:HG13	2.02	0.60
1:B:257:SER:C	4:B:2160:HOH:O	2.41	0.59
1:B:181:TYR:CZ	1:B:223:ARG:HG3	2.38	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:C:133:SER:HB2	1:C:163:GLY:C	2.23	0.59
1:A:18:GLN:HG3	4:A:2020:HOH:O	2.02	0.58
1:C:29:THR:HG21	1:D:314:ARG:HD3	1.85	0.58
1:B:17:LYS:HE2	1:B:245:LYS:HB3	1.86	0.58
1:B:96:HIS:HE1	4:B:2071:HOH:O	1.86	0.57
1:C:129:MET:HE2	1:C:131:ASP:HB2	1.86	0.57
1:B:255:SER:C	4:B:2158:HOH:O	2.42	0.56
1:B:260:SER:HB3	4:B:2163:HOH:O	2.03	0.56
1:C:222:LEU:O	1:C:223:ARG:HG2	2.03	0.56
1:D:79:THR:HG21	1:D:92:LEU:HD21	1.86	0.56
1:D:274:ASN:HD22	1:D:274:ASN:N	2.01	0.56
1:B:17:LYS:HE3	1:B:247:PHE:O	2.06	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:C:254:GLY:C	4:C:2134:HOH:O	2.44	0.55
1:D:53:SER:HA	1:D:95:ASP:HB3	1.88	0.55
1:A:121:GLY:N	4:A:2105:HOH:O	2.39	0.55
1:C:261:GLU:HG2	4:C:2141:HOH:O	2.06	0.55
1:D:325:SER:HB2	4:D:2168:HOH:O	2.06	0.55
1:A:258:LEU:HB2	1:A:261:GLU:CD	2.28	0.55
1:B:260:SER:CB	4:B:2163:HOH:O	2.54	0.55
1:D:107:ARG:HB2	1:D:108:PRO:HD3	1.88	0.54
1:D:122:ASN:HB3	4:D:2006:HOH:O	2.08	0.54
1:B:343:THR:HG22	4:B:2067:HOH:O	2.07	0.54
1:B:38:ILE:HG13	1:B:50:ILE:HD11	1.88	0.54
1:A:54:THR:HG22	1:A:105:TYR:CD2	2.42	0.54
1:A:17:LYS:HE2	1:A:245:LYS:HB3	1.88	0.54
1:A:34:VAL:O	1:A:38:ILE:HG13	2.07	0.53
1:A:308:LYS:HD3	4:B:2085:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:THR:C	4:B:2204:HOH:O	2.46	0.53
1:B:259:LYS:O	1:B:263:GLU:HG2	2.09	0.53
1:D:290:HIS:CG	1:D:316:TYR:HB3	2.44	0.52
1:A:116:ARG:O	4:A:2105:HOH:O	2.19	0.52
1:B:257:SER:CA	4:B:2160:HOH:O	2.57	0.52
1:B:107:ARG:N	1:B:108:PRO:CD	2.73	0.52
1:D:289:GLY:O	1:D:293:THR:HG23	2.08	0.52
1:A:286:PRO:HG2	1:A:320:ALA:HA	1.91	0.52
1:D:54:THR:HG23	4:D:2045:HOH:O	2.09	0.52
1:D:17:LYS:CE	1:D:245:LYS:O	2.58	0.52
1:A:96:HIS:HE1	4:A:2086:HOH:O	1.93	0.52
1:D:244:ALA:O	1:D:246:PRO:HD3	2.10	0.52
1:D:52:PHE:HA	4:D:2031:HOH:O	2.08	0.52
1:D:274:ASN:N	1:D:274:ASN:ND2	2.57	0.52
1:C:143:ILE:O	1:C:146:GLU:HG3	2.10	0.52
1:C:251:PHE:HB2	1:C:270:VAL:HG11	1.92	0.52
1:A:259:LYS:HE3	1:A:334:ASP:OD1	2.10	0.51
1:D:66:LYS:HD3	4:D:2051:HOH:O	2.10	0.51
1:A:110:LEU:HD23	1:A:156:ILE:HD12	1.91	0.51
1:A:243:ASP:CB	4:A:2164:HOH:O	2.58	0.51
1:D:143:ILE:O	1:D:146:GLU:HG3	2.10	0.51
1:A:311:TYR:CE1	1:B:281:TYR:HB2	2.46	0.51
1:B:185:GLU:OE2	1:B:189:LYS:HE2	2.11	0.51
1:B:256:GLY:N	4:B:2159:HOH:O	2.43	0.51
1:D:258:LEU:HD23	1:D:258:LEU:N	2.24	0.51
1:C:312:ASP:OD1	1:C:312:ASP:C	2.50	0.51
