



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:53 am BST

PDB ID : 1E51  
Title : Crystal structure of native human erythrocyte 5-aminolaevulinic acid dehydratase  
Authors : Mills-Davies, N.L.; Thompson, D.; Cooper, J.B.; Shoolingin-Jordan, P.M.  
Deposited on : 2000-07-13  
Resolution : 2.83 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](mailto: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.

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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 : 2.11  
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) : 2.11

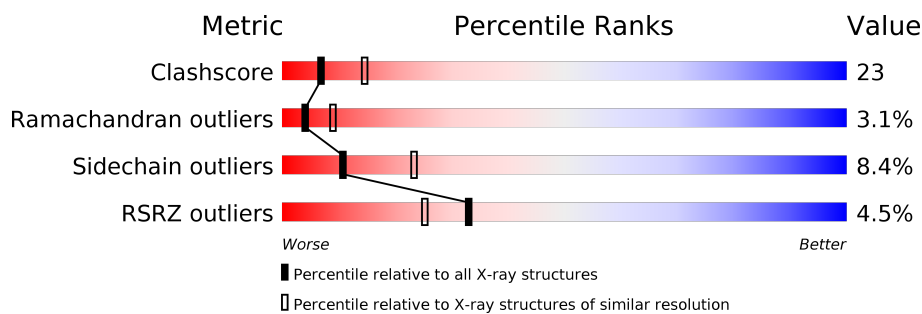
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.83 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))
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	330	 5% 58% 36% 5%
1	B	330	 4% 57% 28% 5% 9%

## 2 Entry composition [i](#)

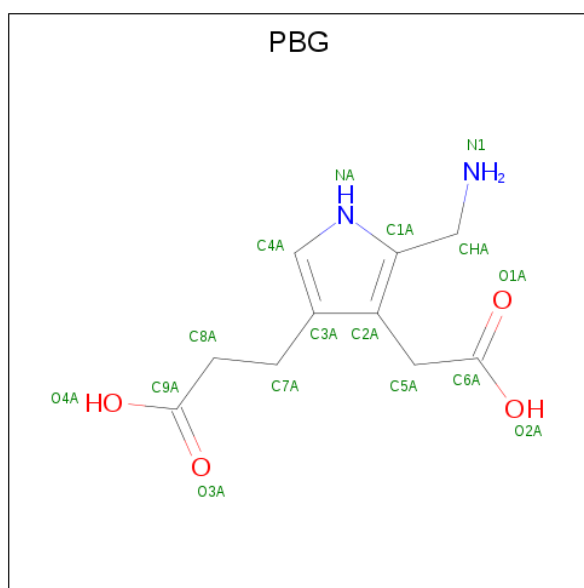
There are 4 unique types of molecules in this entry. The entry contains 4707 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DELTA-AMINOLEVULINIC ACID DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2437	1560	426	432	19			
1	B	299	Total	C	N	O	S	0	0	0
			2243	1442	387	396	18			

- Molecule 2 is 3-[5-(AMINOMETHYL)-4-(CARBOXYMETHYL)-1H-PYRROL-3-YL]PROPANOIC ACID (three-letter code: PBG) (formula:  $C_{10}H_{14}N_2O_4$ ).

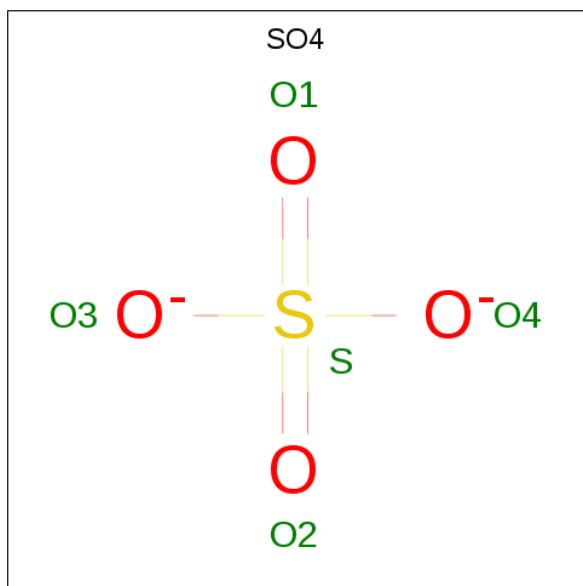


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	10	2	4		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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



