Full wwPDB X-ray Structure Validation Report

May 22, 2020 – 01:29 am BST

PDB ID	:	3LFU
Title	:	Crystal Structure of E. coli UvrD
Authors	:	Korolev, S.; Waksman, G.; Lohman, T.M.
Deposited on	:	2010-01-18
Resolution	:	1.80 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:

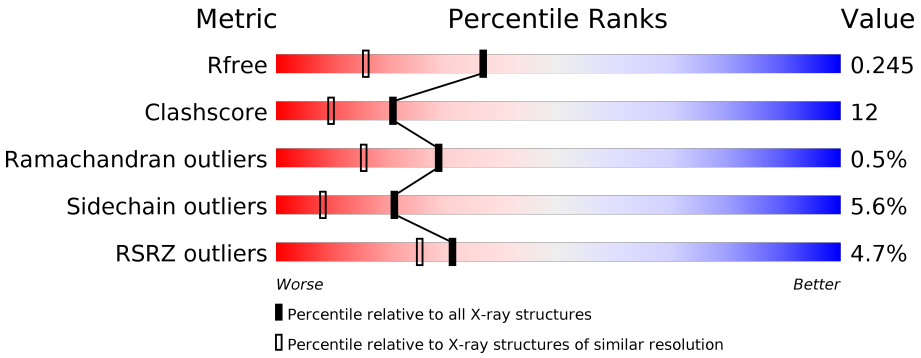
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	647	5% 79% 15%

2 Entry composition

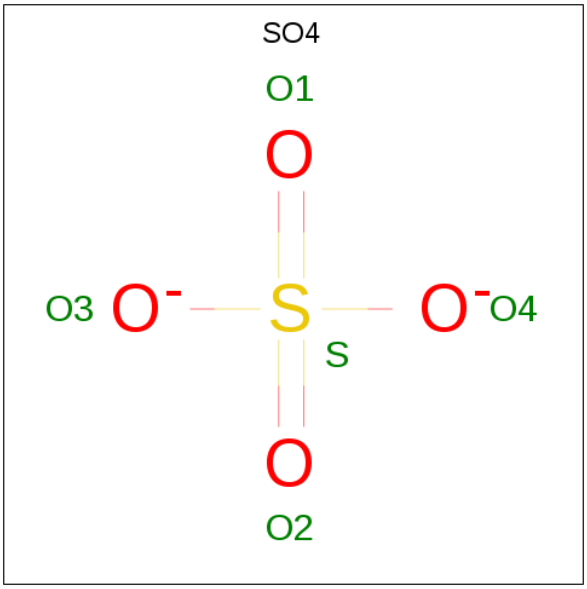
There are 3 unique types of molecules in this entry. The entry contains 5780 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA helicase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	633	5039	3155	920	938	26	0	0	0

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



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

- Molecule 3 is water.

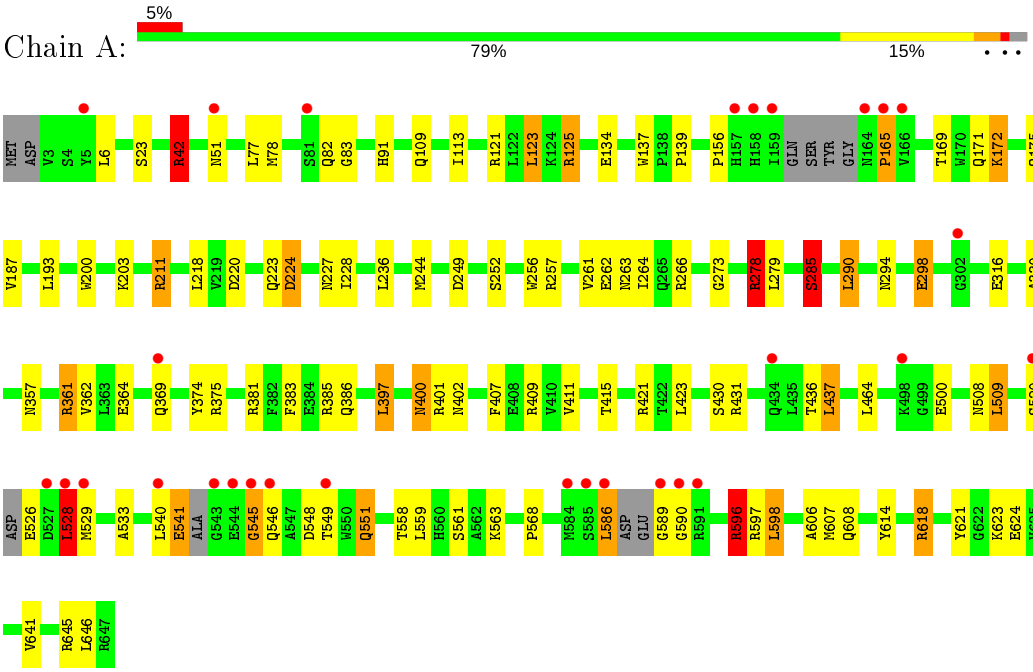
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	721	Total	O	0	0
			721	721		

