Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2024 – 06:55 PM EST

PDB ID	:	1FX7
Title	:	CRYSTAL STRUCTURE OF THE IRON-DEPENDENT REGULATOR (IDER) FROM MYCOBACTERIUM TUBERCULOSIS
Authors	:	Feese, M.D.; Ingason, B.P.; Goranson-Siekierke, J.; Holmes, R.K.; Hol, W.J.G.
Deposited on	:	2000-09-25
Resolution	:	2.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

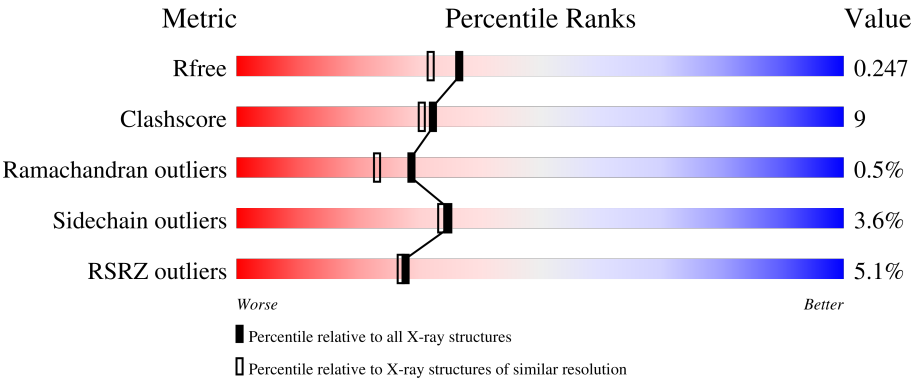
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	230	4% 84% 16%
1	B	230	4% 80% 14%
1	C	230	8% 71% 23%
1	D	230	3% 70% 23%

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	B	1005	-	-	X	-
2	SO4	C	1016	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7817 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.

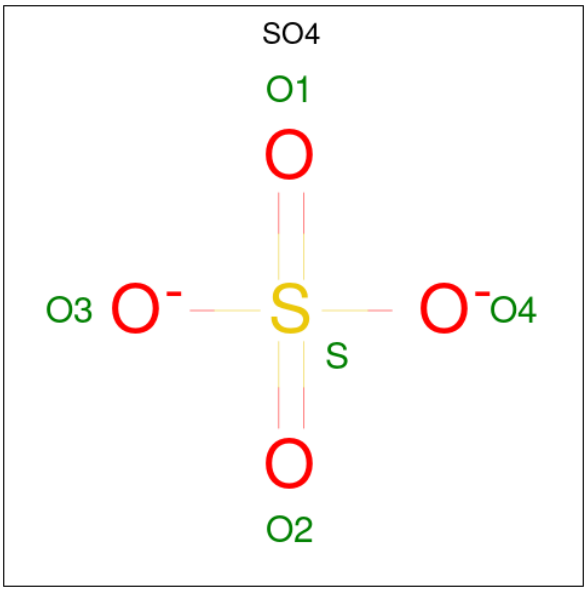
- Molecule 1 is a protein called IRON-DEPENDENT REPRESSOR IDER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	3	0
			1777	1109	322	336	10			
1	B	220	Total	C	N	O	S	0	3	0
			1718	1074	311	323	10			
1	C	220	Total	C	N	O	S	0	4	0
			1716	1074	308	323	11			
1	D	220	Total	C	N	O	S	0	4	0
			1716	1074	308	323	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	ASP	VAL	conflict	UNP P0A672
B	136	ASP	VAL	conflict	UNP P0A672
C	136	ASP	VAL	conflict	UNP P0A672
D	136	ASP	VAL	conflict	UNP P0A672

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



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			
2	A	1	Total	O	S		0	0
			5	4	1			
2	A	1	Total	O	S		0	0
			5	4	1			
2	A	1	Total	O	S		0	0
			5	4	1			
2	A	1	Total	O	S		0	0
			5	4	1			
2	B	1	Total	O	S		0	0
			5	4	1			
2	B	1	Total	O	S		0	0
			5	4	1			
2	B	1	Total	O	S		0	0
			5	4	1			
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	C	1	Total	O	S		0	0
			5	4	1			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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 COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Co 3 3	0	0
3	B	3	Total Co 3 3	0	0
3	C	3	Total Co 3 3	0	0
3	D	4	Total Co 4 4	0	0

- Molecule 4 is water.