- Molecule 1: DELTA-AMINOLEVULINIC ACID DEHYDRATASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.53Å 125.53Å 200.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.38 – 2.83 44.38 – 2.83	Depositor EDS
% Data completeness (in resolution range)	95.5 (44.38-2.83) 95.7 (44.38-2.83)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.213 , 0.270 0.215 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.4	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 83.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4707	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: ZN, PBG, 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	0.42	0/2496	0.73	2/3398 (0.1%)
1	B	0.41	0/2294	0.69	1/3124 (0.0%)
All	All	0.42	0/4790	0.71	3/6522 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	GLY	O-C-N	-5.99	113.12	122.70
1	A	26	LEU	CA-CB-CG	5.56	128.09	115.30
1	B	10	GLY	O-C-N	-5.20	114.39	122.70

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	2437	0	2378	126	0
1	B	2243	0	2203	101	0
2	A	16	0	12	6	0
3	A	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4707	0	4593	215	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 23.

All (215) 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:227:PRO:HG2	1:A:230:ALA:HB2	1.36	1.08
1:B:11:TYR:HD1	1:B:11:TYR:N	1.49	1.07
1:B:40:VAL:HB	1:B:43:ASP:HB2	1.11	1.06
1:B:11:TYR:N	1:B:11:TYR:CD1	2.18	1.05
1:A:40:VAL:HB	1:A:43:ASP:HB2	1.39	1.04
1:A:11:TYR:CD1	1:A:11:TYR:N	2.26	1.02
1:B:170:MET:HE2	1:B:199:LYS:H	1.28	0.98
1:A:95:ASP:HB3	1:A:153:VAL:HG13	1.44	0.95
1:A:11:TYR:HD1	1:A:11:TYR:N	1.61	0.95
1:B:11:TYR:HD1	1:B:11:TYR:H	1.00	0.93
1:A:27:ASN:H	1:A:30:ASN:HD22	1.19	0.90
1:B:260:ILE:O	1:B:264:VAL:HG13	1.75	0.85
1:A:209:ARG:HA	1:A:209:ARG:HH11	1.41	0.85
1:A:252:LYS:CE	2:A:500:PBG:H7A2	2.08	0.83
1:A:227:PRO:HG2	1:A:230:ALA:CB	2.07	0.83
1:B:227:PRO:HG2	1:B:230:ALA:HB2	1.63	0.81
1:B:40:VAL:HB	1:B:43:ASP:CB	2.05	0.79
1:A:202:SER:HB2	1:B:302:GLU:OE2	1.82	0.79
1:A:44:ILE:O	1:A:44:ILE:HG23	1.83	0.79
1:B:123:LEU:C	1:B:125:PRO:HD2	2.05	0.78
1:A:119:CYS:HB2	1:A:162:CYS:SG	2.24	0.76
1:A:43:ASP:O	1:A:60:ARG:HD3	1.86	0.76
1:A:258:LEU:HD21	1:A:306:ALA:HB1	1.68	0.75
1:B:86:PRO:O	1:B:87:LYS:CB	2.34	0.75
1:A:255:MET:HA	1:A:258:LEU:HD13	1.68	0.74
1:A:207:PRO:HB2	1:A:279:SER:HB2	1.69	0.74
1:B:235:LEU:HD11	1:B:263:GLU:HG2	1.70	0.74
1:A:18:ALA:HA	1:A:21:THR:HG22	1.69	0.74
1:A:260:ILE:O	1:A:264:VAL:HG13	1.87	0.74
1:B:95:ASP:HA	1:B:126:TYR:CG	2.23	0.73
1:A:40:VAL:CB	1:A:43:ASP:HB2	2.17	0.73
1:B:11:TYR:O	1:B:16:LEU:HD23	1.88	0.72
