Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 10:30 PM BST

PDB ID	:	6R8H
Title	:	Triosephosphate isomerase from liver fluke (Fasciola hepatica).
Authors	:	Ferraro, F.; Corvo, I.; Bergalli, L.; Ilarraz, A.; Cabrera, M.; Gil, J.; Susuki, B.; Caffrey, C.; Timson, D.J.; Robert, X.; Guillon, C.; Alvarez, G.
Deposited on	:	2019-04-01
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

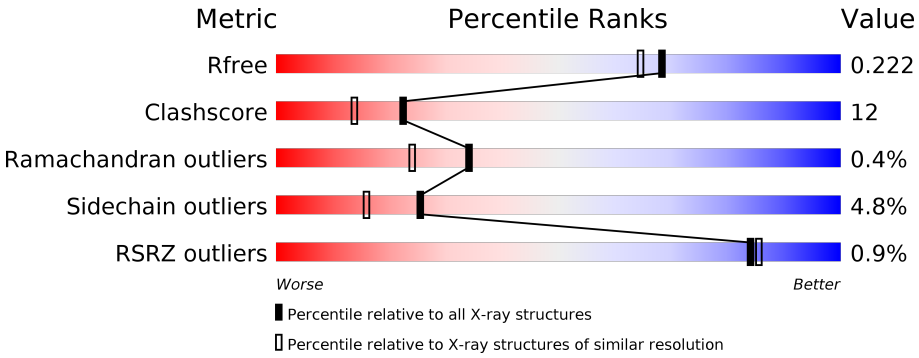
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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	250	79% 18%
1	B	250	% 77% 22%
1	C	250	% 74% 24%
1	D	250	80% 18%
1	E	250	% 78% 18%
1	F	250	2% 78% 20%

2 Entry composition

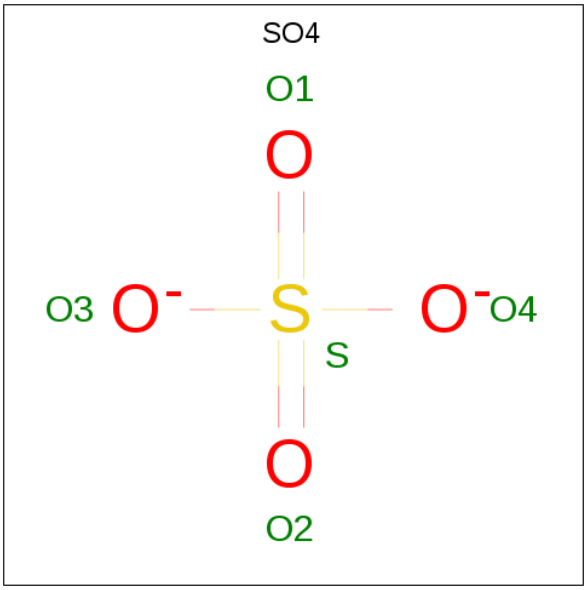
There are 3 unique types of molecules in this entry. The entry contains 12745 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Triosephosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1928	1214	343	361	10			
1	B	250	Total	C	N	O	S	0	0	0
			1928	1214	343	361	10			
1	C	250	Total	C	N	O	S	0	0	0
			1928	1214	343	361	10			
1	D	250	Total	C	N	O	S	0	2	0
			1948	1225	349	364	10			
1	E	250	Total	C	N	O	S	0	0	0
			1928	1214	343	361	10			
1	F	250	Total	C	N	O	S	0	1	0
			1939	1220	347	362	10			

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



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

- Molecule 3 is water.

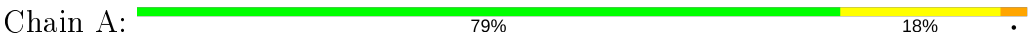
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	139	Total O 139 139	0	0
3	B	231	Total O 231 231	0	0
3	C	181	Total O 181 181	0	0
3	D	145	Total O 145 145	0	0
3	E	184	Total O 184 184	0	0
3	F	236	Total O 236 236	0	0

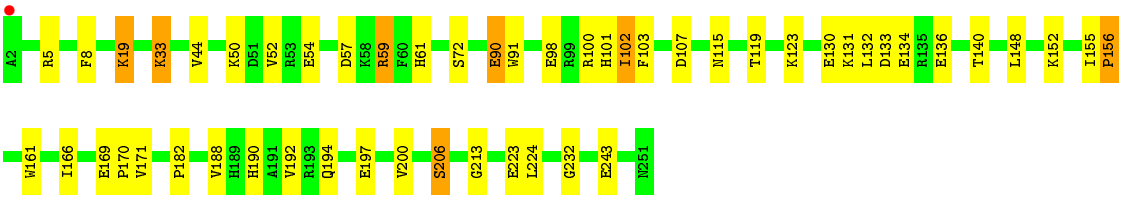
3 Residue-property plots (i)