1:C:2:PRO:HB2	4:C:2001:HOH:O	2.11	0.51
1:C:258:LEU:HB2	1:C:261:GLU:HG3	1.93	0.50
1:D:276:ASP:O	1:D:280:GLN:HG3	2.11	0.50
1:D:153:ALA:HB3	4:D:2095:HOH:O	2.10	0.50
1:D:26:ILE:HD13	1:D:275:VAL:HG22	1.93	0.50
1:D:141:LEU:O	1:D:145:GLN:HG3	2.11	0.50
1:C:262:ILE:O	1:C:266:LEU:HG	2.12	0.50
4:A:2180:HOH:O	1:B:308:LYS:HG2	2.11	0.50
1:B:9:TYR:O	1:B:12:MET:HB2	2.11	0.50
1:B:5:THR:OG1	1:B:8:VAL:HG13	2.12	0.50
1:B:39:LYS:HG2	4:B:2031:HOH:O	2.10	0.49
1:D:255:SER:CB	2:D:1345:SO4:O3	2.59	0.49
1:A:78:PHE:CE1	1:B:74:ALA:HB1	2.47	0.49
1:C:273:MET:CE	1:C:335:LEU:HD21	2.43	0.49
1:A:333:ASN:HB3	4:A:2209:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LYS:HE3	1:A:247:PHE:O	2.12	0.49
1:C:273:MET:HE1	1:C:335:LEU:HD21	1.94	0.49
1:C:51:GLN:HA	1:C:93:HIS:O	2.12	0.49
1:D:162:ILE:CD1	1:D:204:LEU:HD11	2.43	0.49
1:C:240:LEU:HB3	1:C:241:PRO:HD2	1.93	0.49
1:C:267:ARG:CA	4:C:2033:HOH:O	2.44	0.49
4:C:2039:HOH:O	1:D:32:GLU:HG3	2.12	0.48
1:B:303:GLY:N	4:B:2180:HOH:O	2.46	0.48
1:A:255:SER:HB2	2:A:1344:SO4:O4	2.13	0.48
1:A:308:LYS:CD	4:B:2085:HOH:O	2.62	0.48
1:C:161:GLU:HG3	1:C:205:ALA:HB3	1.96	0.48
1:C:283:PHE:O	1:C:286:PRO:HD2	2.14	0.48
1:C:32:GLU:HB2	4:C:2041:HOH:O	2.13	0.48
1:D:21:TYR:CE2	1:D:340:LYS:HD3	2.49	0.48
1:A:9:TYR:CD2	1:A:126:GLN:HB3	2.50	0.47
1:D:244:ALA:C	1:D:246:PRO:HD3	2.33	0.47
1:A:31:SER:HB2	1:A:78:PHE:CZ	2.50	0.47
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:B:31:SER:HB2	1:B:78:PHE:CZ	2.49	0.47
1:D:17:LYS:HE3	1:D:247:PHE:O	2.15	0.47
1:B:3:ILE:HD11	1:B:79:THR:HG22	1.97	0.47
1:B:113:SER:O	1:B:117:VAL:HG23	2.15	0.47
1:B:295:TYR:CG	1:B:296:ASP:N	2.83	0.46
1:C:4:ALA:HB1	1:C:8:VAL:HG23	1.97	0.46
1:D:240:LEU:N	1:D:240:LEU:HD12	2.29	0.46
1:C:57:ALA:O	1:C:71:GLY:HA3	2.16	0.46
1:D:254:GLY:O	1:D:256:GLY:N	2.48	0.46
1:A:122:ASN:HB3	4:A:2005:HOH:O	2.15	0.46
1:B:273:MET:CE	1:B:335:LEU:HD21	2.46	0.46
1:A:95:ASP:OD1	1:A:96:HIS:CD2	2.68	0.46
1:D:102:LEU:HD23	1:D:106:VAL:HB	1.98	0.46
1:A:312:ASP:OD1	1:A:312:ASP:C	2.51	0.46
1:C:188:GLU:HG3	4:C:2113:HOH:O	2.16	0.46
1:C:190:THR:HG23	1:C:194:LEU:HD12	1.97	0.46
1:C:267:ARG:NE	4:C:2143:HOH:O	2.48	0.46
1:D:17:LYS:HD3	1:D:248:ASP:OD1	2.16	0.46
1:B:201:LYS:HB3	1:B:201:LYS:HE2	1.70	0.46
1:A:259:LYS:O	1:A:263:GLU:HG2	2.16	0.45
1:B:135:VAL:HB	1:B:136:PRO:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:THR:HG22	1:A:56:GLY:HA3	1.98	0.45
1:A:252:HIS:HB3	4:A:2087:HOH:O	2.16	0.45
1:C:295:TYR:CG	1:C:296:ASP:N	2.84	0.45
