Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:30 PM GMT

PDB ID	:	1B4K
Title	:	High resolution crystal structure of a MG2-dependent 5-aminolevulinic acid dehydratase
Authors	:	Frankenberg, N.; Jahn, D.; Heinz, D.W.
Deposited on	:	1998-12-22
Resolution	:	1.67 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

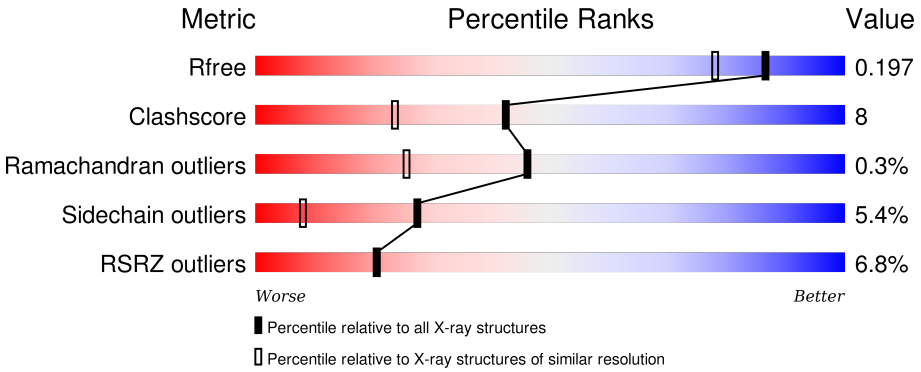
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.67 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}	91344	4802 (1.70-1.66)
Clashscore	102246	5317 (1.70-1.66)
Ramachandran outliers	100387	5225 (1.70-1.66)
Sidechain outliers	100360	5224 (1.70-1.66)
RSRZ outliers	91569	4813 (1.70-1.66)

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. 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	337	3%, 81%, 14%
1	B	337	10%, 75%, 15%, 5%

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	A	401	-	-	-	X
4	SHF	A	403	-	-	-	X

2 Entry composition

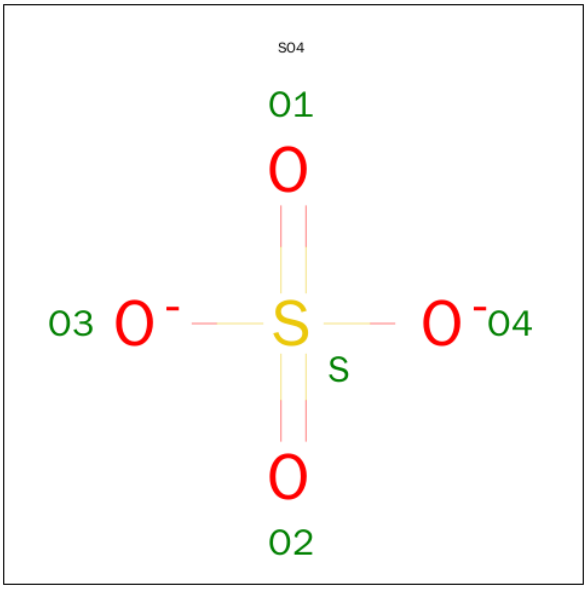
There are 5 unique types of molecules in this entry. The entry contains 5604 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (5-AMINOLEVULINIC ACID DEHYDRATASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2522	1586	443	483	10			
1	B	320	Total	C	N	O	S	0	0	0
			2485	1563	437	475	10			

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

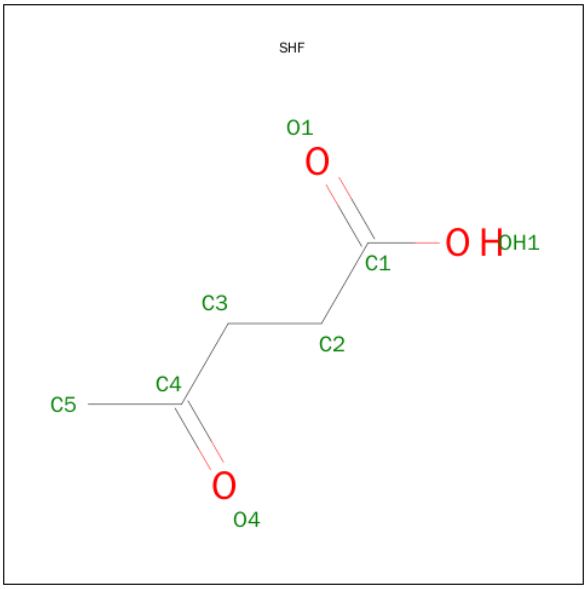


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is LAEVULINIC ACID (three-letter code: SHF) (formula: $C_5H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 5 2	0	0
4	B	1	Total C O 7 5 2	0	0

- Molecule 5 is water.