1:B:44:ILE:O	1:B:44:ILE:HG23	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ILE:HG12	1:B:211:ALA:HA	1.71	0.72
1:A:234:ALA:O	1:A:238:VAL:HG23	1.90	0.71
1:B:207:PRO:HB2	1:B:279:SER:HB2	1.74	0.70
1:B:11:TYR:O	1:B:12:PHE:CG	2.45	0.69
1:A:119:CYS:HB2	1:A:162:CYS:HG	1.57	0.69
1:A:27:ASN:HA	1:A:327:LEU:HD21	1.75	0.69
1:B:12:PHE:C	1:B:12:PHE:CD1	2.66	0.69
1:B:50:LEU:CD1	1:B:53:VAL:HB	2.22	0.69
1:A:252:LYS:CE	2:A:500:PBG:C7A	2.70	0.69
1:B:144:GLU:CD	1:B:144:GLU:H	1.96	0.68
1:B:11:TYR:O	1:B:12:PHE:CD2	2.45	0.68
1:A:12:PHE:C	1:A:12:PHE:CD1	2.67	0.67
1:A:122:CYS:SG	1:A:132:CYS:HB3	2.34	0.67
1:B:12:PHE:O	1:B:12:PHE:HD1	1.78	0.67
1:A:3:PRO:C	1:A:5:SER:H	1.99	0.65
1:A:221:ARG:O	1:A:225:GLN:HB2	1.96	0.65
1:A:125:PRO:HA	1:A:214:SER:OG	1.96	0.65
1:B:101:ALA:O	1:B:105:ILE:HG13	1.98	0.64
1:A:13:HIS:HB3	1:A:16:LEU:HB2	1.79	0.63
1:A:11:TYR:O	1:A:16:LEU:HD23	1.98	0.62
1:A:40:VAL:HB	1:A:43:ASP:CB	2.23	0.62
1:B:125:PRO:O	1:B:126:TYR:C	2.37	0.62
1:B:60:ARG:HD2	1:B:63:GLU:OE2	2.01	0.61
1:B:22:ALA:O	1:B:23:THR:CB	2.49	0.61
1:A:221:ARG:HG2	1:A:224:TYR:OH	2.01	0.60
1:A:235:LEU:HD22	1:A:267:LYS:HD2	1.83	0.60
1:B:3:PRO:C	1:B:5:SER:H	2.02	0.60
1:B:12:PHE:CD1	1:B:12:PHE:O	2.55	0.60
1:B:46:PRO:HA	1:B:54:ALA:CB	2.32	0.60
1:A:147:ARG:HD2	1:B:1:MET:HE2	1.82	0.60
1:B:325:GLN:O	1:B:328:LYS:HD3	2.01	0.60
1:A:13:HIS:CG	1:A:14:PRO:HD2	2.37	0.59
1:B:124:CYS:N	1:B:125:PRO:HD2	2.18	0.59
1:A:11:TYR:O	1:A:12:PHE:CG	2.55	0.59
1:A:327:LEU:O	1:A:328:LYS:HG2	2.02	0.59
1:A:60:ARG:HB3	1:A:60:ARG:HH11	1.68	0.58
1:B:95:ASP:HA	1:B:126:TYR:CD2	2.39	0.58
1:B:168:SER:HB3	1:B:196:TYR:CE1	2.39	0.57
1:A:50:LEU:HD21	1:A:279:SER:HB2	1.85	0.57
1:A:223:CYS:SG	1:B:12:PHE:HA	2.45	0.56
1:B:124:CYS:N	1:B:125:PRO:CD	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ALA:HA	1:B:194:MET:O	2.06	0.56
1:A:3:PRO:O	1:A:5:SER:N	2.39	0.56
1:A:119:CYS:CB	1:A:162:CYS:HG	2.17	0.55
1:B:4:GLN:HG3	1:B:4:GLN:O	2.06	0.55
1:B:7:LEU:O	1:B:10:GLY:N	2.31	0.55
1:A:252:LYS:HG3	1:A:276:TYR:HB3	1.87	0.55
1:A:174:ARG:HG2	1:A:175:VAL:N	2.21	0.55
1:B:247:ASP:HB3	1:B:248:MET:CE	2.37	0.54
1:A:252:LYS:HE2	2:A:500:PBG:H7A2	1.88	0.54
1:B:3:PRO:O	1:B:5:SER:N	2.40	0.54
1:B:176:GLU:O	1:B:180:GLU:HG3	2.07	0.54
1:B:170:MET:HE2	1:B:199:LYS:N	2.11	0.54
1:B:27:ASN:O	1:B:29:SER:N	2.41	0.54
1:A:119:CYS:HB3	1:A:157:TYR:HD2	1.73	0.54
1:A:320:THR:O	1:A:324:LEU:HG	2.09	0.53
1:A:44:ILE:O	1:A:44:ILE:CG2	2.56	0.53
1:B:105:ILE:O	1:B:109:ARG:HG2	2.09	0.53
1:A:147:ARG:HD2	1:B:1:MET:CE	2.39	0.53
1:A:125:PRO:HG2	1:A:126:TYR:CD2	2.44	0.52
1:B:27:ASN:HA	1:B:327:LEU:HD13	1.91	0.52
1:B:13:HIS:HB3	1:B:16:LEU:HB2	1.91	0.52
1:B:50:LEU:HD13	1:B:53:VAL:HB	1.91	0.52