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: Triosephosphate isomerase

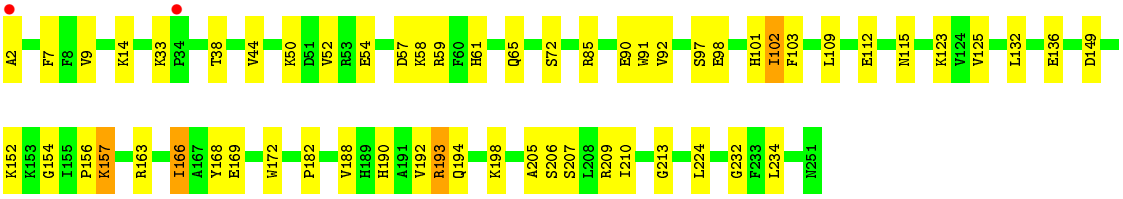
Chain A:





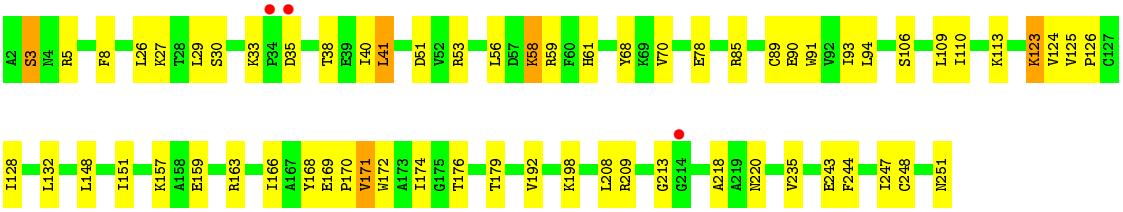
- Molecule 1: Triosephosphate isomerase

Chain B:



- Molecule 1: Triosephosphate isomerase

Chain C:



- Molecule 1: Triosephosphate isomerase

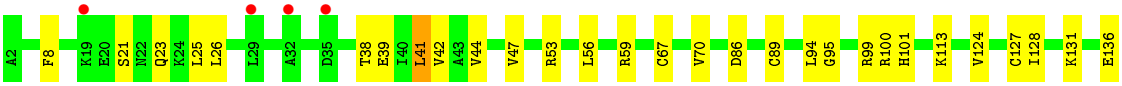
Chain D:

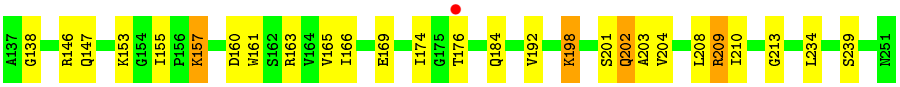
- Molecule 1: Triosephosphate isomerase

Chain E:

- Molecule 1: Triosephosphate isomerase

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	87.42Å 87.42Å 186.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.3 (20.00-1.90) 90.4 (20.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	17.91 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.194 , 0.224 0.194 , 0.222	Depositor DCC
R_{free} test set	5584 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	17.1	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.125 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12745	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7582e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.72	0/1966	0.92	0/2655
1	B	0.70	0/1966	0.92	0/2655
1	C	0.70	0/1966	0.94	0/2655
1	D	0.71	0/1986	0.94	0/2681
1	E	0.69	0/1966	0.92	0/2655
1	F	0.70	0/1977	0.93	0/2669
All	All	0.70	0/11827	0.93	0/15970