1:A:243:ASP:HB3	4:A:2164:HOH:O	2.17	0.45
1:D:16:ALA:HB1	1:D:21:TYR:O	2.17	0.45
1:A:313:PRO:HD2	1:B:280:GLN:HG2	1.98	0.45
4:A:2180:HOH:O	1:B:308:LYS:CG	2.65	0.45
1:A:117:VAL:HA	4:A:2105:HOH:O	2.16	0.44
1:C:254:GLY:HA3	1:C:274:ASN:O	2.17	0.44
1:C:274:ASN:HB3	4:C:2035:HOH:O	2.17	0.44
1:D:95:ASP:O	1:D:96:HIS:C	2.55	0.44
1:C:54:THR:HG22	1:C:105:TYR:CD2	2.52	0.44
1:B:163:GLY:C	1:B:207:THR:HG21	2.38	0.44
1:C:117:VAL:HA	1:C:121:GLY:O	2.18	0.44
1:D:122:ASN:HB3	1:D:123:PRO:HD2	1.99	0.44
1:D:240:LEU:HB3	1:D:241:PRO:CD	2.46	0.43
1:B:343:THR:HA	4:B:2067:HOH:O	2.17	0.43
1:C:107:ARG:HB2	1:C:108:PRO:HD3	2.00	0.43
1:D:188:GLU:HG3	1:D:233:VAL:CG1	2.49	0.43
1:D:303:GLY:C	4:D:2158:HOH:O	2.56	0.43
1:B:244:ALA:O	1:B:246:PRO:HD3	2.19	0.43
1:D:244:ALA:HA	4:D:2135:HOH:O	2.17	0.43
1:D:245:LYS:N	4:D:2137:HOH:O	2.38	0.43
1:B:313:PRO:O	1:B:317:LEU:HG	2.19	0.43
1:A:122:ASN:HB3	1:A:123:PRO:HD2	2.01	0.43
1:C:298:VAL:HA	1:C:311:TYR:HB3	1.99	0.43
1:C:98:PRO:HB2	1:C:100:ASP:OD1	2.19	0.43
1:C:185:GLU:O	1:C:188:GLU:HB2	2.19	0.43
1:A:285:ARG:N	1:A:286:PRO:HD2	2.33	0.43
1:B:257:SER:HB2	1:B:262:ILE:HD11	1.99	0.43
1:C:17:LYS:HD3	1:C:248:ASP:OD1	2.18	0.43
1:D:210:ASN:HB3	1:D:222:LEU:HD21	2.01	0.43
1:A:240:LEU:HB3	1:A:241:PRO:HD2	2.00	0.42
1:B:312:ASP:OD1	1:B:312:ASP:C	2.58	0.42
1:B:228:ALA:O	1:B:232:GLN:HG3	2.19	0.42
1:C:185:GLU:CA	4:C:2113:HOH:O	2.64	0.42
1:D:17:LYS:O	1:D:245:LYS:HE3	2.20	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:D:285:ARG:N	1:D:286:PRO:HD2	2.33	0.42
1:C:158:LEU:O	1:C:202:TYR:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:ARG:HB3	1:C:286:PRO:HD3	2.02	0.42
1:A:36:ALA:HB2	1:A:321:GLU:HG3	2.00	0.42
1:D:51:GLN:HA	1:D:93:HIS:O	2.19	0.42
1:A:231:GLN:NE2	1:A:249:PHE:CE2	2.87	0.42
1:A:5:THR:N	1:A:8:VAL:CG1	2.82	0.42
1:C:79:THR:HG21	1:C:92:LEU:HD21	2.01	0.42
1:A:204:LEU:O	1:A:249:PHE:HA	2.20	0.41
1:B:51:GLN:HA	1:B:93:HIS:O	2.20	0.41
1:D:57:ALA:O	1:D:71:GLY:HA3	2.20	0.41
1:C:184:PRO:HG3	1:C:229:GLN:OE1	2.19	0.41
1:C:229:GLN:O	1:C:233:VAL:HG23	2.20	0.41
1:A:285:ARG:HB3	1:A:286:PRO:HD3	2.01	0.41
1:D:290:HIS:CD2	1:D:316:TYR:HB3	2.54	0.41
1:A:181:TYR:CD1	1:A:181:TYR:N	2.89	0.41
1:C:19:ASN:O	1:C:20:SER:HB2	2.20	0.41
1:C:74:ALA:HB1	1:D:78:PHE:CD1	2.56	0.41
1:D:31:SER:HB2	1:D:78:PHE:CZ	2.56	0.41
1:B:109:LEU:HA	1:B:109:LEU:HD23	1.86	0.41
1:C:268:TYR:CD1	1:C:268:TYR:N	2.87	0.41
1:B:54:THR:HG22	1:B:105:TYR:CD2	2.55	0.41
1:B:107:ARG:HB2	1:B:108:PRO:HD3	2.03	0.41