1:A:226:LEU:HD21	1:A:234:ALA:HA	1.91	0.52
1:A:302:GLU:OE2	1:B:202:SER:CB	2.58	0.52
1:A:147:ARG:NH1	1:B:1:MET:HB2	2.24	0.51
1:B:227:PRO:HG2	1:B:230:ALA:CB	2.35	0.51
1:A:78:ILE:HD11	1:A:108:LEU:HD12	1.92	0.51
1:A:39:ASP:OD2	1:A:83:SER:N	2.44	0.51
1:B:319:TYR:HD1	1:B:322:GLN:HG3	1.76	0.51
1:B:300:VAL:O	1:B:304:MET:HG2	2.11	0.51
1:B:194:MET:HB2	1:B:248:MET:HG3	1.91	0.51
1:A:176:GLU:O	1:A:180:GLU:HB2	2.11	0.51
1:A:252:LYS:HE3	2:A:500:PBG:H7A2	1.89	0.51
1:A:169:ASP:O	1:A:170:MET:HB2	2.10	0.50
1:A:259:ASP:OD2	1:B:309:ARG:HD2	2.11	0.50
1:A:11:TYR:C	1:A:13:HIS:H	2.15	0.50
1:A:11:TYR:O	1:A:13:HIS:N	2.45	0.50
1:B:239:ASP:O	1:B:243:ARG:HG3	2.11	0.50
1:A:221:ARG:HA	1:A:224:TYR:CE1	2.47	0.50
1:A:66:ARG:N	1:A:67:PRO:HD2	2.27	0.50
1:A:262:ARG:O	1:A:262:ARG:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:PRO:HG3	1:A:126:TYR:CD1	2.47	0.49
1:A:302:GLU:OE2	1:B:202:SER:HB2	2.12	0.49
1:A:27:ASN:N	1:A:30:ASN:HD22	1.99	0.49
1:B:50:LEU:O	1:B:50:LEU:HD12	2.13	0.49
1:B:255:MET:HA	1:B:258:LEU:HD13	1.93	0.49
1:A:116:LEU:HD11	1:A:164:VAL:HG21	1.95	0.49
1:A:3:PRO:C	1:A:5:SER:N	2.65	0.48
1:A:170:MET:HE1	1:A:196:TYR:O	2.14	0.48
1:A:80:GLY:HA3	1:A:126:TYR:OH	2.13	0.48
1:A:47:ILE:HD13	1:A:211:ALA:CB	2.44	0.48
1:A:209:ARG:CA	1:A:209:ARG:HH11	2.21	0.48
1:A:12:PHE:C	1:A:12:PHE:HD1	2.17	0.48
1:B:167:PRO:HD2	1:B:195:SER:HA	1.96	0.47
1:B:192:SER:HB2	1:B:248:MET:HE3	1.94	0.47
1:B:1:MET:HG2	1:B:2:GLN:H	1.78	0.47
1:B:170:MET:HB2	1:B:224:TYR:HD2	1.78	0.47
1:A:212:ALA:C	1:A:214:SER:H	2.17	0.47
1:B:3:PRO:C	1:B:5:SER:N	2.68	0.47
1:B:119:CYS:HB2	1:B:162:CYS:SG	2.55	0.47
1:A:91:GLY:C	1:A:93:ALA:H	2.17	0.47
1:A:322:GLN:O	1:A:325:GLN:HB3	2.15	0.47
1:A:60:ARG:HB3	1:A:60:ARG:NH1	2.29	0.47
1:A:149:ARG:O	1:A:153:VAL:HG23	2.15	0.47
1:A:224:TYR:CD1	1:A:224:TYR:N	2.83	0.47
1:B:58:VAL:HG11	1:B:103:GLU:CB	2.45	0.47
1:B:226:LEU:HD21	1:B:234:ALA:HA	1.97	0.46
1:A:133:GLY:HA3	1:A:171:MET:HE1	1.96	0.46
1:B:247:ASP:HB3	1:B:248:MET:HE3	1.96	0.46
1:A:171:MET:O	1:A:174:ARG:HD2	2.15	0.46
1:A:252:LYS:HE3	2:A:500:PBG:H8A1	1.96	0.46
1:A:47:ILE:HD13	1:A:211:ALA:HB2	1.97	0.46
1:B:327:LEU:O	1:B:328:LYS:HG3	2.15	0.46
1:B:262:ARG:O	1:B:262:ARG:HD3	2.16	0.46
1:B:58:VAL:HG11	1:B:103:GLU:HB3	1.98	0.46
1:A:122:CYS:SG	1:A:123:LEU:N	2.88	0.45
1:A:179:LYS:HE2	1:A:247:ASP:OD2	2.16	0.45
1:A:255:MET:HA	1:A:258:LEU:CD1	2.43	0.45
1:A:40:VAL:CG1	1:A:43:ASP:HB2	2.47	0.45
1:B:49:SER:O	1:B:51:PRO:HD3	2.16	0.45
1:A:212:ALA:O	1:A:214:SER:N	2.50	0.44
1:A:27:ASN:HA	1:A:327:LEU:CD2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLN:HB3	1:A:4:GLN:HE21	1.54	0.44
1:A:278:VAL:HG22	1:A:281:GLU:OE2	2.17	0.44
