

# Full wwPDB X-ray Structure Validation Report (i)

#### Jan 13, 2021 – 12:11 PM JST

PDB ID	:	7CLG
Title	:	Crystal structure of the ATP-dependent restriction endonuclease SauUSI
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Deposited on	:	2020-07-21
Resolution	:	3.10  Å(reported)

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

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

The 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	:	2.16
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)	:	2.16

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 3.10 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 cha	ain		
1	А	953	3% 61%	25%	•	12%
1	В	953	3% 56%	26%	•	15%

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	В	1003	-	-	Х	-



#### $7 \mathrm{CLG}$

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12328 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 Putative helicase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	А	838	Total 6233	C 3976	N 1028	O 1211	${ m S} { m 3}$	${ m Se} 15$	0	0	0
1	В	806	Total 6042	C 3872	N 992	O 1162	${ m S} { m 3}$	Se 13	0	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	15	Total O 15 15	0	0
3	В	18	Total         O           18         18	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: Putative helicase





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	86.58Å 175.68Å $89.38$ Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $115.68^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	56.79 - 3.10	Depositor
Resolution (A)	80.55 - 3.10	EDS
% Data completeness	99.6 (56.79-3.10)	Depositor
(in resolution range)	$99.7 \ (80.55 - 3.10)$	EDS
R <sub>merge</sub>	0.11	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.59 (at 3.13 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
D D.	0.245 , $0.297$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.246 , $0.298$	DCC
$R_{free}$ test set	2019 reflections $(4.64\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	98.4	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32, 123.2	EDS
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12328	wwPDB-VP
Average B, all atoms $(Å^2)$	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: 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).

Mal	Chain	Bond	lengths	Bond angles		
Mol Chain		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.30	0/6320	0.50	0/8556	
1	В	0.30	0/6135	0.50	0/8306	
All	All	0.30	0/12455	0.50	0/16862	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	6233	0	5647	154	0
1	В	6042	0	5559	194	0
2	А	5	0	0	0	0
2	В	15	0	0	3	0
3	А	15	0	0	1	0
3	В	18	0	0	0	0
All	All	12328	0	11206	339	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 14.

All (339) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

A + 1	A + 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:567:ILE:HG13	1:B:568:PRO:HD3	1.46	0.97
1:B:481:LEU:HD21	1:B:493:VAL:HG21	1.57	0.86
1:B:403:CYS:SG	1:B:549:LYS:NZ	2.55	0.80
1:B:86:LEU:HD22	1:B:175:TRP:HE3	1.47	0.80
1:A:268:PRO:HG2	1:A:338:TYR:HB2	1.64	0.80
1:B:531:SER:HB3	1:B:534:ILE:HD13	1.64	0.79
1:A:246:LEU:HD23	1:A:380:PHE:N	1.99	0.77
1:B:925:LYS:HG2	1:B:932:VAL:HG22	1.69	0.74
1:B:925:LYS:HD3	1:B:926:MSE:H	1.52	0.74
1:B:806:TYR:CE1	1:B:944:ARG:HB2	2.23	0.73
1:B:97:LYS:NZ	1:B:447:TYR:O	2.21	0.73
1:B:531:SER:HA	1:B:566:LEU:HD21	1.70	0.72
1:A:89:ASN:ND2	3:A:1101:HOH:O	2.23	0.71
1:B:328:PHE:HD1	1:B:358:TYR:HE2	1.37	0.70
1:A:914:ALA:HB2	1:A:939:LEU:HD23	1.73	0.69
1:B:925:LYS:HB2	1:B:931:ASN:HA	1.72	0.69
1:A:104:LYS:NZ	1:A:443:ASP:O	2.22	0.69
1:A:868:TRP:HD1	1:A:935:MSE:HE2	1.56	0.69
1:A:713:ASP:HA	1:A:716:LYS:HB3	1.75	0.67
1:B:271:PHE:HB3	1:B:314:TYR:HD1	1.59	0.67
1:A:733:THR:HA	1:A:819:ASN:OD1	1.93	0.67
1:B:275:VAL:HG11	1:B:281:LEU:HB2	1.75	0.67
1:B:70:LYS:NZ	1:B:101:GLU:OE1	2.24	0.67
1:B:568:PRO:HG2	1:B:608:ILE:HG21	1.77	0.67
1:A:441:LYS:NZ	1:A:601:GLU:OE2	2.28	0.66
1:B:115:ILE:HD11	1:B:118:PHE:HD1	1.61	0.66
1:B:86:LEU:HD22	1:B:175:TRP:CE3	2.30	0.66
1:A:263:VAL:HA	1:A:338:TYR:HE2	1.61	0.66
1:B:810:SER:HB2	1:B:906:ILE:HA	1.78	0.65
1:A:736:ARG:NH1	1:A:739:ASP:OD1	2.30	0.65
1:A:369:ALA:O	1:A:537:GLN:NE2	2.30	0.65
1:A:579:LYS:NZ	1:A:615:VAL:O	2.25	0.65
1:B:238:ARG:NH2	1:B:262:ASP:OD2	2.27	0.65
1:A:456:ILE:HG12	1:A:524:VAL:HB	1.80	0.64
1:A:247:ILE:HG12	1:A:367:MSE:HG2	1.80	0.64
1:A:571:LEU:HD13	1:A:598:ILE:HD13	1.81	0.63
1:B:303:LEU:HB3	1:B:317:ALA:HB2	1.81	0.63
1:B:577:GLN:H	1:B:653:VAL:HG21	1.63	0.63
1:B:259:CYS:HB2	1:B:367:MSE:HE1	1.81	0.63
1:B:477:LYS:CB	1:B:503:ASN:H	2.11	0.63
1:B:872:SER:HA	1:B:932:VAL:HG12	1.80	0.63