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

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	1928	0	1923	40	0
1	B	1928	0	1923	49	0
1	C	1928	0	1923	57	0
1	D	1948	0	1942	33	0
1	E	1928	0	1923	44	0
1	F	1939	0	1935	52	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	139	0	0	2	0
3	B	231	0	0	10	0
3	C	181	0	0	13	0
3	D	145	0	0	5	0
3	E	184	0	0	6	0
3	F	236	0	0	16	0
All	All	12745	0	11569	269	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (269) 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:F:169:GLU:OE1	1:F:234:LEU:HB3	1.78	0.84
1:F:25:LEU:HG	3:F:446:HOH:O	1.81	0.80
1:E:101:HIS:O	1:E:102:ILE:HG13	1.85	0.76
1:E:90:GLU:HG2	1:E:91:TRP:HD1	1.50	0.76
1:A:101:HIS:O	1:A:102:ILE:HG13	1.86	0.76
1:C:41:LEU:HD22	1:C:61:HIS:HB2	1.66	0.76
1:B:169:GLU:HG2	1:B:213:GLY:HA3	1.69	0.73
1:B:2:ALA:HB3	3:B:552:HOH:O	1.89	0.72
1:E:148:LEU:HD21	1:E:166:ILE:HD13	1.71	0.71
1:E:131:LYS:HA	1:E:171:VAL:HB	1.74	0.69
1:B:132:LEU:O	1:B:136:GLU:HG3	1.92	0.68
1:E:90:GLU:HG2	1:E:91:TRP:CD1	2.29	0.68
1:E:132:LEU:HB2	1:E:172:TRP:HB3	1.76	0.68
1:F:169:GLU:HG2	1:F:213:GLY:CA	2.24	0.68
1:E:38:THR:O	1:E:59:ARG:NH2	2.20	0.67
1:D:131:LYS:HA	1:D:171:VAL:HB	1.77	0.65
1:F:174:ILE:O	1:F:176:THR:HG23	1.97	0.64
1:C:38:THR:HB	3:C:437:HOH:O	1.96	0.64
1:F:23:GLN:HA	1:F:23:GLN:OE1	1.97	0.63
1:C:58:LYS:HD2	3:C:452:HOH:O	1.99	0.62
1:D:201:SER:HB3	1:D:204:VAL:H	1.64	0.62
1:C:132:LEU:HB2	1:C:172:TRP:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:LEU:HD22	1:D:56:LEU:HD13	1.82	0.62
1:C:85:ARG:HD2	1:C:90:GLU:OE2	2.00	0.61
1:C:26:LEU:HD22	1:C:56:LEU:HD13	1.83	0.61
1:C:109:LEU:O	1:C:113:LYS:HG3	2.01	0.61
1:C:123:LYS:HD3	1:C:123:LYS:N	2.16	0.61
1:C:93:ILE:HD13	1:C:125:VAL:HB	1.81	0.61
1:D:109:LEU:O	1:D:113:LYS:HG3	2.00	0.60
1:D:41:LEU:HD13	1:D:42:VAL:N	2.16	0.60
1:F:41:LEU:HD13	1:F:42:VAL:N	2.15	0.60
1:A:90:GLU:HG2	1:A:91:TRP:CD1	2.36	0.60
1:E:166:ILE:HG22	1:E:208:LEU:HD21	1.84	0.60
1:E:152:LYS:HD3	1:E:161:TRP:HZ2	1.67	0.60
1:B:90:GLU:HG2	1:B:123:LYS:HD2	1.85	0.59
1:B:182:PRO:HG3	1:B:224:LEU:HD22	1.84	0.59
1:F:100[B]:ARG:NH2	3:F:405:HOH:O	2.32	0.59
1:E:91:TRP:CZ2	1:E:123:LYS:HD2	2.38	0.59
1:A:131:LYS:HA	1:A:171:VAL:HB	1.85	0.59
1:E:133:ASP:OD1	1:E:134:GLU:HG3	2.03	0.59
1:B:152:LYS:HE2	3:B:536:HOH:O	2.02	0.59
1:B:101:HIS:O	1:B:102:ILE:HG13	2.03	0.58
1:F:94:LEU:HD12	1:F:124:VAL:HG23	1.85	0.58
1:A:19:LYS:HE3	1:D:86:ASP:O	2.04	0.58
1:E:148:LEU:HD12	3:E:534:HOH:O	2.04	0.58
1:F:157:LYS:NZ	1:F:160:ASP:OD1	2.37	0.58