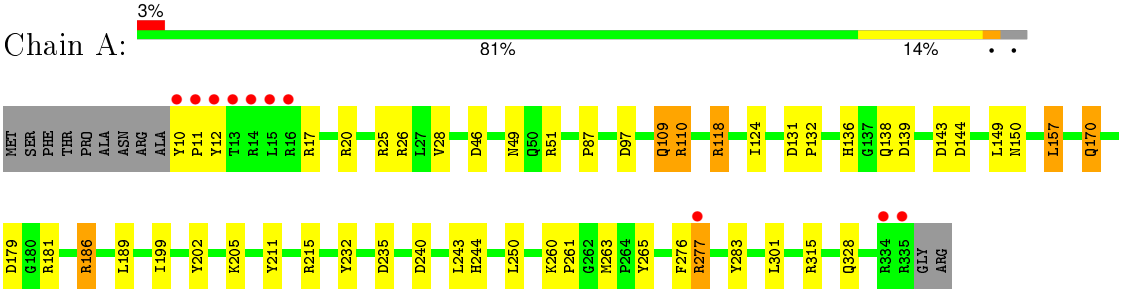
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	322	Total O 322 322	0	0
5	B	250	Total O 250 250	0	0

3 Residue-property plots (i)

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.

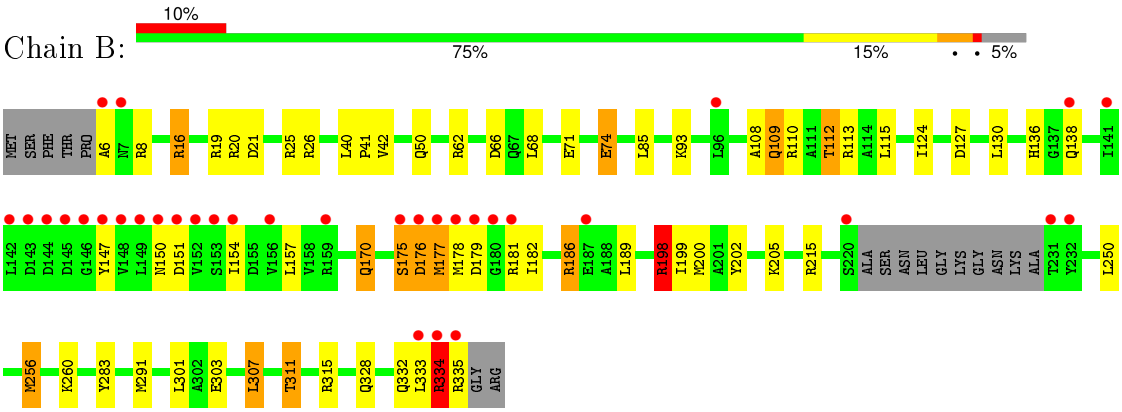
- Molecule 1: PROTEIN (5-AMINOLEVULINIC ACID DEHYDRATASE)

Chain A:



- Molecule 1: PROTEIN (5-AMINOLEVULINIC ACID DEHYDRATASE)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	128.24Å 128.24Å 86.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.30 – 1.67 51.45 – 1.67	Depositor EDS
% Data completeness (in resolution range)	98.2 (51.30-1.67) 95.3 (51.45-1.67)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.25 (at 1.67Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.178 , 0.208 0.170 , 0.197	Depositor DCC
R_{free} test set	4104 reflections (5.43%)	DCC
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 81819 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5604	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, SO4, SHF