		Interatomic Clash		
Atom-1 Atom-2		distance (Å)	overlap (Å)	
1:B:309:ASP:OD1	1:B:309:ASP:N	2.31	0.63	
1:A:814:PHE:CE2	1:A:839:PRO:HG3	2.34	0.62	
1:A:170:GLU:HG2	1:B:34:ASN:ND2	2.14	0.62	
1:A:525:MSE:HE3	1:A:527:ARG:HH11	1.64	0.62	
1:A:118:PHE:HA	1:B:149:TYR:HB3	1.82	0.61	
1:B:441:LYS:NZ	1:B:601:GLU:OE2	2.33	0.61	
1:B:644:ILE:HD11	1:B:788:LEU:HD13	1.80	0.61	
1:A:577:GLN:HB3	1:A:617:LEU:HD23	1.81	0.61	
1:B:124:ILE:HD11	1:B:167:VAL:HG11	1.82	0.61	
1:A:337:ASP:HA	1:A:361:PRO:HB2	1.81	0.61	
1:A:271:PHE:HD2	1:A:338:TYR:HB3	1.66	0.61	
1:B:246:LEU:HD12	1:B:247:ILE:H	1.66	0.61	
1:A:896:ILE:HD11	1:A:911:LEU:HB2	1.82	0.60	
1:B:101:GLU:HA	1:B:104:LYS:HD2	1.83	0.60	
1:A:674:LEU:CB	1:A:775:ASN:HD21	2.15	0.60	
1:B:525:MSE:HE3	1:B:556:ASP:HB2	1.82	0.60	
1:A:381:GLU:HG3	1:A:382:LEU:HD12	1.83	0.59	
1:B:332:ASP:HB3	1:B:335:GLU:HB3	1.82	0.59	
1:B:289:LYS:HG3	1:B:300:PHE:CE1	2.36	0.59	
1:B:119:HIS:NE2	2:B:1001:SO4:O1	2.34	0.59	
1:B:342:ASP:OD2	1:B:342:ASP:N	2.34	0.59	
1:B:328:PHE:HD1	1:B:358:TYR:CE2	2.19	0.58	
1:A:227:GLN:O	1:A:231:LEU:HG	2.01	0.58	
1:A:833:ILE:HB	1:A:838:MSE:HG3	1.84	0.58	
1:B:687:SER:O	1:B:691:ALA:N	2.28	0.58	
1:B:430:THR:O	1:B:434:ARG:HB2	2.04	0.57	
1:A:90:TYR:CD1	1:A:117:GLY:HA2	2.40	0.57	
1:B:14:LYS:NZ	1:B:864:ASP:OD2	2.31	0.57	
1:B:662:TYR:HA	1:B:665:LEU:HD12	1.87	0.57	
1:A:301:GLY:N	1:A:314:TYR:O	2.37	0.57	
1:A:137:SER:OG	1:A:150:GLU:HG3	2.04	0.57	
1:A:318:THR:HG23	1:A:321:THR:H	1.68	0.57	
1:B:582:TYR:O	1:B:586:LEU:HB2	2.04	0.57	
1:B:840:ILE:HD12	1:B:894:MSE:HE3	1.86	0.57	
1:B:643:PHE:HB3	1:B:649:ILE:O	2.05	0.56	
1:B:471:LEU:O	1:B:476:ILE:HB	2.04	0.56	
1:B:806:TYR:HE1	1:B:944:ARG:HB2	1.70	0.56	
1:A:686:PHE:CE1	1:A:782:LEU:HD13	2.40	0.56	
1:A:831:TYR:HB3	1:A:868:TRP:HZ2	1.70	0.56	
1:B:271:PHE:HB3	1:B:314:TYR:CD1	2.40	0.56	
1:B:693:GLY:HA3	1:B:793:ASN:HB2	1.87	0.56	