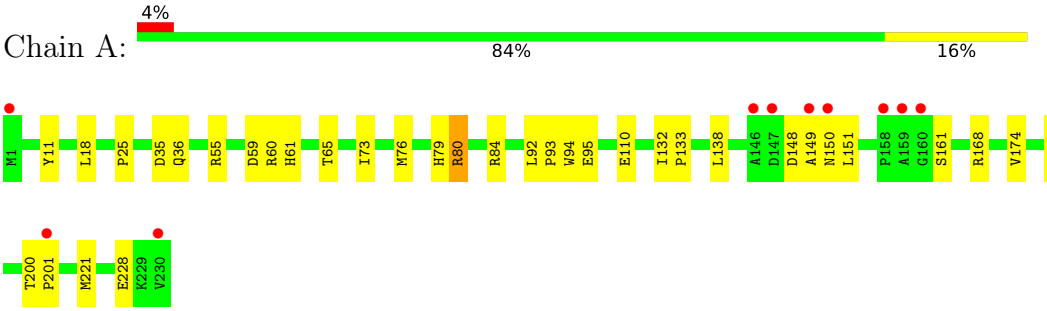
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	263	Total O 263 263	0	0
4	B	208	Total O 208 208	0	0
4	C	139	Total O 139 139	0	0
4	D	182	Total O 182 182	0	0

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.

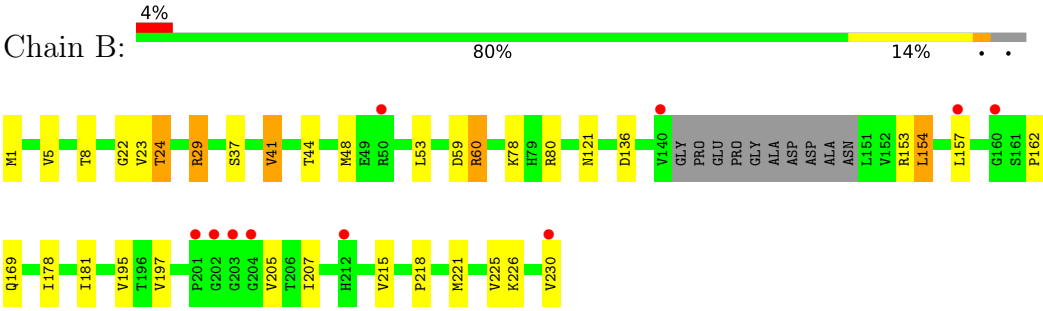
• Molecule 1: IRON-DEPENDENT REPRESSOR IDER

Chain A:



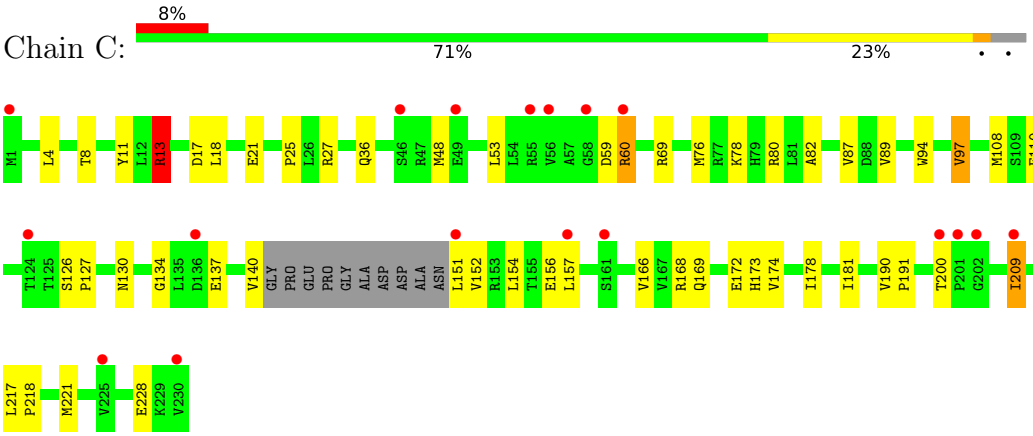
• Molecule 1: IRON-DEPENDENT REPRESSOR IDER

Chain B:



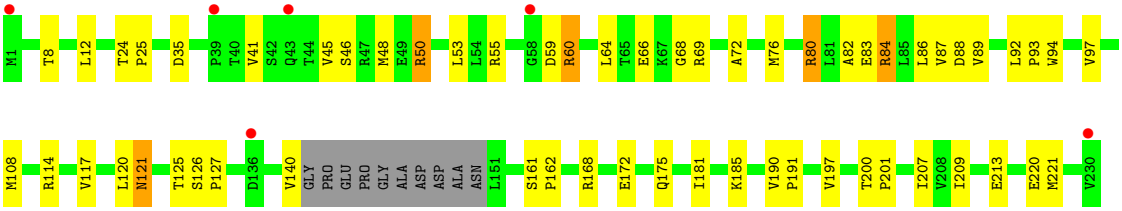
• Molecule 1: IRON-DEPENDENT REPRESSOR IDER

Chain C:



• Molecule 1: IRON-DEPENDENT REPRESSOR IDER

Chain D:


M1 T8 L12 T24 P25 D35 P39 T40 V41 S42 Q43 T44 V45 S46 R47 M48 E49 R50 L53 L54 R55 G58 D59 R60 L64 T65 E66 K67 G68 R69 A72 M76 R80 L81 A82 E83 R84 L85 L86 V87 D88 V89 L92 P93 W94 V97
M108 R114 V117 L120 N121 T125 S126 P127 D136 V140 GLY PRO GLU PRO GLY ALA ASP ASP ALA ASN L151 S161 P162 R168 E172 Q175 I181 K185 V190 P191 V197 T200 P201 I207 V208 I209 E213 E220 M221 V230

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	46.31Å 113.97Å 236.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.96 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.6 (20.00-2.00) 83.1 (19.96-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 1.80Å)	Xtriage
Refinement program	REFMAC, TNT	Depositor
R, R_{free}	0.214 , 0.272 0.202 , 0.247	Depositor DCC
R_{free} test set	4839 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.853	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 70.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7817	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO, 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	0.44	0/1818	1.08	6/2474 (0.2%)
1	B	0.41	0/1756	1.02	4/2386 (0.2%)
1	C	0.38	0/1758	0.96	4/2389 (0.2%)
1	D	0.39	0/1758	1.01	4/2389 (0.2%)
All	All	0.41	0/7090	1.02	18/9638 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	B	80	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	84	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	A	168	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	80	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	D	80	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	168	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	A	94	TRP	CA-CB-CG	6.04	125.19	113.70
1	D	114	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	D	60	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	C	114	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	80	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	D	168	ARG	CD-NE-CZ	5.67	131.53	123.60
1	C	13	ARG	CG-CD-NE	5.65	123.67	111.80
1	A	61	HIS	CA-CB-CG	5.41	122.79	113.60
1	C	13	ARG	CD-NE-CZ	5.32	131.05	123.60
1	B	29	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	60	ARG	CD-NE-CZ	5.23	130.92	123.60

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	1777	0	1806	25	0
1	B	1718	0	1759	26	0
1	C	1716	0	1753	38	0
1	D	1716	0	1753	36	0
2	A	30	0	0	0	0
2	B	25	0	0	2	0
2	C	20	0	0	0	0
2	D	10	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	4	0	0	0	0
4	A	263	0	0	1	0
4	B	208	0	0	3	0
4	C	139	0	0	2	0
4	D	182	0	0	1	0
All	All	7817	0	7071	124	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 9.