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 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: DNA helicase II

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	194.54Å 58.74Å 69.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.54 – 1.80 29.54 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.0 (29.54-1.80) 91.0 (29.54-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.76 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, R_{free}	0.199 , 0.248 0.198 , 0.245	Depositor DCC
R_{free} test set	3393 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	22.7	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.58$, $< L^2 > = 0.43$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5780	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: 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	0.53	0/5127	1.02	26/6918 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	596	ARG	NE-CZ-NH2	-18.40	111.10	120.30
1	A	42	ARG	NE-CZ-NH1	15.84	128.22	120.30
1	A	596	ARG	NE-CZ-NH1	14.04	127.32	120.30
1	A	278	ARG	NE-CZ-NH1	-13.27	113.66	120.30
1	A	361	ARG	NE-CZ-NH2	-11.44	114.58	120.30
1	A	42	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	A	278	ARG	NE-CZ-NH2	8.38	124.49	120.30
1	A	618	ARG	CG-CD-NE	-7.75	95.52	111.80
1	A	361	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	224	ASP	CB-CG-OD1	7.23	124.81	118.30
1	A	290	LEU	CB-CG-CD1	7.20	123.25	111.00
1	A	220	ASP	CB-CG-OD1	7.06	124.65	118.30
1	A	211	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	A	437	LEU	CB-CG-CD1	6.63	122.27	111.00
1	A	618	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	165	PRO	N-CA-CB	6.32	110.89	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	596	ARG	CD-NE-CZ	6.30	132.42	123.60
1	A	285	SER	CB-CA-C	6.20	121.88	110.10
1	A	211	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	A	509	LEU	CB-CG-CD1	6.09	121.36	111.00
1	A	109	GLN	C-N-CA	-6.07	106.53	121.70
1	A	397	LEU	CB-CG-CD1	6.03	121.24	111.00
1	A	42	ARG	CD-NE-CZ	5.81	131.73	123.60
1	A	249	ASP	CB-CG-OD1	5.74	123.46	118.30
1	A	224	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	A	279	LEU	CB-CG-CD1	5.35	120.10	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	GLY	Peptide
1	A	528	LEU	Peptide
1	A	596	ARG	Sidechain
1	A	618	ARG	Sidechain

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	5039	0	4945	123	0
2	A	20	0	0	0	0
3	A	721	0	0	61	0
All	All	5780	0	4945	123	0