1:C:148:LEU:HD11	1:C:192:VAL:HG13	1.85	0.57
1:B:224:LEU:HD21	3:B:465:HOH:O	2.03	0.57
1:F:155:ILE:HD12	1:F:161:TRP:CE2	2.39	0.57
1:C:41:LEU:CD2	3:C:402:HOH:O	2.51	0.57
1:C:157:LYS:NZ	3:C:405:HOH:O	2.31	0.57
1:E:91:TRP:CE2	1:E:123:LYS:HD2	2.39	0.57
1:F:94:LEU:HD12	1:F:124:VAL:CG2	2.33	0.57
1:C:123:LYS:HD2	1:C:163:ARG:HD2	1.87	0.57
1:E:251:ASN:OD1	3:E:401:HOH:O	2.18	0.56
1:A:155:ILE:O	1:A:156:PRO:C	2.40	0.56
1:E:7:PHE:CZ	1:E:232:GLY:HA2	2.41	0.56
1:B:102:ILE:HG22	1:B:103:PHE:CD2	2.41	0.56
1:E:50:LYS:HG3	1:E:51:ASP:N	2.21	0.56
1:F:169:GLU:HG2	1:F:213:GLY:HA3	1.88	0.56
1:A:91:TRP:CZ2	1:A:123:LYS:HD2	2.41	0.56
1:F:8:PHE:CE2	1:F:165:VAL:HG21	2.40	0.56
1:B:85:ARG:NH1	1:B:90:GLU:OE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ILE:HG12	1:C:208:LEU:HD21	1.88	0.56
1:C:38:THR:HG21	1:C:248:CYS:O	2.05	0.55
1:B:109:LEU:HA	1:B:112:GLU:OE1	2.06	0.55
1:D:85:ARG:HD2	1:D:90:GLU:OE2	2.07	0.55
1:B:156:PRO:HB2	3:B:409:HOH:O	2.07	0.55
1:A:155:ILE:O	1:A:156:PRO:O	2.25	0.55
1:C:41:LEU:CD2	1:C:61:HIS:HB2	2.36	0.55
1:B:188:VAL:O	1:B:192:VAL:HG23	2.07	0.55
1:B:206:SER:OG	1:B:207:SER:N	2.40	0.55
1:E:152:LYS:HD3	1:E:161:TRP:CZ2	2.41	0.55
1:E:58:LYS:HG3	3:E:507:HOH:O	2.07	0.55
1:B:190:HIS:CE1	1:B:194:GLN:OE1	2.60	0.54
1:A:50:LYS:NZ	1:A:54:GLU:OE2	2.40	0.54
1:B:97:SER:HB3	3:B:512:HOH:O	2.07	0.54
1:A:148:LEU:HD11	1:A:192:VAL:HG13	1.90	0.54
1:C:35:ASP:N	1:C:35:ASP:OD1	2.40	0.54
1:B:193:ARG:HD3	1:B:205:ALA:O	2.08	0.54
1:E:58:LYS:HE2	3:E:513:HOH:O	2.07	0.54
1:A:223:GLU:H	1:A:223:GLU:CD	2.12	0.53
1:E:166:ILE:HG22	1:E:208:LEU:CD2	2.38	0.53
1:B:163:ARG:NH1	3:B:416:HOH:O	2.39	0.53
1:C:132:LEU:O	1:C:132:LEU:HG	2.09	0.53
1:A:90:GLU:HG2	1:A:91:TRP:HD1	1.71	0.53
1:F:163:ARG:NE	3:F:415:HOH:O	2.42	0.53
1:B:50:LYS:NZ	1:B:54:GLU:OE2	2.43	0.52
1:C:29:LEU:HD11	1:C:244:PHE:HD2	1.74	0.52
1:A:115:ASN:HA	1:A:156:PRO:HD3	1.91	0.52
1:C:128:ILE:HD11	1:C:151:ILE:CD1	2.39	0.52
1:F:146:ARG:NH2	3:F:408:HOH:O	2.43	0.52
1:D:20:GLU:O	1:D:23[A]:GLN:HB2	2.10	0.52
1:E:61:HIS:HB3	1:E:91:TRP:CD1	2.46	0.51
1:E:109:LEU:O	1:E:113:LYS:HG3	2.11	0.51
1:E:79:ILE:HD12	1:F:47:VAL:HG13	1.91	0.51
1:D:3:SER:OG	1:D:5:ARG:HG2	2.11	0.51
1:F:202:GLN:HG2	3:F:489:HOH:O	2.10	0.51
1:C:171:VAL:HG22	3:C:495:HOH:O	2.11	0.50
1:C:166:ILE:CG1	1:C:208:LEU:HD21	2.41	0.50
1:C:85:ARG:CD	1:C:90:GLU:OE2	2.59	0.50
1:A:91:TRP:CE2	1:A:123:LYS:HD2	2.46	0.50
1:C:53:ARG:HB2	1:C:89:CYS:SG	2.51	0.50
1:B:190:HIS:NE2	1:B:194:GLN:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:GLY:O	1:B:156:PRO:HD3	2.11	0.50