All (124) 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:76[A]:MET:HE2	1:A:80:ARG:HG3	1.46	0.98
1:B:48[A]:MET:HG2	1:B:53:LEU:HD12	1.45	0.95
1:C:209:ILE:HD11	1:C:212:HIS:HB2	1.55	0.89
1:A:76[A]:MET:CE	1:A:80:ARG:HG3	2.07	0.84
1:D:76[A]:MET:HE2	1:D:80:ARG:NE	1.97	0.80
1:C:8:THR:HA	1:C:48[B]:MET:HE1	1.63	0.80
1:C:130:ASN:HD22	1:C:169:GLN:HE21	1.28	0.78
1:A:95:GLU:OE2	1:A:185:LYS:HD3	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASP:O	1:B:60:ARG:HB2	1.88	0.73
1:D:83:GLU:HG2	1:D:97:VAL:HG13	1.74	0.70
1:D:59:ASP:O	1:D:60:ARG:HB2	1.92	0.69
1:B:48[A]:MET:HG2	1:B:53:LEU:CD1	2.23	0.68
1:A:76[A]:MET:HE3	1:A:79:HIS:HB3	1.74	0.68
1:C:89:VAL:HG11	1:D:89:VAL:HG11	1.78	0.64
1:C:209:ILE:H	1:C:214:ASN:ND2	1.95	0.64
1:A:59:ASP:O	1:A:60:ARG:HB2	1.97	0.62
1:C:17:ASP:O	1:C:21:GLU:HG2	1.99	0.62
1:A:18:LEU:HD13	1:A:25:PRO:HA	1.83	0.60
1:C:48[B]:MET:HG2	1:C:53:LEU:HD12	1.82	0.60
1:C:87:VAL:HG23	1:C:97:VAL:HG21	1.82	0.60
1:C:130:ASN:HD22	1:C:169:GLN:NE2	1.99	0.60
1:C:154:LEU:HD12	1:C:217:LEU:HD22	1.83	0.60
1:C:18:LEU:HD13	1:C:25:PRO:HA	1.83	0.59
1:D:200:THR:HB	1:D:201:PRO:CD	2.33	0.58
1:C:59:ASP:O	1:C:60:ARG:HB2	2.02	0.58
1:D:87:VAL:HG13	1:D:97:VAL:HG21	1.86	0.58
1:B:22:GLY:HA3	1:B:153:ARG:NH1	2.20	0.57
1:D:200:THR:HB	1:D:201:PRO:HD2	1.86	0.57
1:C:11:TYR:OH	1:C:36:GLN:NE2	2.38	0.57
1:A:200:THR:HG23	1:A:201:PRO:HD2	1.87	0.57
1:C:209:ILE:H	1:C:214:ASN:HD22	1.53	0.57
1:D:8:THR:HA	1:D:48[B]:MET:HE1	1.87	0.56
1:C:218:PRO:HD2	1:C:221[B]:MET:HG3	1.87	0.55
1:D:190:VAL:HB	1:D:191:PRO:HD2	1.89	0.55
1:C:117:VAL:HG11	1:C:140:VAL:HG11	1.87	0.55
1:A:190:VAL:HB	1:A:191:PRO:HD2	1.89	0.54
1:D:76[A]:MET:HE2	1:D:80:ARG:HE	1.73	0.54
1:C:178:ILE:O	1:C:181:ILE:HG22	2.08	0.54
1:A:76[A]:MET:HE3	1:A:79:HIS:CD2	2.43	0.53
1:C:134:GLY:HA2	1:C:137:GLU:OE1	2.09	0.53
1:C:117:VAL:HG11	1:C:140:VAL:HG21	1.92	0.52
1:C:152:VAL:CG2	1:C:156:GLU:HB2	2.40	0.52
1:C:76[A]:MET:HE2	1:C:172:GLU:OE2	2.09	0.51
1:B:1:MET:HE1	1:B:5:VAL:HA	1.90	0.51
1:D:76[A]:MET:HE3	1:D:80:ARG:HG3	1.92	0.51
1:A:76[A]:MET:HE3	1:A:79:HIS:CG	2.45	0.51
1:B:23:VAL:HG23	2:B:1005:SO4:S	2.50	0.51
1:A:76[A]:MET:HE3	1:A:79:HIS:CB	2.38	0.51
1:D:94:TRP:CE3	1:D:185:LYS:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:VAL:HB	1:A:191:PRO:CD	2.41	0.50
1:D:161:SER:HB3	1:D:162:PRO:HD2	1.92	0.50
1:A:11:TYR:OH	1:A:36:GLN:NE2	2.44	0.50
1:B:166:VAL:HG23	1:B:230:VAL:HG22	1.94	0.50
1:B:162:PRO:HA	1:B:197:VAL:O	2.12	0.50
1:D:46:SER:O	1:D:50:ARG:HG2	2.11	0.50
1:D:84:ARG:HD2	1:D:125:THR:O	2.12	0.50
1:B:178:ILE:HA	1:B:181:ILE:HG22	1.94	0.49
1:D:8:THR:HA	1:D:48[B]:MET:CE	2.42	0.49
1:C:173:HIS:HD2	4:C:2026:HOH:O	1.96	0.49
1:B:44:THR:HG22	1:B:48[A]:MET:CE	2.43	0.49
1:D:175:GLN:HA	1:D:181:ILE:HG13	1.94	0.49
1:B:48[A]:MET:CG	1:B:53:LEU:HD12	2.32	0.48
1:B:169:GLN:HB2	1:B:226:LYS:HB2	1.95	0.48
1:C:27:ARG:NH2	1:C:60:ARG:HG2	2.28	0.48