1:B:66:ARG:HB3	1:B:67:PRO:HD3	1.99	0.44
1:A:182:LEU:HD13	1:A:191:VAL:HB	2.00	0.44
1:A:226:LEU:CD2	1:A:234:ALA:HA	2.47	0.44
1:B:73:LEU:HD21	1:B:76:VAL:CG1	2.48	0.44
1:A:58:VAL:HG21	1:A:103:GLU:CB	2.47	0.44
1:A:58:VAL:HG21	1:A:103:GLU:HB3	1.99	0.44
1:A:124:CYS:N	1:A:125:PRO:CD	2.81	0.43
1:B:47:ILE:HG12	1:B:211:ALA:CA	2.44	0.43
1:A:167:PRO:HD2	1:A:195:SER:HA	1.99	0.43
1:B:170:MET:HB2	1:B:224:TYR:CD2	2.53	0.43
1:A:1:MET:HB2	1:B:147:ARG:NH1	2.34	0.43
1:B:62:GLU:HB2	1:B:111:THR:HG21	2.00	0.43
1:B:205:TYR:HE1	1:B:278:VAL:HG11	1.84	0.43
1:A:124:CYS:N	1:A:125:PRO:HD2	2.34	0.43
1:B:264:VAL:CG2	1:B:265:LYS:N	2.80	0.42
1:A:262:ARG:HA	1:A:310:ALA:O	2.19	0.42
1:A:60:ARG:CB	1:A:60:ARG:NH1	2.83	0.42
1:A:22:ALA:O	1:A:23:THR:CB	2.66	0.42
1:A:170:MET:CE	1:A:196:TYR:O	2.67	0.42
1:B:44:ILE:O	1:B:44:ILE:CG2	2.61	0.42
1:A:230:ALA:HB1	1:A:233:LEU:HB2	2.01	0.42
1:A:168:SER:HB3	1:A:196:TYR:CE1	2.55	0.42
1:A:209:ARG:NH2	2:A:500:PBG:O2A	2.53	0.42
1:B:38:THR:HG22	1:B:56:TYR:O	2.18	0.42
1:A:27:ASN:H	1:A:30:ASN:ND2	2.01	0.42
1:B:167:PRO:HG3	1:B:178:ILE:CD1	2.49	0.42
1:B:38:THR:HG22	1:B:56:TYR:C	2.39	0.42
1:A:74:ARG:HB3	1:A:74:ARG:NH1	2.35	0.41
1:A:248:MET:HB3	1:A:248:MET:HE3	1.91	0.41
1:A:250:MET:HG2	1:A:251:VAL:N	2.35	0.41
1:B:125:PRO:HB2	1:B:126:TYR:H	1.57	0.41
1:B:197:SER:HB3	1:B:238:VAL:HG22	2.01	0.41
1:A:147:ARG:NH1	1:B:1:MET:HE2	2.36	0.41
1:A:212:ALA:C	1:A:214:SER:N	2.74	0.41
1:B:8:HIS:C	1:B:10:GLY:N	2.72	0.41
1:A:150:LEU:CD2	1:A:174:ARG:HB2	2.51	0.41
1:A:286:TRP:O	1:A:290:GLN:HG2	2.20	0.41
1:B:123:LEU:C	1:B:125:PRO:CD	2.81	0.41
1:A:16:LEU:HA	1:A:16:LEU:HD12	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:CYS:HB2	1:B:125:PRO:HD3	2.03	0.41
1:A:287:HIS:CD2	1:B:291:ALA:HB2	2.55	0.41
1:B:239:ASP:OD1	1:B:268:HIS:HE1	2.03	0.41
1:A:141:PHE:CD1	1:A:171:MET:HE1	2.56	0.41
1:A:284:MET:HG2	1:B:284:MET:HB2	2.03	0.41
1:A:173:GLY:HA2	1:A:244:GLU:OE2	2.21	0.41
1:A:42:ASP:HA	1:A:60:ARG:HD2	2.02	0.41
1:B:1:MET:HG2	1:B:2:GLN:N	2.36	0.41
1:B:66:ARG:HB3	1:B:67:PRO:CD	2.51	0.40
1:A:167:PRO:HG3	1:A:178:ILE:HD12	2.03	0.40
1:B:122:CYS:SG	1:B:124:CYS:SG	3.19	0.40
1:B:247:ASP:HB3	1:B:248:MET:HE2	2.02	0.40
1:B:50:LEU:HD23	1:B:279:SER:CB	2.51	0.40
1:A:150:LEU:HD23	1:A:174:ARG:HB2	2.04	0.40
1:A:282:PHE:CD2	1:A:319:TYR:CE2	3.09	0.40
1:B:221:ARG:HA	1:B:224:TYR:CE1	2.56	0.40
1:A:259:ASP:O	1:A:263:GLU:HB2	2.22	0.40
1:A:250:MET:HA	1:A:274:ALA:O	2.20	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	322/330 (98%)	273 (85%)	39 (12%)	10 (3%)	4	9
1	B	291/330 (88%)	259 (89%)	23 (8%)	9 (3%)	4	9
All	All	613/660 (93%)	532 (87%)	62 (10%)	19 (3%)	4	9