1:B:44:VAL:HG11	1:B:52:VAL:HG11	1.93	0.50
1:C:41:LEU:HD21	1:C:61:HIS:ND1	2.27	0.50
1:C:3:SER:OG	1:C:5:ARG:HG2	2.12	0.50
1:C:26:LEU:HD22	1:C:56:LEU:CD1	2.42	0.50
1:E:152:LYS:HE2	1:E:200:VAL:HG13	1.93	0.49
1:F:53:ARG:HB2	1:F:89:CYS:SG	2.52	0.49
1:A:188:VAL:O	1:A:192:VAL:HG23	2.12	0.49
1:B:149:ASP:OD2	3:B:401:HOH:O	2.19	0.49
1:C:85:ARG:HD3	1:C:90:GLU:OE1	2.13	0.49
1:D:29:LEU:HD11	1:D:244:PHE:CD2	2.47	0.49
1:E:169:GLU:HG2	1:E:213:GLY:HA3	1.95	0.49
1:F:201:SER:CB	1:F:204:VAL:H	2.25	0.49
1:F:169:GLU:OE1	1:F:213:GLY:HA3	2.13	0.49
1:F:163:ARG:NH2	3:F:415:HOH:O	2.45	0.49
1:A:8:PHE:O	1:A:232:GLY:HA3	2.12	0.49
1:B:168:TYR:O	1:B:213:GLY:N	2.44	0.49
1:C:68:TYR:HB2	1:C:78:GLU:OE1	2.12	0.49
1:F:23:GLN:CA	1:F:23:GLN:OE1	2.61	0.49
1:D:118:LEU:O	1:D:163[B]:ARG:NH1	2.36	0.48
1:D:41:LEU:HD22	1:D:61:HIS:HB2	1.94	0.48
1:E:19:LYS:HE2	1:F:86:ASP:O	2.13	0.48
1:B:50:LYS:HE2	1:C:51:ASP:OD2	2.12	0.48
1:D:108:GLU:HB3	1:F:138:GLY:O	2.12	0.48
1:F:155:ILE:HD12	1:F:161:TRP:CD2	2.49	0.48
1:F:239:SER:HB2	3:F:516:HOH:O	2.14	0.48
1:C:26:LEU:O	1:C:30:SER:N	2.39	0.48
1:A:152:LYS:HD3	1:A:161:TRP:HZ2	1.78	0.48
1:D:23[B]:GLN:OE1	1:D:23[B]:GLN:HA	2.14	0.48
1:E:39:GLU:OE2	3:E:402:HOH:O	2.20	0.48
1:C:41:LEU:CD2	1:C:61:HIS:ND1	2.77	0.48
1:D:175:GLY:HA3	3:D:524:HOH:O	2.14	0.48
1:A:61:HIS:HB3	1:A:91:TRP:CD1	2.49	0.47
1:D:135:ARG:HH21	1:D:140:THR:HG21	1.79	0.47
1:F:42:VAL:HG12	1:F:44:VAL:HG13	1.95	0.47
1:B:58:LYS:NZ	3:B:405:HOH:O	2.27	0.47
1:F:146:ARG:NH1	3:F:405:HOH:O	2.48	0.47
1:A:152:LYS:HD3	1:A:161:TRP:CZ2	2.49	0.47
1:D:157:LYS:NZ	3:D:408:HOH:O	2.36	0.47
1:B:166:ILE:HG22	1:B:210:ILE:HA	1.96	0.47
1:E:168:TYR:CE1	1:E:188:VAL:HG11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:ASP:HB3	3:E:522:HOH:O	2.15	0.47
1:A:115:ASN:O	1:A:119:THR:HG23	2.15	0.47
1:C:218:ALA:HB2	1:C:243:GLU:HB2	1.97	0.47
1:C:171:VAL:HA	1:C:174:ILE:HD12	1.97	0.46
1:E:115:ASN:HA	1:E:156:PRO:HD3	1.97	0.46
1:E:76:THR:O	1:F:99:ARG:NH1	2.47	0.46
1:B:169:GLU:HA	1:B:213:GLY:O	2.15	0.46
1:F:131:LYS:HB3	3:F:439:HOH:O	2.15	0.46
1:C:41:LEU:HD23	3:C:402:HOH:O	2.13	0.46
1:E:155:ILE:O	1:E:156:PRO:C	2.52	0.46
1:F:163:ARG:CZ	3:F:415:HOH:O	2.63	0.46
1:D:94:LEU:HD12	1:D:124:VAL:CG2	2.46	0.46
1:B:9:VAL:HG12	1:B:38:THR:HG22	1.97	0.45
1:E:46:PHE:CE1	1:E:64:ALA:HB1	2.51	0.45
1:C:3:SER:N	3:C:413:HOH:O	2.50	0.45
1:D:35:ASP:O	1:D:59:ARG:NH2	2.49	0.45
1:B:132:LEU:HB2	1:B:172:TRP:HB3	1.97	0.45
1:B:149:ASP:HB2	3:B:520:HOH:O	2.16	0.45
1:F:201:SER:HB2	1:F:204:VAL:H	1.82	0.45