1:B:207:ILE:HB	1:B:215:VAL:HG13	1.95	0.48
1:A:174:VAL:HA	1:A:221[B]:MET:HE1	1.96	0.47
1:B:37:SER:O	1:B:41:VAL:HG13	2.14	0.47
1:D:120:LEU:O	1:D:121:ASN:HB2	2.15	0.47
1:B:23:VAL:HG23	2:B:1005:SO4:O3	2.15	0.47
1:D:12:LEU:HB3	1:D:72:ALA:HB2	1.97	0.47
1:C:78:LYS:HE3	4:C:2048:HOH:O	2.14	0.47
1:C:110:GLU:OE1	1:C:114:ARG:NH2	2.47	0.47
1:D:41:VAL:O	1:D:45:VAL:HG23	2.14	0.47
1:D:87:VAL:CG1	1:D:97:VAL:HG21	2.45	0.47
1:D:190:VAL:HB	1:D:191:PRO:CD	2.44	0.47
1:A:76[A]:MET:HE2	1:A:80:ARG:CG	2.33	0.46
1:B:154:LEU:HD22	1:B:225:VAL:HB	1.96	0.46
1:C:82:ALA:HB2	1:C:108[B]:MET:SD	2.56	0.46
1:A:65:THR:HB	4:A:2180:HOH:O	2.14	0.46
1:A:174:VAL:HA	1:A:221[B]:MET:CE	2.46	0.45
1:A:80:ARG:HB2	1:A:132:ILE:HG12	1.97	0.45
1:D:117:VAL:HG11	1:D:140:VAL:HG21	1.97	0.45
1:B:195:VAL:HG21	1:B:207:ILE:HG23	1.99	0.45
1:C:130:ASN:ND2	1:C:169:GLN:HE21	2.04	0.45
1:A:151:LEU:HD12	1:A:228:GLU:HG3	1.99	0.45
1:C:190:VAL:HB	1:C:191:PRO:HD2	1.98	0.45
1:C:166:VAL:HG23	1:C:228:GLU:HB3	2.00	0.44
1:C:13:ARG:HD2	1:C:76[A]:MET:SD	2.58	0.44
1:C:152:VAL:HG23	1:C:156:GLU:HB2	2.00	0.44
1:C:130:ASN:ND2	1:C:169:GLN:HB3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:VAL:HG21	4:B:2182:HOH:O	2.17	0.44
1:D:197:VAL:HG12	1:D:207:ILE:HD13	2.00	0.43
1:A:92:LEU:HD12	1:A:93:PRO:HD2	1.99	0.43
1:D:24:THR:HA	1:D:25:PRO:HD3	1.87	0.43
1:D:87:VAL:HG23	1:D:88:ASP:N	2.34	0.43
1:D:76[A]:MET:HE2	1:D:80:ARG:CZ	2.46	0.43
1:D:82:ALA:HB2	1:D:108[B]:MET:SD	2.58	0.43
1:D:220:GLU:HG3	1:D:221[B]:MET:HE3	1.99	0.43
1:D:76[A]:MET:HE2	1:D:172:GLU:OE2	2.19	0.43
1:D:83:GLU:O	1:D:87:VAL:HG22	2.19	0.43
1:B:23:VAL:HG22	1:B:24:THR:N	2.33	0.43
1:D:86:LEU:HB3	1:D:97:VAL:HG22	2.00	0.43
1:B:218:PRO:HD2	1:B:221[B]:MET:HG3	2.01	0.42
1:B:154:LEU:O	1:B:205:VAL:HG21	2.19	0.42
1:C:59:ASP:O	1:C:60:ARG:CB	2.67	0.42
1:A:73:ILE:HG23	1:A:133:PRO:HB2	2.02	0.42
1:B:195:VAL:HG23	4:B:2103:HOH:O	2.18	0.42
1:C:126:SER:HB2	1:C:127:PRO:HD2	2.01	0.42
1:D:126:SER:HB2	1:D:127:PRO:CD	2.51	0.41
1:D:69:ARG:HD3	4:D:2192:HOH:O	2.20	0.41
1:A:190:VAL:O	1:A:191:PRO:C	2.59	0.41
1:D:53:LEU:O	1:D:68:GLY:HA3	2.21	0.41
1:A:110:GLU:HG3	1:A:138:LEU:CD2	2.50	0.41
1:B:181:ILE:HG21	4:B:2031:HOH:O	2.20	0.41
1:C:166:VAL:CG2	1:C:228:GLU:HB3	2.51	0.41
1:C:190:VAL:HB	1:C:191:PRO:CD	2.50	0.41
1:D:92:LEU:HD12	1:D:93:PRO:HD2	2.03	0.41
1:C:174:VAL:HA	1:C:221[B]:MET:HE2	2.04	0.40
1:B:8:THR:HG23	1:B:48[A]:MET:SD	2.61	0.40
1:B:197:VAL:HG12	1:B:207:ILE:HD13	2.04	0.40
1:C:151:LEU:HD11	1:C:168:ARG:HB2	2.03	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	231/230 (100%)	222 (96%)	7 (3%)	2 (1%)	17 11
1	B	219/230 (95%)	214 (98%)	5 (2%)	0	100 100
1	C	220/230 (96%)	214 (97%)	5 (2%)	1 (0%)	29 23
1	D	220/230 (96%)	213 (97%)	6 (3%)	1 (0%)	29 23
All	All	890/920 (97%)	863 (97%)	23 (3%)	4 (0%)	29 30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ASP
1	A	149	ALA
1	C	60	ARG
1	D	121	ASN