		Interatomic Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:448:SER:HB3	1:A:551:TYR:CE1	2.41	0.55
1:A:887:HIS:O	1:A:891:GLY:N	2.39	0.55
1:A:461:LYS:HB3	1:A:482:THR:HG21	1.89	0.55
1:A:806:TYR:OH	1:A:943:VAL:HA	2.06	0.55
1:B:394:GLN:NE2	1:B:571:LEU:O	2.40	0.55
1:A:432:ASP:O	1:A:436:ASN:ND2	2.33	0.54
1:A:446:GLY:O	1:A:553:THR:HG21	2.07	0.54
1:A:247:ILE:HG22	1:A:388:ALA:HB3	1.88	0.54
1:B:45:ILE:HD12	1:B:72:GLN:HG3	1.90	0.54
1:A:14:LYS:NZ	1:A:19:LYS:O	2.41	0.54
1:A:294:ILE:HG22	1:A:295:LYS:H	1.72	0.54
1:B:580:ASP:OD1	1:B:950:TYR:OH	2.23	0.54
1:A:263:VAL:HA	1:A:338:TYR:CE2	2.42	0.54
1:B:60:PHE:HD1	1:B:93:PHE:CD2	2.26	0.54
1:B:66:LEU:HD11	1:B:105:LEU:HD11	1.90	0.54
1:A:719:MSE:HA	1:A:719:MSE:HE2	1.91	0.53
1:B:407:TYR:OH	1:B:556:ASP:OD2	2.24	0.53
1:A:833:ILE:HA	1:A:838:MSE:HA	1.90	0.53
1:A:811:ARG:HD3	1:A:841:PHE:CD1	2.42	0.53
1:B:262:ASP:OD2	1:B:338:TYR:OH	2.24	0.53
1:B:814:PHE:HE1	1:B:839:PRO:HG3	1.73	0.53
1:A:97:LYS:NZ	1:A:101:GLU:OE2	2.40	0.53
1:B:634:LEU:HD12	1:B:636:HIS:H	1.74	0.53
1:A:522:GLN:HG2	1:A:553:THR:HG23	1.90	0.53
1:B:489:TYR:O	1:B:493:VAL:HG22	2.09	0.53
1:A:167:VAL:HG22	1:B:32:LEU:HD22	1.90	0.53
1:A:86:LEU:HD21	1:A:174:LEU:HD12	1.91	0.53
1:A:868:TRP:CD1	1:A:935:MSE:HE2	2.41	0.52
1:B:472:SER:HA	1:B:476:ILE:O	2.09	0.52
1:B:925:LYS:HG3	1:B:930:SER:O	2.09	0.52
1:A:519:GLU:OE2	1:A:519:GLU:N	2.40	0.52
1:A:644:ILE:HD13	1:A:791:TYR:CE1	2.44	0.52
1:A:704:GLU:O	1:A:708:ASN:N	2.42	0.52
1:A:113:THR:HB	1:A:178:SER:HB3	1.90	0.52
1:B:143:ASN:ND2	2:B:1003:SO4:O3	2.43	0.52
1:A:223:PRO:HB3	1:A:261:LEU:HD21	1.90	0.52
1:A:170:GLU:HG2	1:B:34:ASN:HD22	1.74	0.52
1:B:734:SER:O	1:B:738:LEU:HD12	2.10	0.52
1:B:295:LYS:HD2	1:B:298:SER:H	1.75	0.51
1:B:281:LEU:HD11	1:B:316:PHE:HB3	1.91	0.51
1:A:542:GLY:O	1:A:549:LYS:NZ	2.37	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:138:SER:CB	1:A:152:ASN:HD21	2.23	0.51
1:B:303:LEU:HB2	1:B:315:LEU:HD11	1.93	0.51
1:A:797:GLN:OE1	1:A:809:TYR:OH	2.26	0.51
1:B:481:LEU:HD21	1:B:493:VAL:CG2	2.34	0.51
1:B:574:ASP:HB3	1:B:582:TYR:CE1	2.45	0.51
1:A:5:LEU:HG	1:A:158:MSE:HE1	1.91	0.51
1:B:810:SER:O	1:B:813:ASP:N	2.45	0.50
1:B:274:ILE:HG22	1:B:319:ILE:HG12	1.94	0.50
1:A:259:CYS:O	1:A:263:VAL:HG23	2.11	0.50
1:B:471:LEU:HD13	1:B:476:ILE:HG21	1.92	0.50
1:B:452:LEU:HD21	1:B:504:TYR:CZ	2.46	0.50
1:B:874:ARG:N	1:B:931:ASN:O	2.45	0.50
1:A:413:TYR:CZ	1:A:433:GLU:HB3	2.46	0.50