1:B:115:GLN:O	1:B:119:LYS:HG2	2.20	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:HB1	2.56	0.41
1:A:209:GLY:C	1:A:222:LEU:HD23	2.41	0.41
1:A:222:LEU:HD12	1:A:261:GLU:OE1	2.20	0.41
1:B:36:ALA:HB2	1:B:321:GLU:HG3	2.02	0.41
1:C:113:SER:HB3	1:C:123:PRO:HB3	2.03	0.41
1:D:77:GLU:OE1	1:D:77:GLU:HA	2.21	0.41
1:D:231:GLN:HA	1:D:231:GLN:OE1	2.20	0.41
1:B:122:ASN:HB3	1:B:123:PRO:HD2	2.02	0.41
1:B:285:ARG:HB3	1:B:286:PRO:HD3	2.03	0.41
1:C:32:GLU:OE1	1:D:32:GLU:OE1	2.39	0.41
1:A:117:VAL:CA	4:A:2105:HOH:O	2.69	0.40
1:B:49:ILE:HG12	1:B:91:ALA:HB3	2.03	0.40
1:B:97:CYS:HA	1:B:98:PRO:HD2	1.98	0.40
1:B:290:HIS:CG	1:B:316:TYR:HB3	2.55	0.40
1:C:303:GLY:N	4:C:2159:HOH:O	2.45	0.40
1:B:13:LEU:HD13	1:B:203:LEU:HD21	2.04	0.40
1:C:184:PRO:HG3	1:C:229:GLN:CD	2.42	0.40
1:C:267:ARG:N	4:C:2033:HOH:O	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ASP:OD1	1:D:101:LYS:HG3	2.21	0.40
1:C:34:VAL:O	1:C:38:ILE:HG13	2.21	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	Interatomic distance (Å)	Clash overlap (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 (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	308/344 (90%)	297 (96%)	10 (3%)	1 (0%)	41	47
1	B	308/344 (90%)	293 (95%)	12 (4%)	3 (1%)	15	15
1	C	308/344 (90%)	290 (94%)	14 (4%)	4 (1%)	12	10
1	D	308/344 (90%)	296 (96%)	10 (3%)	2 (1%)	25	27
All	All	1232/1376 (90%)	1176 (96%)	46 (4%)	10 (1%)	19	20

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

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Mol	Chain	Res	Type
1	B	256	GLY
1	C	256	GLY
1	C	223	ARG

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	242/266 (91%)	237 (98%)	5 (2%)	53	65
1	B	242/266 (91%)	236 (98%)	6 (2%)	47	58
1	C	242/266 (91%)	234 (97%)	8 (3%)	38	46
1	D	242/266 (91%)	236 (98%)	6 (2%)	47	58
All	All	968/1064 (91%)	943 (97%)	25 (3%)	46	56

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

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Mol	Chain	Res	Type
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	B	51	GLN
1	B	122	ASN
1	C	252	HIS
1	D	326	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	D	1345	-	4,4,4	0.17	0	6,6,6	0.31	0
2	SO4	B	1345	-	4,4,4	0.22	0	6,6,6	0.17	0
2	SO4	D	1344	-	4,4,4	0.15	0	6,6,6	0.31	0
2	SO4	A	1345	-	4,4,4	0.15	0	6,6,6	0.19	0
2	SO4	A	1344	-	4,4,4	0.11	0	6,6,6	0.12	0
2	SO4	B	1344	-	4,4,4	0.12	0	6,6,6	0.25	0
2	SO4	C	1345	-	4,4,4	0.15	0	6,6,6	0.24	0