1:E:8:PHE:O	1:E:232:GLY:HA3	2.16	0.45
1:B:182:PRO:HA	1:B:224:LEU:HD13	1.99	0.45
1:F:160:ASP:HA	3:F:517:HOH:O	2.17	0.45
1:C:94:LEU:HD12	1:C:124:VAL:HG21	1.98	0.45
1:B:168:TYR:CE1	1:B:188:VAL:HG11	2.52	0.45
1:D:85:ARG:CD	1:D:90:GLU:OE2	2.65	0.45
1:F:201:SER:HB2	1:F:204:VAL:HB	1.99	0.45
1:F:95:GLY:O	1:F:127:CYS:HB2	2.17	0.45
1:C:235:VAL:HG21	1:C:247:ILE:HG21	1.98	0.44
1:C:8:PHE:CZ	1:C:41:LEU:HG	2.51	0.44
1:A:130:GLU:CD	1:A:140:THR:HG23	2.37	0.44
1:C:94:LEU:O	1:C:126:PRO:HA	2.17	0.44
1:B:166:ILE:CG2	1:B:210:ILE:HA	2.47	0.44
1:D:202:GLN:HG2	3:D:451:HOH:O	2.16	0.44
1:A:170:PRO:HD2	1:A:213:GLY:O	2.17	0.44
1:B:125:VAL:HG12	1:B:125:VAL:O	2.17	0.44
1:F:100[B]:ARG:NH1	3:F:405:HOH:O	2.49	0.44
1:A:190:HIS:CE1	1:A:194:GLN:OE1	2.70	0.44
1:B:7:PHE:CZ	1:B:232:GLY:HA2	2.53	0.44
1:C:168:TYR:CE2	1:C:170:PRO:HD3	2.53	0.44
1:F:234:LEU:HD12	1:F:234:LEU:HA	1.77	0.44
1:C:94:LEU:HD12	1:C:124:VAL:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:479:HOH:O	1:D:136:GLU:HG2	2.16	0.44
1:E:170:PRO:HD2	1:E:213:GLY:O	2.17	0.44
1:A:50:LYS:HB3	1:A:50:LYS:HE3	1.85	0.43
1:B:156:PRO:O	1:B:157:LYS:HB2	2.18	0.43
1:D:113:LYS:NZ	3:D:416:HOH:O	2.51	0.43
1:A:132:LEU:HD22	1:A:136:GLU:CD	2.39	0.43
1:A:90:GLU:HB2	3:A:493:HOH:O	2.18	0.43
1:C:123:LYS:CD	1:C:123:LYS:N	2.81	0.43
1:F:201:SER:HB3	1:F:203:ALA:N	2.33	0.43
1:A:102:ILE:HG22	1:A:103:PHE:CD2	2.53	0.43
1:B:209:ARG:NH2	3:B:429:HOH:O	2.51	0.43
1:C:40:ILE:O	3:C:402:HOH:O	2.21	0.43
1:F:100[B]:ARG:HD3	1:F:101:HIS:NE2	2.33	0.43
1:B:115:ASN:HA	1:B:156:PRO:HD3	1.99	0.43
1:C:179:THR:HG21	1:C:220:ASN:ND2	2.34	0.43
1:C:29:LEU:HD11	1:C:244:PHE:CD2	2.52	0.43
1:F:67:CYS:O	1:F:113:LYS:HD3	2.18	0.43
1:E:33:LYS:HD3	1:E:34:PRO:HD2	2.00	0.43
1:B:61:HIS:HB3	1:B:91:TRP:CD1	2.53	0.43
1:E:155:ILE:HG22	1:E:155:ILE:O	2.19	0.43
1:F:184:GLN:HA	3:F:461:HOH:O	2.19	0.43
1:A:132:LEU:CD2	1:A:136:GLU:HG3	2.49	0.43
1:B:101:HIS:O	1:B:102:ILE:CB	2.66	0.43
1:B:9:VAL:HG12	1:B:38:THR:CG2	2.48	0.43
1:D:212:TYR:O	1:D:233:PHE:HA	2.19	0.43
1:F:26:LEU:HD22	1:F:56:LEU:HD13	2.00	0.43
1:A:100:ARG:NH1	1:A:107:ASP:OD1	2.52	0.43
1:C:8:PHE:HZ	1:C:41:LEU:HG	1.83	0.43
1:E:50:LYS:HE2	1:E:50:LYS:HB2	1.82	0.43
1:A:133:ASP:OD1	1:A:134:GLU:HG3	2.19	0.42
1:B:14:LYS:HA	1:B:65:GLN:OE1	2.19	0.42
1:C:163:ARG:NH1	3:C:418:HOH:O	2.52	0.42
1:D:166:ILE:CG1	1:D:208:LEU:HD21	2.49	0.42
1:D:53:ARG:HB2	1:D:89:CYS:SG	2.59	0.42
1:C:106:SER:O	1:C:110:ILE:HG12	2.18	0.42
1:C:251:ASN:O	3:C:401:HOH:O	2.21	0.42
1:C:61:HIS:HB3	1:C:91:TRP:CD1	2.54	0.42