1:A:458:VAL:HB	1:A:463:GLU:CD	2.32	0.50
1:B:894:MSE:HE1	1:B:937:LEU:HG	1.94	0.50
1:B:58:VAL:HG21	1:B:140:LEU:HB2	1.94	0.49
1:A:394:GLN:NE2	1:A:571:LEU:O	2.45	0.49
1:B:633:ARG:HG2	1:B:646:GLN:HG3	1.94	0.49
1:B:691:ALA:HB3	1:B:692:PRO:HD3	1.94	0.49
1:B:577:GLN:H	1:B:653:VAL:CG2	2.24	0.49
1:A:486:SER:O	1:A:490:ARG:HG3	2.12	0.49
1:A:686:PHE:HE1	1:A:782:LEU:HD13	1.76	0.49
1:A:525:MSE:HE3	1:A:527:ARG:NH1	2.26	0.49
1:A:589:ASN:O	1:A:592:ILE:HG22	2.12	0.49
1:B:690:ILE:O	1:B:789:SER:HB2	2.12	0.49
1:A:836:GLN:NE2	1:A:891:GLY:O	2.45	0.49
1:B:682:ASN:O	1:B:686:PHE:HB2	2.13	0.49
1:B:41:LEU:O	1:B:45:ILE:HG12	2.13	0.49
1:A:663:GLU:O	1:A:667:ARG:HB2	2.12	0.49
1:A:907:TYR:C	1:A:908:PHE:HD1	2.15	0.49
1:B:238:ARG:HH22	1:B:262:ASP:CG	2.16	0.49
1:B:451:ILE:O	1:B:521:ASN:ND2	2.46	0.49
1:B:634:LEU:HD13	1:B:636:HIS:HB2	1.94	0.49
1:A:461:LYS:HD2	1:A:462:LYS:H	1.77	0.49
1:B:682:ASN:HB2	1:B:778:PHE:HZ	1.77	0.49
1:B:919:GLY:N	1:B:921:GLU:OE1	2.46	0.49
1:A:507:THR:HG21	1:A:510:LEU:HB2	1.95	0.48
1:B:39:LYS:HD3	1:B:146:LYS:O	2.13	0.48
1:B:539:LEU:O	1:B:543:LEU:HG	2.13	0.48
1:B:140:LEU:HD12	1:B:145:LEU:HD11	1.95	0.48
1:B:13:HIS:HA	1:B:17:ILE:HD12	1.95	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:246:LEU:CD2	1:B:380:PHE:HB2	2.43	0.48
1:B:921:GLU:HB2	1:B:935:MSE:HA	1.95	0.48
1:A:828:ILE:HG23	1:A:832:MSE:HB3	1.94	0.48
1:A:163:LEU:HD21	1:B:153:VAL:HG21	1.95	0.48
1:A:266:VAL:O	1:A:268:PRO:HD3	2.13	0.48
1:A:481:LEU:O	1:A:507:THR:HG23	2.13	0.48
1:B:287:GLU:OE2	1:B:290:LYS:NZ	2.30	0.48
1:A:97:LYS:O	1:A:100:GLY:N	2.47	0.48
1:A:696:ARG:CB	1:A:793:ASN:HD21	2.27	0.48
1:B:563:THR:HA	1:B:565:TYR:CE1	2.49	0.48
1:B:574:ASP:HB3	1:B:582:TYR:HE1	1.79	0.48
1:B:247:ILE:HB	1:B:367:MSE:HG2	1.95	0.48
1:B:468:ALA:O	1:B:478:SER:OG	2.30	0.48
1:A:34:ASN:ND2	1:A:148:ASN:O	2.39	0.47
1:A:736:ARG:HG2	1:A:819:ASN:HA	1.97	0.47
1:B:527:ARG:NH1	1:B:529:THR:OG1	2.47	0.47
1:B:341:PHE:HZ	1:B:364:MSE:SE	2.48	0.47
1:B:937:LEU:HD13	1:B:937:LEU:H	1.80	0.47
1:B:944:ARG:HD2	1:B:946:ASP:OD1	2.14	0.47
1:A:340:VAL:HA	1:A:365:LEU:O	2.14	0.47
1:B:328:PHE:CD1	1:B:358:TYR:CE2	3.02	0.47
1:A:920:SER:HB2	1:A:936:ASP:H	1.79	0.47
1:B:658:PHE:CD1	1:B:664:PHE:HB2	2.50	0.47
1:B:90:TYR:CE2	1:B:117:GLY:HA2	2.50	0.47
1:B:474:LYS:HA	1:B:474:LYS:HD3	1.59	0.47
1:B:259:CYS:SG	1:B:340:VAL:HG21	2.55	0.47
1:A:124:ILE:HD11	1:A:167:VAL:CG1	2.45	0.47