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	196/195 (100%)	193 (98%)	3 (2%)	65 69
1	B	192/195 (98%)	185 (96%)	7 (4%)	35 34
1	C	192/195 (98%)	183 (95%)	9 (5%)	26 22
1	D	192/195 (98%)	184 (96%)	8 (4%)	30 27
All	All	772/780 (99%)	745 (96%)	27 (4%)	35 35

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	150	ASN
1	A	161	SER
1	B	24	THR

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Mol	Chain	Res	Type
1	B	29	ARG
1	B	41	VAL
1	B	121	ASN
1	B	136	ASP
1	B	154	LEU
1	B	157	LEU
1	C	4	LEU
1	C	13	ARG
1	C	69	ARG
1	C	94	TRP
1	C	97	VAL
1	C	157	LEU
1	C	200	THR
1	C	209	ILE
1	C	213	GLU
1	D	35	ASP
1	D	50	ARG
1	D	55	ARG
1	D	64	LEU
1	D	66	GLU
1	D	84	ARG
1	D	209	ILE
1	D	213	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	150	ASN
1	A	214	ASN
1	B	36	GLN
1	B	130	ASN
1	B	169	GLN
1	C	36	GLN
1	C	130	ASN
1	C	173	HIS
1	C	214	ASN
1	D	36	GLN
1	D	43	GLN
1	D	121	ASN
1	D	130	ASN
1	D	169	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 30 ligands modelled in this entry, 13 are monoatomic - leaving 17 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	B	1014	-	4,4,4	0.62	0	6,6,6	0.24	0
2	SO4	A	1013	-	4,4,4	0.67	0	6,6,6	0.28	0
2	SO4	C	1016	-	4,4,4	0.64	0	6,6,6	0.06	0
2	SO4	B	1002	-	4,4,4	0.65	0	6,6,6	0.24	0
2	SO4	A	1008	-	4,4,4	0.64	0	6,6,6	0.12	0
2	SO4	B	1011	-	4,4,4	0.61	0	6,6,6	0.15	0
2	SO4	A	1006	-	4,4,4	0.65	0	6,6,6	0.15	0
2	SO4	C	1003	-	4,4,4	0.63	0	6,6,6	0.34	0
2	SO4	C	1007	-	4,4,4	0.61	0	6,6,6	0.18	0
2	SO4	A	1004	-	4,4,4	0.46	0	6,6,6	0.37	0
2	SO4	B	1005	-	4,4,4	0.60	0	6,6,6	0.26	0
2	SO4	B	1009	-	4,4,4	0.68	0	6,6,6	0.33	0
2	SO4	D	1012	-	4,4,4	0.59	0	6,6,6	0.13	0
2	SO4	C	1010	-	4,4,4	0.64	0	6,6,6	0.16	0
2	SO4	A	1017	-	4,4,4	0.63	0	6,6,6	0.07	0
2	SO4	A	1001	-	4,4,4	0.55	0	6,6,6	0.34	0
2	SO4	D	1015	-	4,4,4	0.61	0	6,6,6	0.07	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1005	SO4	2	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