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

All (123) 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:407:PHE:O	1:A:411:VAL:HG23	1.42	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ARG:HG2	1:A:278:ARG:HH11	1.05	1.16
1:A:51:ASN:HB3	3:A:740:HOH:O	1.45	1.13
1:A:623:LYS:HE3	3:A:695:HOH:O	1.55	1.05
1:A:278:ARG:HG2	1:A:278:ARG:NH1	1.69	1.00
1:A:415:THR:HG23	3:A:869:HOH:O	1.66	0.95
1:A:123:LEU:HD11	1:A:177:TYR:CD1	2.03	0.94
1:A:558:THR:HG23	1:A:561:SER:H	1.34	0.90
1:A:407:PHE:CE2	1:A:411:VAL:HG21	2.08	0.89
1:A:42:ARG:HD3	3:A:776:HOH:O	1.72	0.88
1:A:121:ARG:HD2	3:A:1170:HOH:O	1.72	0.86
1:A:563:LYS:HE2	3:A:976:HOH:O	1.75	0.86
1:A:278:ARG:CG	1:A:278:ARG:HH11	1.76	0.85
1:A:586:LEU:H	1:A:586:LEU:HD22	1.43	0.83
1:A:589:GLY:HA2	3:A:1011:HOH:O	1.78	0.83
1:A:278:ARG:HD3	3:A:1316:HOH:O	1.77	0.82
1:A:375:ARG:HH22	1:A:551:GLN:HE21	1.24	0.81
1:A:586:LEU:HB3	3:A:1342:HOH:O	1.81	0.81
1:A:407:PHE:CD2	1:A:411:VAL:HG21	2.17	0.79
1:A:464:LEU:HD12	3:A:1347:HOH:O	1.82	0.79
1:A:431:ARG:NH1	3:A:948:HOH:O	2.20	0.75
1:A:386:GLN:HG3	3:A:1372:HOH:O	1.88	0.74
1:A:278:ARG:CD	3:A:1316:HOH:O	2.33	0.73
1:A:278:ARG:CG	1:A:278:ARG:NH1	2.41	0.72
1:A:627:HIS:HE1	3:A:1348:HOH:O	1.71	0.72
1:A:42:ARG:HD2	1:A:244:MET:CE	2.20	0.71
1:A:261:VAL:HG23	3:A:769:HOH:O	1.92	0.70
1:A:627:HIS:HD2	3:A:666:HOH:O	1.75	0.70
1:A:558:THR:HG21	3:A:1364:HOH:O	1.93	0.68
1:A:559:LEU:HD13	1:A:598:LEU:HD13	1.77	0.67
1:A:526:GLU:CB	3:A:1329:HOH:O	2.43	0.67
1:A:528:LEU:HD23	1:A:528:LEU:H	1.60	0.67
1:A:385:ARG:HH11	1:A:508:ASN:ND2	1.95	0.64
1:A:123:LEU:HD11	1:A:177:TYR:HD1	1.58	0.64
1:A:386:GLN:CG	3:A:1372:HOH:O	2.45	0.63
1:A:586:LEU:HD12	3:A:1342:HOH:O	1.97	0.63
1:A:203:LYS:NZ	3:A:1271:HOH:O	2.31	0.63
1:A:156:PRO:HB2	1:A:175:GLN:HG2	1.81	0.62
1:A:285:SER:HB2	1:A:606:ALA:O	1.99	0.62
1:A:193:LEU:HB2	3:A:1344:HOH:O	2.00	0.60
1:A:409:ARG:HD2	3:A:916:HOH:O	1.99	0.60
1:A:540:LEU:HD12	3:A:1124:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:ARG:HD2	3:A:1258:HOH:O	2.04	0.58
1:A:559:LEU:HB2	1:A:598:LEU:HD11	1.86	0.58
1:A:256:TRP:CH2	1:A:257:ARG:NH2	2.72	0.58
1:A:262:GLU:HG2	1:A:266:ARG:NH1	2.19	0.58
1:A:261:VAL:HG21	1:A:597:ARG:NH2	2.19	0.57
1:A:400:ASN:ND2	1:A:402:ASN:H	2.01	0.57
1:A:172:LYS:HD3	3:A:673:HOH:O	2.04	0.57
1:A:464:LEU:CD1	3:A:1347:HOH:O	2.47	0.57
1:A:385:ARG:HH11	1:A:508:ASN:HD21	1.51	0.57
1:A:123:LEU:HD11	1:A:177:TYR:CE1	2.40	0.56
1:A:590:GLY:HA3	3:A:1305:HOH:O	2.05	0.56
1:A:252:SER:OG	1:A:261:VAL:HG22	2.04	0.56
1:A:563:LYS:HD2	3:A:1341:HOH:O	2.05	0.55
1:A:137:TRP:CH2	1:A:169:THR:HB	2.42	0.55
1:A:203:LYS:NZ	3:A:1254:HOH:O	2.33	0.55
1:A:415:THR:HG22	3:A:1191:HOH:O	2.06	0.55
1:A:42:ARG:HD2	1:A:244:MET:HE1	1.88	0.54
1:A:528:LEU:O	1:A:529:MET:HG3	2.08	0.54
1:A:262:GLU:HG3	1:A:266:ARG:CZ	2.37	0.54
1:A:134:GLU:HG3	1:A:139:PRO:HD3	1.90	0.53