1:B:255:LYS:HB2	1:B:255:LYS:HE3	1.58	0.47
1:B:381:GLU:CD	1:B:381:GLU:H	2.14	0.47
1:A:124:ILE:HD11	1:A:167:VAL:HG11	1.96	0.46
1:B:412:ASP:HB3	1:B:437:TYR:CE1	2.50	0.46
1:B:692:PRO:HA	1:B:792:ASN:HD22	1.80	0.46
1:B:387:ILE:HG13	1:B:387:ILE:H	1.55	0.46
1:A:528:PRO:HB3	1:A:561:TYR:CG	2.50	0.46
1:B:899:GLN:HG2	1:B:903:ASP:HB3	1.96	0.46
1:B:914:ALA:HB2	1:B:939:LEU:HD23	1.97	0.46
1:A:468:ALA:HB2	1:A:506:ILE:HD13	1.96	0.46
1:A:897:PHE:HB3	1:A:908:PHE:HB2	1.98	0.46
1:B:397:LEU:HD21	1:B:405:PHE:HE1	1.80	0.46
1:A:224:ASN:OD1	1:A:227:GLN:N	2.49	0.46
1:B:478:SER:O	1:B:478:SER:OG	2.34	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:874:ARG:HA	1:B:874:ARG:HD2	1.65	0.46
1:A:61:ILE:HG23	1:A:140:LEU:HG	1.97	0.45
1:B:945:ASP:O	1:B:949:ARG:HG3	2.16	0.45
1:A:138:SER:OG	1:A:152:ASN:ND2	2.46	0.45
1:A:32:LEU:HB2	1:A:152:ASN:HB2	1.96	0.45
1:B:361:PRO:HG2	1:B:364:MSE:HG2	1.98	0.45
1:B:583:LYS:O	1:B:587:THR:HG22	2.17	0.45
1:A:246:LEU:HD12	1:A:247:ILE:N	2.31	0.45
1:B:574:ASP:O	1:B:582:TYR:OH	2.30	0.45
1:A:937:LEU:H	1:A:937:LEU:HD13	1.82	0.45
1:B:115:ILE:HD11	1:B:118:PHE:CD1	2.47	0.45
1:A:39:LYS:HE2	1:A:146:LYS:O	2.16	0.45
1:B:44:ILE:HG13	1:B:125:PHE:HZ	1.81	0.45
1:A:29:PRO:HB3	1:A:155:LEU:HD23	1.99	0.45
1:A:580:ASP:OD1	1:A:950:TYR:OH	2.23	0.45
1:B:921:GLU:H	1:B:921:GLU:CD	2.20	0.45
1:A:271:PHE:CD2	1:A:338:TYR:HB3	2.50	0.44
1:A:531:SER:HB3	1:A:534:ILE:HD13	1.99	0.44
1:B:944:ARG:NH1	1:B:946:ASP:OD2	2.50	0.44
1:A:640:LEU:HD11	1:A:661:TYR:CG	2.51	0.44
1:B:445:TYR:OH	1:B:601:GLU:OE2	2.27	0.44
1:A:661:TYR:CE1	1:A:665:LEU:HD11	2.52	0.44
1:A:109:GLU:HB3	1:A:175:TRP:HH2	1.82	0.44
1:A:86:LEU:HD21	1:A:174:LEU:CD1	2.47	0.44
1:B:655:PHE:CE1	1:B:687:SER:HB2	2.53	0.44
1:A:711:THR:OG1	1:A:711:THR:O	2.36	0.44
1:A:733:THR:HA	1:A:819:ASN:CG	2.37	0.44
1:A:163:LEU:HD13	1:B:30:LYS:O	2.18	0.44
1:A:658:PHE:CE2	1:A:664:PHE:HD2	2.35	0.44
1:A:842:ILE:HD11	1:A:898:VAL:HG22	2.00	0.44
1:B:157:THR:HG21	1:B:164:VAL:CG2	2.48	0.44
1:A:341:PHE:HB3	1:A:342:ASP:H	1.50	0.44
1:A:174:LEU:HD21	1:B:149:TYR:CZ	2.53	0.44
1:A:496:LYS:HG2	1:A:501:LYS:HB3	2.00	0.43
1:A:54:PHE:CZ	1:A:83:GLY:HA3	2.53	0.43
1:B:627:TYR:CE2	1:B:638:PRO:HD2	2.53	0.43
1:B:340:VAL:HA	1:B:365:LEU:O	2.18	0.43
1:B:519:GLU:N	1:B:519:GLU:OE2	2.51	0.43
1:B:58:VAL:O	1:B:87:THR:HG22	2.18	0.43
1:A:810:SER:H	1:A:813:ASP:HB2	1.82	0.43
1:B:246:LEU:HD12	1:B:247:ILE:N	2.30	0.43