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	ILE
1	A	97	GLU
1	B	28	ALA
1	B	44	ILE
1	B	125	PRO
1	A	96	SER
1	A	143	ALA
1	B	87	LYS
1	A	12	PHE
1	A	28	ALA
1	B	4	GLN
1	B	83	SER
1	A	59	LYS
1	A	213	LYS
1	B	294	PHE
1	A	3	PRO
1	A	188	GLY
1	B	3	PRO
1	B	86	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	241/267 (90%)	220 (91%)	21 (9%)	10	21
1	B	223/267 (84%)	205 (92%)	18 (8%)	11	24
All	All	464/534 (87%)	425 (92%)	39 (8%)	11	23

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	11	TYR
1	A	12	PHE
1	A	26	LEU
1	A	64	MET

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Mol	Chain	Res	Type
1	A	77	LEU
1	A	116	LEU
1	A	124	CYS
1	A	132	CYS
1	A	155	LEU
1	A	174	ARG
1	A	190	ARG
1	A	209	ARG
1	A	240	ARG
1	A	248	MET
1	A	264	VAL
1	A	273	LEU
1	A	276	TYR
1	A	322	GLN
1	A	324	LEU
1	A	327	LEU
1	B	4	GLN
1	B	11	TYR
1	B	12	PHE
1	B	16	LEU
1	B	25	THR
1	B	62	GLU
1	B	66	ARG
1	B	115	LEU
1	B	119	CYS
1	B	228	PRO
1	B	248	MET
1	B	258	LEU
1	B	263	GLU
1	B	264	VAL
1	B	273	LEU
1	B	297	LYS
1	B	322	GLN
1	B	328	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	30	ASN
1	A	114	ASN
1	A	277	HIS