1:A:42:ARG:HD2	1:A:244:MET:HE3	1.90	0.53
1:A:77:LEU:HD12	3:A:1320:HOH:O	2.09	0.53
1:A:23:SER:HB2	3:A:658:HOH:O	2.08	0.53
1:A:125:ARG:CZ	3:A:1174:HOH:O	2.55	0.53
1:A:77:LEU:CD1	3:A:1320:HOH:O	2.56	0.53
1:A:421:ARG:HG3	3:A:1116:HOH:O	2.08	0.53
1:A:528:LEU:HD21	1:A:533:ALA:N	2.24	0.53
1:A:614:TYR:CE1	1:A:629:PRO:HG3	2.43	0.52
1:A:261:VAL:CG2	3:A:1314:HOH:O	2.57	0.52
1:A:263:ASN:ND2	1:A:266:ARG:HH11	2.09	0.51
1:A:113:ILE:HD13	1:A:187:VAL:CG2	2.40	0.51
1:A:193:LEU:HD23	1:A:228:ILE:HG23	1.92	0.51
1:A:252:SER:CB	1:A:261:VAL:HG22	2.41	0.50
1:A:608:GLN:NE2	3:A:1009:HOH:O	2.39	0.50
1:A:134:GLU:CD	3:A:829:HOH:O	2.49	0.50
1:A:548:ASP:CB	3:A:710:HOH:O	2.59	0.50
1:A:82:GLN:NE2	3:A:1214:HOH:O	2.45	0.49
1:A:528:LEU:HD23	1:A:528:LEU:N	2.27	0.48
1:A:211:ARG:HG3	1:A:236:LEU:O	2.14	0.48
1:A:316:GLU:HB3	3:A:690:HOH:O	2.12	0.48
1:A:364:GLU:HG2	1:A:374:TYR:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:THR:HA	3:A:899:HOH:O	2.12	0.48
1:A:294:ASN:O	1:A:298:GLU:HG2	2.13	0.48
1:A:568:PRO:HA	1:A:607:MET:HB2	1.94	0.48
1:A:641:VAL:HG23	3:A:680:HOH:O	2.14	0.47
1:A:223:GLN:CB	3:A:1255:HOH:O	2.62	0.47
1:A:82:GLN:O	1:A:83:GLY:C	2.52	0.47
1:A:400:ASN:HD22	1:A:401:ARG:N	2.13	0.46
1:A:223:GLN:HB2	3:A:1255:HOH:O	2.15	0.46
1:A:278:ARG:HD2	3:A:1316:HOH:O	2.09	0.46
1:A:91:HIS:ND1	3:A:803:HOH:O	2.15	0.46
1:A:123:LEU:CD1	1:A:177:TYR:HD1	2.27	0.46
1:A:261:VAL:HG22	3:A:1314:HOH:O	2.16	0.46
1:A:590:GLY:CA	3:A:1305:HOH:O	2.62	0.46
1:A:528:LEU:CD2	1:A:533:ALA:HB2	2.46	0.45
1:A:586:LEU:HD22	1:A:586:LEU:N	2.19	0.45
1:A:589:GLY:CA	3:A:1011:HOH:O	2.52	0.45
1:A:193:LEU:HD13	3:A:1344:HOH:O	2.16	0.45
1:A:381:ARG:HD2	1:A:545:GLY:HA2	1.99	0.44
1:A:78:MET:HG2	3:A:1136:HOH:O	2.16	0.44
1:A:224:ASP:HB2	3:A:859:HOH:O	2.17	0.44
1:A:520:SER:CB	3:A:1354:HOH:O	2.65	0.43
1:A:407:PHE:CD2	1:A:411:VAL:CG2	2.95	0.43
1:A:187:VAL:HG23	1:A:187:VAL:O	2.18	0.43
1:A:264:ILE:HD12	3:A:1255:HOH:O	2.18	0.43
1:A:171:GLN:O	1:A:175:GLN:HG3	2.18	0.43
1:A:262:GLU:HG3	1:A:266:ARG:NH2	2.33	0.43
1:A:383:PHE:HD1	1:A:541:GLU:HG3	1.82	0.43
1:A:528:LEU:CD2	1:A:528:LEU:N	2.81	0.43
1:A:402:ASN:HB3	1:A:436:THR:HG21	2.01	0.43
1:A:200:TRP:CZ3	1:A:236:LEU:HB2	2.53	0.42
1:A:627:HIS:CD2	3:A:666:HOH:O	2.60	0.42
1:A:42:ARG:HG2	1:A:218:LEU:HD21	2.00	0.42
1:A:172:LYS:HE2	1:A:172:LYS:HB2	1.65	0.42
1:A:596:ARG:NH2	3:A:724:HOH:O	2.42	0.41
1:A:421:ARG:CG	3:A:1116:HOH:O	2.67	0.41
1:A:330:ALA:HB2	1:A:362:VAL:HG12	2.02	0.41
1:A:51:ASN:CB	3:A:740:HOH:O	2.29	0.41
1:A:400:ASN:HD22	1:A:400:ASN:C	2.23	0.40
1:A:175:GLN:NE2	3:A:673:HOH:O	2.52	0.40
1:A:332:PHE:O	1:A:336:ARG:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	623/647 (96%)	608 (98%)	12 (2%)	3 (0%)	29 15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	545	GLY
1	A	546	GLN
1	A	165	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	520/545 (95%)	491 (94%)	29 (6%)	21 8