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	230/230 (100%)	-0.22	10 (4%)	35	34	20, 30, 67, 134	0
1	B	220/230 (95%)	-0.17	10 (4%)	33	32	22, 36, 74, 166	0
1	C	220/230 (95%)	0.21	19 (8%)	10	9	24, 47, 108, 183	0
1	D	220/230 (95%)	-0.14	6 (2%)	54	53	28, 39, 68, 96	0
All	All	890/920 (96%)	-0.08	45 (5%)	28	27	20, 38, 79, 183	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	201	PRO	5.6
1	A	150	ASN	4.8
1	C	58	GLY	4.5
1	C	200	THR	4.4
1	C	230	VAL	4.3
1	D	58	GLY	4.2
1	B	201	PRO	4.1
1	B	230	VAL	3.9
1	D	39	PRO	3.7
1	C	151	LEU	3.7
1	C	1	MET	3.5
1	A	149	ALA	3.4
1	C	60	ARG	3.3
1	C	56	VAL	3.3
1	A	201	PRO	3.2
1	B	202	GLY	3.2
1	C	209	ILE	3.2
1	C	49	GLU	3.1
1	A	159	ALA	3.1
1	B	160	GLY	3.0
1	B	204	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	1	MET	2.9
1	C	124	THR	2.9
1	C	161	SER	2.9
1	A	147	ASP	2.8
1	C	225	VAL	2.7
1	C	202	GLY	2.7
1	C	55	ARG	2.7
1	A	158	PRO	2.5
1	A	160	GLY	2.5
1	A	230	VAL	2.5
1	B	50	ARG	2.5
1	C	46	SER	2.4
1	A	146	ALA	2.4
1	A	1	MET	2.4
1	C	213	GLU	2.3
1	C	157	LEU	2.3
1	B	212	HIS	2.3
1	B	157	LEU	2.2
1	D	230	VAL	2.2
1	C	136	ASP	2.2
1	D	136	ASP	2.1
1	B	203	GLY	2.0
1	D	43	GLN	2.0
1	B	140	VAL	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, 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	1016	5/5	0.22	0.69	201,202,202,203	0
2	SO4	A	1017	5/5	0.84	0.22	94,100,103,103	0
2	SO4	B	1014	5/5	0.88	0.22	48,64,75,80	0
2	SO4	A	1013	5/5	0.89	0.21	38,57,66,78	0
2	SO4	A	1006	5/5	0.94	0.16	41,58,71,75	0
2	SO4	B	1002	5/5	0.94	0.11	62,66,66,69	0
2	SO4	D	1015	5/5	0.94	0.27	83,86,90,95	0
2	SO4	C	1003	5/5	0.95	0.13	41,50,56,60	0
2	SO4	C	1007	5/5	0.95	0.11	50,50,63,66	0
2	SO4	B	1011	5/5	0.96	0.13	55,60,69,72	0
2	SO4	A	1001	5/5	0.96	0.11	37,44,55,58	0
2	SO4	C	1010	5/5	0.97	0.15	54,55,66,67	0
2	SO4	A	1008	5/5	0.97	0.20	46,61,71,74	0
2	SO4	B	1005	5/5	0.97	0.16	52,58,65,71	0
2	SO4	D	1012	5/5	0.98	0.13	44,48,60,65	0
2	SO4	B	1009	5/5	0.98	0.08	42,45,48,59	0
3	CO	B	2010	1/1	0.98	0.02	44,44,44,44	0
3	CO	C	2005	1/1	0.98	0.04	32,32,32,32	0
3	CO	C	2011	1/1	0.98	0.06	44,44,44,44	0
3	CO	A	2009	1/1	0.99	0.04	29,29,29,29	0
3	CO	D	2007	1/1	0.99	0.05	30,30,30,30	0
3	CO	D	2008	1/1	0.99	0.04	31,31,31,31	0
3	CO	D	2012	1/1	0.99	0.03	39,39,39,39	0
3	CO	D	2013	1/1	0.99	0.02	49,49,49,49	0
3	CO	C	2006	1/1	1.00	0.03	31,31,31,31	0
2	SO4	A	1004	5/5	1.00	0.06	30,31,38,39	0
3	CO	B	2003	1/1	1.00	0.06	27,27,27,27	0
3	CO	B	2004	1/1	1.00	0.04	26,26,26,26	0
3	CO	A	2001	1/1	1.00	0.06	21,21,21,21	0
3	CO	A	2002	1/1	1.00	0.08	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.