	A L O	Interatomic	Clash
Atom-1 Atom-2		distance $(\text{\AA})$	overlap (Å)
1:B:459:SER:OG	1:B:463:GLU:OE2	2.27	0.43
1:B:565:TYR:HB3	1:B:612:LEU:HA	2.00	0.43
1:B:739:ASP:OD1	1:B:739:ASP:N	2.51	0.43
1:B:14:LYS:HD2	1:B:23:HIS:ND1	2.33	0.43
1:B:62:THR:HG21	2:B:1003:SO4:O1	2.19	0.43
1:B:72:GLN:O	1:B:76:LEU:HD13	2.19	0.43
1:B:26:ASN:N	1:B:26:ASN:OD1	2.52	0.43
1:B:565:TYR:O	1:B:569:ILE:HG13	2.18	0.43
1:B:876:LEU:HA	1:B:881:VAL:HG21	2.01	0.43
1:A:686:PHE:HB3	1:A:785:LEU:HD13	1.99	0.43
1:A:145:LEU:O	1:A:146:LYS:HG2	2.18	0.43
1:A:687:SER:O	1:A:692:PRO:HD3	2.18	0.43
1:A:246:LEU:HB2	1:A:383:PHE:CD1	2.54	0.43
1:A:246:LEU:HD12	1:A:247:ILE:H	1.83	0.43
1:A:460:SER:C	1:A:508:VAL:HG21	2.40	0.43
1:A:528:PRO:HD3	1:A:561:TYR:CZ	2.54	0.43
1:B:221:ILE:HG21	1:B:291:VAL:HG22	2.01	0.43
1:A:269:ASN:O	1:A:269:ASN:ND2	2.53	0.42
1:A:66:LEU:HA	1:A:66:LEU:HD12	1.90	0.42
1:B:397:LEU:HD21	1:B:405:PHE:CE1	2.53	0.42
1:B:868:TRP:CD1	1:B:935:MSE:HE2	2.53	0.42
1:B:12:LEU:HD12	1:B:12:LEU:HA	1.88	0.42
1:B:111:ARG:HG3	1:B:175:TRP:CH2	2.54	0.42
1:B:580:ASP:OD2	1:B:808:LYS:NZ	2.24	0.42
1:A:158:MSE:HG3	1:B:17:ILE:HA	2.01	0.42
1:A:840:ILE:N	1:A:895:TYR:O	2.47	0.42
1:B:336:PHE:HB2	1:B:339:ILE:HD11	2.01	0.42
1:B:458:VAL:HG21	1:B:464:ALA:HB2	2.00	0.42
1:A:527:ARG:NH2	1:A:529:THR:HA	2.35	0.42
1:A:797:GLN:O	1:A:804:ILE:HD11	2.20	0.42
1:B:341:PHE:CD1	1:B:341:PHE:N	2.87	0.42
1:B:529:THR:HG23	1:B:535:PHE:HB2	2.01	0.42
1:A:182:THR:HG23	1:A:185:TRP:H	1.85	0.42
1:A:248:ILE:O	1:A:391:ILE:N	2.43	0.42
1:A:687:SER:O	1:A:691:ALA:HB3	2.19	0.42
1:B:528:PRO:HD3	1:B:561:TYR:CZ	2.55	0.42
1:B:593:ASN:N	1:B:593:ASN:OD1	2.53	0.42
1:A:523:VAL:HB	1:A:554:VAL:HG22	2.01	0.42
1:B:539:LEU:HG	1:B:543:LEU:HD11	2.02	0.42
1:B:620:ASN:HA	1:B:623:ILE:HG22	2.00	0.42
1:A:623:ILE:HG23	1:A:654:ILE:HG13	2.02	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1.B.289.LYS.HB2	1.B.289.LYS.HE3	1.64	0.42
1:B:408:PHE:CD1	1:B:599:ASN:HB2	2.55	0.42
1:A:226:MSE:HE1	1:A:395:ALA:C	2.41	0.41
1.B.339.ILE.HG13	1·B·361·PRO·HG3	2.02	0.41
1·B·326·ASP·HB3	1·B·329·LVS·HG3	2.02	0.41
1.B.342:ASP:HA	1:B:367:MSE:O	2.20	0.41
1:B:72:GLN:OE1	1.B.599.ASN.ND2	2 43	0.41
1.B.237.ILE.HA	1·B·240·LYS·HG2	2.02	0.41
1:A:14:LYS:HA	1:A:18:ASP:O	2.20	0.41
1:A:158:MSE:HE3	1:B:17:ILE:HG23	2.02	0.41
1:A:102:LEU:HD13	1:A:110:VAL:HG11	2.01	0.41
1:A:146:LYS:HE3	1:A:146:LYS:HB3	1.70	0.41
1:A:894:MSE:HE2	1:A:937:LEU:HG	2.03	0.41
1:B:114:ASP:OD1	1:B:114:ASP:N	2.53	0.41
1:B:141:THB:HG23	1:B:144:ALA:H	1.86	0.41
1.B.397.LEU.HA	1·B·397·LEU·HD12	1.80	0.41
1:B:626:ALA:O	1:B:630:VAL:HG23	2.20	0.41
1:B:618:ASN:HB3	1:B:657:LYS:HD3	2.02	0.41
1:B:181:LEU:HA	1:B:181:LEU:HD12	1.93	0.41
1:B:451:ILE:HD12	1:B:451:ILE:HA	1.87	0.41
1:B:569:ILE:HG12	1:B:582:TYR:CE2	2.56	0.41
1:A:842:ILE:HG22	1:A:868:TRP:CZ3	2.55	0.41
1:B:457:PHE:CE1	1:B:538:GLN:HG2	2.56	0.41
1:A:230:ALA:HB1	1:A:258:LEU:HD21	2.03	0.41
1:A:339:ILE:O	1:A:365:LEU:N	2.48	0.41
1:B:809:TYR:O	1:B:908:PHE:HB2	2.20	0.41
1:B:899:GLN:CG	1:B:903:ASP:HB3	2.50	0.41
1:A:34:ASN:OD1	1:A:40:VAL:HG23	2.20	0.41
1:A:488:ASN:N	1:A:488:ASN:OD1	2.49	0.41
1:A:604:ALA:O	1:A:608:ILE:HD12	2.21	0.41
1:A:127:HIS:N	1:A:127:HIS:ND1	2.69	0.41
1:A:907:TYR:CD2	1:A:907:TYR:N	2.89	0.41
1:B:467:LEU:HD12	1:B:506:ILE:HD13	2.03	0.41
1:B:482:THR:HG22	1:B:483:GLY:N	2.36	0.41
1:A:302:LEU:H	1:A:309:ASP:HB2	1.86	0.40
1:A:567:ILE:HB	1:A:568:PRO:HD3	2.01	0.40
1:A:38:GLU:HA	1:A:590:ASP:OD2	2.20	0.40
1:B:148:ASN:HB3	1:B:150:GLU:HG2	2.02	0.40
1:B:567:ILE:HG21	1:B:567:ILE:HD13	1.90	0.40
1:B:914:ALA:HB1	1:B:937:LEU:HD23	2.02	0.40
1:A:531:SER:OG	1:A:532:SER:N	2.54	0.40