1:F:128:ILE:HG22	1:F:147:GLN:HB3	2.01	0.42
1:C:132:LEU:CB	1:C:172:TRP:HB3	2.49	0.42
1:F:166:ILE:HG12	1:F:208:LEU:HD21	2.02	0.42
1:E:46:PHE:HE1	1:E:64:ALA:HB1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:LYS:HE3	3:F:440:HOH:O	2.20	0.42
1:F:198:LYS:HE2	1:F:198:LYS:O	2.19	0.42
1:C:169:GLU:HG2	1:C:213:GLY:HA3	2.02	0.42
1:C:192:VAL:HA	3:C:532:HOH:O	2.20	0.42
1:D:99:ARG:O	1:D:105:GLU:HG3	2.20	0.42
1:F:41:LEU:HD13	1:F:41:LEU:C	2.41	0.42
1:A:90:GLU:CB	3:A:493:HOH:O	2.67	0.41
1:D:85:ARG:HD3	1:D:90:GLU:OE1	2.20	0.41
1:E:193:ARG:HH11	1:E:193:ARG:HD3	1.75	0.41
1:C:3:SER:HB3	3:C:521:HOH:O	2.20	0.41
1:A:182:PRO:HA	1:A:224:LEU:HD23	2.02	0.41
1:B:98:GLU:O	1:B:102:ILE:HB	2.20	0.41
1:F:192:VAL:CG1	1:F:210:ILE:HD13	2.51	0.41
1:F:38:THR:HG22	1:F:39:GLU:O	2.20	0.41
1:A:133:ASP:OD1	1:A:134:GLU:N	2.53	0.41
1:A:98:GLU:O	1:A:102:ILE:HB	2.20	0.41
1:A:5:ARG:NH1	1:A:206:SER:O	2.48	0.41
1:B:91:TRP:CE2	1:B:123:LYS:HD3	2.56	0.41
1:F:21:SER:CB	3:F:431:HOH:O	2.69	0.41
1:D:166:ILE:HG12	1:D:208:LEU:HD21	2.02	0.41
1:D:193:ARG:NE	1:D:229:ASP:OD1	2.54	0.41
3:D:508:HOH:O	1:F:136:GLU:HG2	2.20	0.41
1:A:44:VAL:HG11	1:A:52:VAL:HG11	2.03	0.41
1:F:209:ARG:NH2	3:F:403:HOH:O	2.27	0.41
1:C:124:VAL:HG22	1:C:125:VAL:N	2.36	0.41
1:E:172:TRP:O	1:E:176:THR:OG1	2.30	0.41
1:A:152:LYS:HE2	1:A:200:VAL:HG13	2.02	0.40
1:B:91:TRP:NE1	1:B:123:LYS:HD3	2.35	0.40
1:D:26:LEU:O	1:D:30:SER:N	2.45	0.40
1:A:101:HIS:O	1:A:102:ILE:CG1	2.64	0.40
1:A:169:GLU:HG2	1:A:213:GLY:HA3	2.02	0.40
1:A:33:LYS:HB3	1:A:33:LYS:HZ2	1.86	0.40
1:B:101:HIS:O	1:B:102:ILE:HB	2.22	0.40
1:C:78:GLU:HA	1:C:78:GLU:OE2	2.21	0.40
1:E:152:LYS:HA	1:E:155:ILE:HG12	2.03	0.40
1:E:66:ASN:OD1	1:E:113:LYS:NZ	2.53	0.40
1:B:234:LEU:HD12	1:B:234:LEU:HA	1.90	0.40
1:D:179:THR:HG21	1:D:220:ASN:ND2	2.36	0.40
1:D:39:GLU:HG2	1:D:61:HIS:NE2	2.36	0.40
1:A:59:ARG:HD3	1:A:59:ARG:C	2.42	0.40
1:B:85:ARG:HH11	1:B:85:ARG:HG3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:VAL:CG1	1:E:238:ALA:HB3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	248/250 (99%)	238 (96%)	8 (3%)	2 (1%)	19 9
1	B	248/250 (99%)	231 (93%)	15 (6%)	2 (1%)	19 9
1	C	248/250 (99%)	236 (95%)	12 (5%)	0	100 100
1	D	250/250 (100%)	241 (96%)	9 (4%)	0	100 100
1	E	248/250 (99%)	233 (94%)	13 (5%)	2 (1%)	19 9
1	F	249/250 (100%)	237 (95%)	12 (5%)	0	100 100
All	All	1491/1500 (99%)	1416 (95%)	69 (5%)	6 (0%)	34 24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ILE
1	B	102	ILE
1	E	102	ILE
1	A	156	PRO
1	B	157	LYS
1	E	156	PRO