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	0.58	0/2569	1.36	30/3486 (0.9%)
1	B	0.54	0/2531	1.41	27/3435 (0.8%)
All	All	0.56	0/5100	1.39	57/6921 (0.8%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	113	ARG	CD-NE-CZ	23.96	157.14	123.60
1	B	198	ARG	CD-NE-CZ	18.87	150.01	123.60
1	A	25	ARG	NE-CZ-NH2	-15.91	112.34	120.30
1	B	19	ARG	NE-CZ-NH2	-15.52	112.54	120.30
1	A	10	TYR	CB-CG-CD1	-14.77	112.14	121.00
1	A	10	TYR	CB-CG-CD2	12.95	128.77	121.00
1	B	19	ARG	NE-CZ-NH1	12.83	126.72	120.30
1	B	198	ARG	NE-CZ-NH1	-11.94	114.33	120.30
1	A	25	ARG	CD-NE-CZ	11.23	139.32	123.60
1	B	25	ARG	NE-CZ-NH1	10.82	125.71	120.30
1	B	315	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	A	118	ARG	CD-NE-CZ	9.67	137.14	123.60
1	B	16	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	A	215	ARG	CD-NE-CZ	8.78	135.90	123.60
1	A	315	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	B	113	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	51	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	A	25	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	B	291	MET	CG-SD-CE	7.71	112.53	100.20
1	A	157	LEU	CB-CG-CD1	7.46	123.69	111.00
1	B	198	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	B	20	ARG	NE-CZ-NH1	7.05	123.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	186	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	B	26	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	263	MET	CG-SD-CE	-6.87	89.21	100.20
1	B	110	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	202	TYR	CB-CG-CD1	6.68	125.01	121.00
1	B	74	GLU	OE1-CD-OE2	-6.58	115.40	123.30
1	A	202	TYR	CB-CG-CD2	-6.54	117.08	121.00
1	A	131	ASP	CB-CG-OD2	6.49	124.14	118.30
1	B	62	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	B	186	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	139	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	118	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	B	176	ASP	CB-CG-OD1	6.05	123.74	118.30
1	A	186	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	16	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	144	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	235	ASP	CB-CG-OD1	5.68	123.42	118.30
1	B	20	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	110	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	B	66	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	20	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	232	TYR	CA-CB-CG	5.45	123.75	113.40
1	B	215	ARG	CD-NE-CZ	5.44	131.22	123.60
1	A	118	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	A	97	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	26	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	118	ARG	NH1-CZ-NH2	-5.22	113.66	119.40
1	B	147	TYR	CA-CB-CG	-5.18	103.55	113.40
1	B	303	GLU	OE1-CD-OE2	5.17	129.50	123.30
1	A	144	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	A	10	TYR	CA-CB-CG	-5.08	103.74	113.40
1	B	110	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	26	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	110	ARG	CG-CD-NE	5.03	122.37	111.80
1	A	277	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	2522	0	2490	38	0
1	B	2485	0	2449	46	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
4	A	7	0	7	0	0
4	B	7	0	7	1	0
5	A	322	0	0	8	0
5	B	250	0	0	5	0
All	All	5604	0	4953	83	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 8.