2	SO4	C	1344	-	4,4,4	0.14	0	6,6,6	0.14	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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1345	SO4	2	0
2	A	1345	SO4	1	0
2	A	1344	SO4	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.70	20 (6%)	19	28	14, 26, 52, 81	0
1	B	314/344 (91%)	0.63	16 (5%)	28	40	15, 26, 49, 91	0
1	C	314/344 (91%)	0.88	27 (8%)	10	16	18, 34, 62, 99	0
1	D	314/344 (91%)	0.64	16 (5%)	28	40	15, 26, 49, 77	0
All	All	1256/1376 (91%)	0.71	79 (6%)	20	29	14, 28, 55, 99	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	163	GLY	7.3
1	A	254	GLY	7.2
1	A	242	ALA	6.9
1	C	256	GLY	6.1
1	B	257	SER	5.9
1	A	258	LEU	5.7
1	C	254	GLY	5.6
1	C	257	SER	5.4
1	B	255	SER	5.3
1	B	256	GLY	4.7
1	C	255	SER	4.6
1	C	111	ALA	4.4
1	C	267	ARG	4.1
1	B	258	LEU	4.1
1	A	163	GLY	4.0
1	D	255	SER	4.0
1	B	254	GLY	3.9
1	C	181	TYR	3.9
1	D	163	GLY	3.8
1	A	223	ARG	3.6
1	D	305	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	343	THR	3.6
1	D	223	ARG	3.6
1	C	260	SER	3.6
1	C	192	GLU	3.5
1	C	222	LEU	3.4
1	A	243	ASP	3.4
1	B	163	GLY	3.3
1	A	256	GLY	3.3
1	C	305	VAL	3.3
1	C	138	ASP	3.2
1	C	258	LEU	3.1
1	B	242	ALA	3.1
1	D	225	ASP	3.1
1	C	102	LEU	3.0
1	A	259	LYS	3.0
1	D	258	LEU	2.9
1	D	257	SER	2.9
1	D	238	LEU	2.9
1	A	238	LEU	2.9
1	B	343	THR	2.8
1	B	244	ALA	2.8
1	A	185	GLU	2.8
1	A	222	LEU	2.7
1	D	254	GLY	2.7
1	C	193	ALA	2.6
1	A	244	ALA	2.5
1	D	343	THR	2.5
1	D	222	LEU	2.5
1	C	259	LYS	2.5
1	A	240	LEU	2.5
1	A	276	ASP	2.5
1	A	255	SER	2.4
1	A	257	SER	2.4
1	B	243	ASP	2.4
1	C	243	ASP	2.4
1	B	222	LEU	2.4
1	C	103	ASP	2.4
1	C	188	GLU	2.4
1	D	303	GLY	2.4
1	D	304	GLU	2.4
1	B	261	GLU	2.3
1	C	261	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	115	GLN	2.3
1	C	119	LYS	2.3
1	B	241	PRO	2.3
1	D	244	ALA	2.2
1	A	261	GLU	2.2
1	C	335	LEU	2.2
1	B	223	ARG	2.2
1	D	261	GLU	2.2
1	A	16	ALA	2.2
1	C	276	ASP	2.2
1	A	342	LEU	2.1
1	C	199	HIS	2.1
1	C	228	ALA	2.1
1	A	225	ASP	2.1
1	D	262	ILE	2.0
1	B	259	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	D	1344	5/5	0.80	0.16	38,43,63,87	0
2	SO4	B	1345	5/5	0.81	0.20	50,54,67,83	0
3	NA	A	1347	1/1	0.83	0.28	43,43,43,43	0
2	SO4	D	1345	5/5	0.84	0.21	57,59,68,88	0
2	SO4	C	1345	5/5	0.84	0.21	50,50,68,80	0
2	SO4	C	1344	5/5	0.85	0.22	51,67,74,83	0
3	NA	A	1346	1/1	0.90	0.22	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	1345	5/5	0.92	0.15	38,46,52,60	0
2	SO4	B	1344	5/5	0.93	0.16	41,44,65,75	0
2	SO4	A	1344	5/5	0.96	0.10	52,55,64,65	0

6.5 Other polymers (i)

There are no such residues in this entry.