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	42	ARG
1	A	123	LEU
1	A	125	ARG
1	A	172	LYS
1	A	186	LEU
1	A	227	ASN
1	A	278	ARG

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Mol	Chain	Res	Type
1	A	285	SER
1	A	290	LEU
1	A	298	GLU
1	A	357	ASN
1	A	361	ARG
1	A	369	GLN
1	A	397	LEU
1	A	400	ASN
1	A	423	LEU
1	A	430	SER
1	A	437	LEU
1	A	500	GLU
1	A	509	LEU
1	A	528	LEU
1	A	541	GLU
1	A	551	GLN
1	A	586	LEU
1	A	598	LEU
1	A	621	TYR
1	A	624	GLU
1	A	646	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	76	GLN
1	A	82	GLN
1	A	102	HIS
1	A	131	ASN
1	A	260	GLN
1	A	263	ASN
1	A	343	ASN
1	A	357	ASN
1	A	400	ASN
1	A	480	GLN
1	A	508	ASN
1	A	551	GLN
1	A	569	GLN
1	A	608	GLN
1	A	627	HIS

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	1002	-	4,4,4	0.20	0	6,6,6	0.56	0
2	SO4	A	1001	-	4,4,4	0.24	0	6,6,6	0.74	0
2	SO4	A	1003	-	4,4,4	0.15	0	6,6,6	0.74	0
2	SO4	A	1000	-	4,4,4	0.29	0	6,6,6	1.69	2 (33%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1000	SO4	O4-S-O3	2.66	120.41	109.06
2	A	1000	SO4	O3-S-O2	-2.09	98.42	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	633/647 (97%)	0.06	30 (4%) 31 25	11, 22, 42, 76	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	ASN	10.7
1	A	590	GLY	9.4
1	A	546	GLN	8.2
1	A	158	HIS	7.1
1	A	527	ASP	6.4
1	A	528	LEU	5.8
1	A	159	ILE	5.8
1	A	165	PRO	5.1
1	A	544	GLU	5.0
1	A	545	GLY	4.4
1	A	543	GLY	4.2
1	A	166	VAL	4.1
1	A	586	LEU	3.9
1	A	626	TYR	3.7
1	A	520	SER	3.7
1	A	157	HIS	3.6
1	A	540	LEU	3.6
1	A	434	GLN	3.6
1	A	584	MET	3.4
1	A	589	GLY	3.1
1	A	81	SER	2.7
1	A	529	MET	2.6
1	A	369	GLN	2.6
1	A	302	GLY	2.4
1	A	591	ARG	2.3
1	A	549	THR	2.3
1	A	498	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	5	TYR	2.1
1	A	51	ASN	2.1
1	A	585	SER	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^{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	A	1003	5/5	0.98	0.09	29,30,37,41	0
2	SO4	A	1001	5/5	0.99	0.06	25,26,33,35	0
2	SO4	A	1002	5/5	0.99	0.08	26,28,29,29	0
2	SO4	A	1000	5/5	0.99	0.10	18,20,27,31	0

6.5 Other polymers (i)

There are no such residues in this entry.