All (83) 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)
4:B:402:SHF:H51	5:B:690:HOH:O	1.48	1.11
1:A:150:ASN:HD21	1:A:179:ASP:H	1.19	0.87
1:B:175:SER:HA	1:B:202:TYR:CD1	2.14	0.82
1:A:170:GLN:HE21	1:A:170:GLN:H	1.28	0.81
1:A:189:LEU:CD1	1:A:199:ILE:HD11	2.10	0.80
1:A:189:LEU:HD12	1:A:199:ILE:HD11	1.64	0.79
1:A:136:HIS:HD2	1:A:138:GLN:H	1.30	0.79
1:B:170:GLN:HE21	1:B:170:GLN:H	1.36	0.74
1:A:186:ARG:NH1	1:A:199:ILE:HD13	2.04	0.73
1:B:136:HIS:HD2	1:B:138:GLN:H	1.35	0.73
1:B:198:ARG:N	1:B:198:ARG:HD3	2.02	0.73
1:B:200:MET:HA	1:B:256:MET:HG2	1.74	0.70
1:A:186:ARG:CZ	1:A:199:ILE:HD13	2.23	0.69
1:A:150:ASN:HD21	1:A:179:ASP:N	1.90	0.68
1:A:87:PRO:HD2	5:A:637:HOH:O	1.93	0.68
1:B:176:ASP:OD2	1:B:181:ARG:HD2	1.93	0.68
1:B:205:LYS:HE3	1:B:260:LYS:HE2	1.76	0.67
1:A:205:LYS:HE3	1:A:260:LYS:HE2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ARG:CZ	1:B:199:ILE:HD13	2.25	0.66
1:B:307:LEU:O	1:B:311:THR:HG23	1.95	0.66
1:B:189:LEU:HD12	1:B:199:ILE:HD11	1.79	0.64
1:B:108:ALA:O	1:B:112:THR:HG23	1.99	0.63
1:B:157:LEU:HD13	1:B:181:ARG:HD3	1.81	0.62
1:B:109:GLN:HE21	1:B:109:GLN:H	1.48	0.61
1:A:150:ASN:HD22	1:B:16:ARG:HH11	1.47	0.61
1:B:124:ILE:H	1:B:170:GLN:NE2	1.99	0.61
1:B:178:MET:HG3	1:B:181:ARG:CZ	2.31	0.61
1:B:189:LEU:CD1	1:B:199:ILE:HD11	2.31	0.60
1:A:186:ARG:NH2	1:A:199:ILE:HD13	2.18	0.59
1:A:136:HIS:CD2	1:A:138:GLN:H	2.17	0.59
1:B:40:LEU:HD23	1:B:41:PRO:O	2.03	0.59
1:B:186:ARG:NH2	1:B:199:ILE:HD13	2.19	0.58
1:A:328:GLN:HG3	5:A:735:HOH:O	2.04	0.57
1:A:132:PRO:HG3	5:A:784:HOH:O	2.04	0.57
1:B:136:HIS:CD2	1:B:138:GLN:H	2.20	0.56
1:B:109:GLN:H	1:B:109:GLN:NE2	2.03	0.55
1:B:182:ILE:HD13	5:B:723:HOH:O	2.06	0.55
1:A:124:ILE:H	1:A:170:GLN:NE2	2.05	0.54
1:A:109:GLN:HE21	1:A:109:GLN:H	1.56	0.54
1:A:243:LEU:H	1:A:243:LEU:HD22	1.73	0.54
1:B:200:MET:HG3	1:B:256:MET:HG3	1.90	0.53
1:B:112:THR:HB	1:B:124:ILE:HG21	1.90	0.53
1:B:124:ILE:H	1:B:170:GLN:HE22	1.55	0.52
1:A:170:GLN:N	1:A:170:GLN:HE21	2.04	0.52
1:B:40:LEU:HD22	1:B:42:VAL:CG1	2.39	0.52
1:A:136:HIS:HE1	5:A:527:HOH:O	1.94	0.51
1:B:6:ALA:HA	5:B:696:HOH:O	2.11	0.50
1:A:109:GLN:NE2	1:A:109:GLN:H	2.09	0.50
1:A:186:ARG:HH12	1:A:199:ILE:HD13	1.75	0.50
1:B:177:MET:HG2	1:B:205:LYS:HB3	1.94	0.49
1:A:240:ASP:HA	1:A:243:LEU:HD23	1.94	0.49
1:B:130:LEU:HG	1:B:157:LEU:HD21	1.96	0.47
1:A:276:PHE:O	1:A:277:ARG:HG2	2.13	0.47
1:B:332:GLN:O	1:B:334:ARG:N	2.47	0.47
1:A:205:LYS:CE	1:A:260:LYS:HE2	2.42	0.47
1:A:243:LEU:N	1:A:243:LEU:HD22	2.30	0.47
1:B:136:HIS:CD2	1:B:138:GLN:HB2	2.50	0.47
1:B:85:LEU:HD12	1:B:112:THR:HG22	1.96	0.46
1:B:178:MET:HG3	1:B:181:ARG:NE	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ASP:OD1	1:B:175:SER:HB3	2.15	0.46
1:B:334:ARG:O	1:B:335:ARG:C	2.54	0.45
1:B:68:LEU:HD21	1:B:115:LEU:HD11	1.98	0.45
1:A:124:ILE:H	1:A:170:GLN:HE22	1.62	0.45
1:B:21:ASP:HA	5:B:512:HOH:O	2.17	0.45
1:A:261:PRO:HD2	1:A:265:TYR:CE2	2.53	0.45
1:B:170:GLN:HE21	1:B:170:GLN:N	2.11	0.44
1:B:178:MET:HG3	1:B:181:ARG:NH2	2.31	0.44
1:B:328:GLN:HG2	5:B:749:HOH:O	2.18	0.44
1:B:175:SER:HA	1:B:202:TYR:CG	2.52	0.44
1:A:211:TYR:CE1	1:A:260:LYS:HE3	2.53	0.43
1:A:143:ASP:HB3	1:A:149:LEU:HD21	2.00	0.43
1:A:244:HIS:CD2	1:B:8:ARG:HH11	2.37	0.43
1:A:28:VAL:HG13	5:A:623:HOH:O	2.19	0.42
1:B:71:GLU:HA	1:B:74:GLU:OE1	2.19	0.42
1:A:46:ASP:OD1	1:A:110:ARG:NH2	2.48	0.42
1:A:211:TYR:HB2	5:A:590:HOH:O	2.19	0.42
1:B:186:ARG:NH1	1:B:199:ILE:HD13	2.35	0.42
1:B:40:LEU:HD22	1:B:42:VAL:HG13	2.02	0.42
1:A:12:TYR:HB2	5:A:749:HOH:O	2.19	0.42
1:A:150:ASN:ND2	1:A:179:ASP:H	2.01	0.41
1:A:11:PRO:O	1:A:17:ARG:NH2	2.54	0.41
1:A:277:ARG:HB3	5:A:736:HOH:O	2.20	0.40
1:B:175:SER:HB2	1:B:202:TYR:CE1	2.56	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	324/337 (96%)	317 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	316/337 (94%)	307 (97%)	7 (2%)	2 (1%)	30 11
All	All	640/674 (95%)	624 (98%)	14 (2%)	2 (0%)	46 25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	333	LEU
1	B	334	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	261/269 (97%)	252 (97%)	9 (3%)	44 19
1	B	257/269 (96%)	238 (93%)	19 (7%)	17 3
All	All	518/538 (96%)	490 (95%)	28 (5%)	27 8