Atom-1	Atom-2	Interatomic	Clash
	1100111-2	distance $(Å)$	overlap (Å)
1:A:842:ILE:HG22	1:A:868:TRP:HZ3	1.86	0.40
1:B:303:LEU:HD13	1:B:308:ARG:HA	2.03	0.40
1:A:899:GLN:HB2	1:A:908:PHE:CG	2.57	0.40
1:B:396:ALA:HB1	1:B:402:LEU:HD13	2.03	0.40
1:B:46:ASP:OD1	1:B:949:ARG:HD3	2.21	0.40
1:A:479:VAL:O	1:A:505:ILE:HA	2.21	0.40
1:B:143:ASN:O	1:B:148:ASN:HB2	2.21	0.40
1:B:33:VAL:CG2	1:B:152:ASN:HB2	2.51	0.40
1:B:304:THR:C	1:B:321:THR:HG21	2.42	0.40
1:B:623:ILE:HD11	1:B:654:ILE:HG12	2.03	0.40
1:B:680:SER:OG	1:B:681:LYS:N	2.55	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	А	810/953~(85%)	743~(92%)	66~(8%)	1 (0%)	51 83
1	В	784/953~(82%)	729~(93%)	55~(7%)	0	100 100
All	All	1594/1906~(84%)	1472 (92%)	121 (8%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	361	PRO