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Mol	Chain	Res	Type
1	A	290	GLN
1	B	2	GLN
1	B	20	GLN
1	B	30	ASN
1	B	114	ASN
1	B	225	GLN
1	B	268	HIS
1	B	290	GLN
1	B	322	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	PBG	A	500	1,3	9,16,16	5.14	6 (66%)	9,21,21	1.31	1 (11%)
4	SO4	A	502	-	4,4,4	0.60	0	6,6,6	0.13	0
4	SO4	B	503	-	4,4,4	0.55	0	6,6,6	0.11	0



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PBG	A	500	1,3	-	1/5/11/11	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	PBG	C2A-C1A	8.57	1.52	1.39
2	A	500	PBG	C4A-NA	8.36	1.48	1.36
2	A	500	PBG	C3A-C2A	6.15	1.51	1.40
2	A	500	PBG	C4A-C3A	5.94	1.53	1.37
2	A	500	PBG	CHA-C1A	3.39	1.55	1.51
2	A	500	PBG	C7A-C3A	2.57	1.56	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	PBG	CHA-C1A-C2A	-2.75	124.74	130.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	PBG	C2A-C3A-C7A-C8A

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	PBG	6	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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	326/330 (98%)	0.04	16 (4%)	29 22	21, 50, 117, 153	0
1	B	299/330 (90%)	-0.07	12 (4%)	38 30	18, 47, 116, 149	0
All	All	625/660 (94%)	-0.01	28 (4%)	33 25	18, 48, 117, 153	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	PRO	5.7
1	A	96	SER	4.3
1	A	219	GLY	3.7
1	B	87	LYS	3.6
1	A	95	ASP	3.2
1	A	218	PHE	3.2
1	B	223	CYS	3.0
1	B	126	TYR	2.9
1	B	84	ARG	2.9
1	A	94	ALA	2.9
1	A	98	GLU	2.8
1	B	224	TYR	2.8
1	A	220	ASP	2.7
1	A	142	ARG	2.5
1	B	1	MET	2.5
1	B	96	SER	2.5
1	B	83	SER	2.4
1	A	135	LEU	2.4
1	A	111	THR	2.4
1	A	140	ALA	2.3
1	A	97	GLU	2.3
1	B	212	ALA	2.2
1	B	211	ALA	2.2
1	B	5	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	222	ARG	2.2
1	A	69	VAL	2.1
1	A	42	ASP	2.1
1	A	217	ALA	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 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	PBG	A	500	16/16	0.81	0.36	45,45,45,45	0
4	SO4	A	502	5/5	0.96	0.21	39,39,39,39	0
4	SO4	B	503	5/5	0.99	0.09	39,39,39,39	0
3	ZN	A	501	1/1	0.99	0.18	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.