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	109	GLN
1	A	118	ARG
1	A	157	LEU
1	A	170	GLN
1	A	181	ARG
1	A	250	LEU
1	A	283	TYR
1	A	301	LEU
1	B	50	GLN
1	B	93	LYS
1	B	109	GLN
1	B	112	THR
1	B	150	ASN

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Mol	Chain	Res	Type
1	B	151	ASP
1	B	154	ILE
1	B	170	GLN
1	B	175	SER
1	B	177	MET
1	B	179	ASP
1	B	198	ARG
1	B	250	LEU
1	B	256	MET
1	B	283	TYR
1	B	301	LEU
1	B	307	LEU
1	B	311	THR
1	B	334	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	109	GLN
1	A	136	HIS
1	A	150	ASN
1	A	170	GLN
1	A	223	ASN
1	A	244	HIS
1	A	328	GLN
1	B	50	GLN
1	B	109	GLN
1	B	136	HIS
1	B	170	GLN

5.3.3 RNA

There are no RNA molecules 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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	401	-	4,4,4	0.97	0	6,6,6	0.45	0
4	SHF	A	403	1	3,6,7	1.04	0	3,6,8	1.77	1 (33%)
2	SO4	B	401	-	4,4,4	0.96	0	6,6,6	0.10	0
4	SHF	B	402	1	3,6,7	0.85	0	3,6,8	1.96	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	401	-	-	0/0/0/0	0/0/0/0
4	SHF	A	403	1	-	0/2/4/5	0/0/0/0
2	SO4	B	401	-	-	0/0/0/0	0/0/0/0
4	SHF	B	402	1	-	0/2/4/5	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	403	SHF	C3-C2-C1	2.88	128.10	112.58
4	B	402	SHF	C3-C2-C1	3.21	129.90	112.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	402	SHF	1	0

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, 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	326/337 (96%)	-0.11	10 (3%) 52 55	11, 16, 30, 76	0
1	B	320/337 (94%)	0.33	34 (10%) 8 8	12, 20, 54, 68	0
All	All	646/674 (95%)	0.11	44 (6%) 20 20	11, 18, 44, 76	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	TYR	13.1
1	A	10	TYR	10.6
1	B	335	ARG	8.9
1	B	147	TYR	8.8
1	A	11	PRO	8.4
1	B	175	SER	5.8
1	B	6	ALA	5.8
1	B	334	ARG	5.7
1	B	144	ASP	5.4
1	B	142	LEU	5.3
1	B	145	ASP	5.3
1	B	176	ASP	5.1
1	A	335	ARG	4.9
1	B	146	GLY	4.7
1	B	177	MET	4.7
1	A	14	ARG	4.4
1	B	152	VAL	4.4
1	A	13	THR	4.4
1	B	179	ASP	4.3
1	B	151	ASP	4.2
1	B	143	ASP	4.0
1	B	156	VAL	3.8
1	B	150	ASN	3.8
1	B	141	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	16	ARG	3.4
1	A	277	ARG	3.4
1	B	96	LEU	3.3
1	B	149	LEU	3.2
1	B	220	SER	3.2
1	B	138	GLN	3.1
1	B	178	MET	3.1
1	B	181	ARG	3.0
1	B	232	TYR	2.6
1	A	15	LEU	2.5
1	B	231	THR	2.5
1	B	7	ASN	2.4
1	B	154	ILE	2.3
1	A	334	ARG	2.3
1	B	187	GLU	2.2
1	B	180	GLY	2.2
1	B	159	ARG	2.2
1	B	148	VAL	2.2
1	B	153	SER	2.1
1	B	333	LEU	2.1

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 carbohydrates 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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	401	5/5	0.76	0.22	7.21	52,53,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SHF	A	403	7/8	0.87	0.13	2.50	14,15,17,17	0
2	SO4	B	401	5/5	0.85	0.14	0.62	76,76,76,76	0
4	SHF	B	402	7/8	0.90	0.14	0.45	17,17,23,24	0
3	MG	A	402	1/1	0.99	0.06	-0.29	12,12,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.