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	205/205 (100%)	195 (95%)	10 (5%)	25 15
1	B	205/205 (100%)	197 (96%)	8 (4%)	32 23
1	C	205/205 (100%)	192 (94%)	13 (6%)	18 8
1	D	207/205 (101%)	200 (97%)	7 (3%)	37 28
1	E	205/205 (100%)	191 (93%)	14 (7%)	16 7
1	F	206/205 (100%)	199 (97%)	7 (3%)	37 28
All	All	1233/1230 (100%)	1174 (95%)	59 (5%)	25 16

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	33	LYS
1	A	57	ASP
1	A	59	ARG
1	A	72	SER
1	A	90	GLU
1	A	166	ILE
1	A	197	GLU
1	A	206	SER
1	A	243	GLU
1	B	33	LYS
1	B	57	ASP
1	B	59	ARG
1	B	72	SER
1	B	92	VAL
1	B	166	ILE
1	B	193	ARG
1	B	198	LYS
1	C	3	SER
1	C	27	LYS
1	C	33	LYS
1	C	41	LEU
1	C	58	LYS
1	C	59	ARG
1	C	70	VAL
1	C	123	LYS

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Mol	Chain	Res	Type
1	C	159	GLU
1	C	171	VAL
1	C	176	THR
1	C	198	LYS
1	C	209	ARG
1	D	3	SER
1	D	58	LYS
1	D	59	ARG
1	D	123	LYS
1	D	178	LYS
1	D	201	SER
1	D	202	GLN
1	E	3	SER
1	E	33	LYS
1	E	50	LYS
1	E	51	ASP
1	E	57	ASP
1	E	58	LYS
1	E	59	ARG
1	E	72	SER
1	E	85	ARG
1	E	90	GLU
1	E	142	GLN
1	E	166	ILE
1	E	193	ARG
1	E	209	ARG
1	F	41	LEU
1	F	59	ARG
1	F	70	VAL
1	F	157	LYS
1	F	198	LYS
1	F	202	GLN
1	F	209	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

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)

6 ligands are modelled in this entry.

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	C	301	-	4,4,4	1.43	0	6,6,6	0.87	0
2	SO4	E	301	-	4,4,4	0.52	0	6,6,6	0.20	0
2	SO4	D	301	-	4,4,4	0.42	0	6,6,6	0.44	0
2	SO4	B	301	-	4,4,4	0.46	0	6,6,6	0.61	0
2	SO4	A	301	-	4,4,4	0.47	0	6,6,6	0.37	0
2	SO4	F	301	-	4,4,4	0.57	0	6,6,6	0.61	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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

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, 95^{th} 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	250/250 (100%)	-0.40	1 (0%) 92 93	5, 13, 24, 37	6 (2%)
1	B	250/250 (100%)	0.09	2 (0%) 86 87	10, 18, 29, 46	44 (17%)
1	C	250/250 (100%)	0.11	3 (1%) 79 81	8, 19, 33, 49	55 (22%)
1	D	250/250 (100%)	-0.40	0 100 100	4, 13, 25, 41	7 (2%)
1	E	250/250 (100%)	0.15	3 (1%) 79 81	9, 19, 35, 53	43 (17%)
1	F	250/250 (100%)	0.05	5 (2%) 65 68	7, 18, 30, 51	49 (19%)
All	All	1500/1500 (100%)	-0.07	14 (0%) 84 85	4, 16, 31, 53	204 (13%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	6.2
1	A	2	ALA	4.9
1	E	2	ALA	3.5
1	C	35	ASP	3.3
1	C	214	GLY	3.0
1	B	34	PRO	2.7
1	F	32	ALA	2.7
1	F	35	ASP	2.5
1	F	19	LYS	2.5
1	F	176	THR	2.5
1	C	34	PRO	2.4
1	E	40	ILE	2.3
1	E	138	GLY	2.3
1	F	29	LEU	2.1

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 (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, 95^{th} 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	C	301	5/5	0.98	0.07	24,26,29,33	5
2	SO4	E	301	5/5	0.98	0.07	22,23,26,27	5
2	SO4	B	301	5/5	0.98	0.07	14,17,17,18	5
2	SO4	F	301	5/5	0.98	0.06	20,24,25,26	0
2	SO4	A	301	5/5	0.99	0.08	18,19,25,27	0
2	SO4	D	301	5/5	0.99	0.04	15,18,22,26	0

6.5 Other polymers (i)

There are no such residues in this entry.