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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.





Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	605/848~(71%)	556~(92%)	49 (8%)	11 39
1	В	600/848~(71%)	548 (91%)	52 (9%)	10 36
All	All	1205/1696~(71%)	1104 (92%)	101 (8%)	11 38

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

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	8	PHE
1	А	26	ASN
1	А	53	THR
1	А	68	SER
1	А	76	LEU
1	А	86	LEU
1	А	89	ASN
1	А	93	PHE
1	А	111	ARG
1	А	121	LYS
1	А	127	HIS
1	А	128	LYS
1	А	130	TYR
1	А	140	LEU
1	А	150	GLU
1	А	151	HIS
1	А	158	MSE
1	А	173	LEU
1	А	229	GLU
1	А	264	ARG
1	А	269	ASN
1	А	286	GLU
1	А	307	HIS
1	А	308	ARG
1	А	338	TYR
1	А	343	GLU
1	А	355	VAL
1	А	402	LEU
1	А	429	LEU
1	А	441	LYS
1	А	461	LYS
1	А	474	LYS
1	А	527	ARG



Mol	Chain	Res	Type
1	А	575	GLN
1	А	619	GLN
1	А	667	ARG
1	А	685	PHE
1	А	688	ARG
1	А	714	GLU
1	А	736	ARG
1	А	781	PHE
1	А	783	GLU
1	А	803	LEU
1	А	804	ILE
1	А	811	ARG
1	А	866	LEU
1	А	881	VAL
1	А	900	LYS
1	А	937	LEU
1	В	52	GLU
1	В	62	THR
1	В	72	GLN
1	В	86	LEU
1	В	111	ARG
1	В	151	HIS
1	В	152	ASN
1	В	176	GLN
1	В	182	THR
1	В	227	GLN
1	В	229	GLU
1	В	274	ILE
1	В	309	ASP
1	В	341	PHE
1	В	342	ASP
1	В	357	ASN
1	В	364	MSE
1	В	380	PHE
1	В	387	ILE
1	В	397	LEU
1	В	443	ASP
1	В	469	ASP
1	В	474	LYS
1	В	488	ASN
1	В	513	GLU
1	В	527	ARG



Mol	Chain	Res	Type
1	В	574	ASP
1	В	577	GLN
1	В	590	ASP
1	В	596	SER
1	В	603	VAL
1	В	633	ARG
1	В	634	LEU
1	В	636	HIS
1	В	641	MSE
1	В	660	ASN
1	В	662	TYR
1	В	667	ARG
1	В	668	TYR
1	В	681	LYS
1	В	686	PHE
1	В	743	TYR
1	В	781	PHE
1	В	807	ASN
1	В	859	GLU
1	В	864	ASP
1	В	874	ARG
1	В	890	LYS
1	В	893	LYS
1	В	925	LYS
1	В	937	LEU
1	В	951	LEU

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

#### 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)

4 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).

Mal	Turne	Chain	Dec	Tink	B	ond leng	$\operatorname{gths}$	B	Bond ang	gles
WIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	SO4	В	1002	-	4,4,4	0.15	0	$6,\!6,\!6$	0.08	0
2	SO4	А	1001	-	4,4,4	0.15	0	$6,\!6,\!6$	0.18	0
2	SO4	В	1001	-	4,4,4	0.16	0	$6,\!6,\!6$	0.21	0
2	SO4	В	1003	-	4,4,4	0.15	0	$6,\!6,\!6$	0.17	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1001	SO4	1	0
2	В	1003	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 (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  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	< <b>RSRZ</b> >	#RSRZ>2	2	$\mathbf{OWAB}(\mathbf{A}^2)$	Q<0.9
1	А	822/953~(86%)	0.20	32 (3%) 39	20	62,128,221,288	0
1	В	792/953~(83%)	0.19	27 (3%) 45	24	59, 119, 196, 286	0
All	All	1614/1906~(84%)	0.20	59 (3%) 41	21	59, 124, 211, 288	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	661	TYR	4.1
1	А	511	PHE	4.0
1	А	274	ILE	4.0
1	А	275	VAL	4.0
1	А	380	PHE	3.6
1	В	299	ASP	3.6
1	А	292	LEU	3.6
1	В	664	PHE	3.5
1	А	887	HIS	3.5
1	А	304	THR	3.4
1	В	705	LEU	3.4
1	В	515	ILE	3.4
1	А	651	PRO	3.3
1	А	701	VAL	3.3
1	А	273	PHE	3.3
1	В	680	SER	3.2
1	В	888	ARG	3.1
1	В	788	LEU	3.0
1	А	509	ASP	3.0
1	А	623	ILE	2.9
1	А	896	ILE	2.9
1	Α	16	PHE	2.9
1	А	951	LEU	2.8
1	В	87	THR	2.8



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Mol	Chain	Res	Type	RSRZ
1	А	86	LEU	2.7
1	В	668	TYR	2.6
1	В	633	ARG	2.6
1	А	301	GLY	2.5
1	А	272	LEU	2.5
1	А	654	ILE	2.5
1	В	649	ILE	2.5
1	В	480	ALA	2.4
1	В	435	VAL	2.4
1	В	654	ILE	2.4
1	В	407	TYR	2.4
1	А	799	GLY	2.4
1	А	860	PHE	2.4
1	В	539	LEU	2.4
1	А	567	ILE	2.3
1	В	896	ILE	2.3
1	В	151	HIS	2.3
1	А	664	PHE	2.2
1	А	686	PHE	2.2
1	А	481	LEU	2.2
1	В	651	PRO	2.2
1	А	387	ILE	2.1
1	В	221	ILE	2.1
1	В	660	ASN	2.1
1	А	457	PHE	2.1
1	В	653	VAL	2.1
1	А	154	LEU	2.1
1	В	785	LEU	2.1
1	А	564	ASN	2.0
1	В	28	THR	2.0
1	В	57	SER	2.0
1	А	66	LEU	2.0
1	А	181	LEU	2.0
1	А	316	PHE	2.0
1	В	507	THR	2.0

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## 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	$B-factors(A^2)$	Q<0.9
2	SO4	В	1001	5/5	0.89	0.23	102,127,135,139	0
2	SO4	В	1002	5/5	0.93	0.20	140,141,142,152	0
2	SO4	А	1001	5/5	0.97	0.18	72,78,94,94	0
2	SO4	В	1003	5/5	0.98	0.15	54,85,88,94	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

