Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:34 PM GMT

PDB ID	:	1U6Z
Title	:	Structure of an E. coli Exopolyphosphatase: Insight into the processive hydrolysis of polyphosphate and its regulation
Authors	:	Hasson, M.S.; Alvarado, J.; Sanders, D.A.
Deposited on	:	2004-08-02
Resolution	:	1.90 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 ⓘ symbol.

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

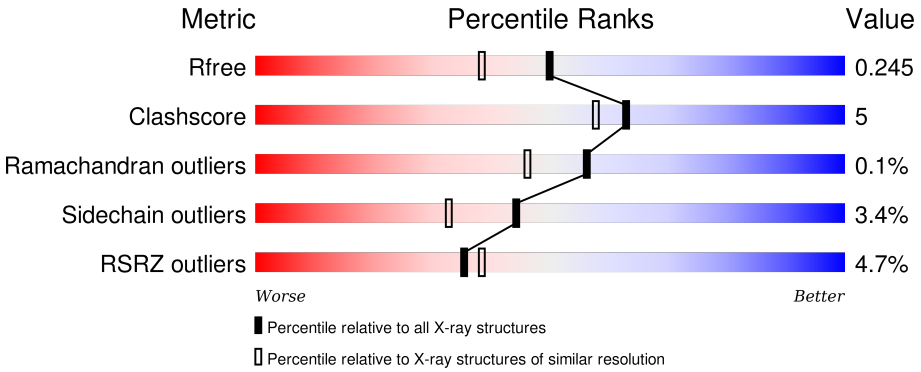
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	513	6%, 81%, 16%
1	B	513	3%, 88%, 8%

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	701	-	-	-	X
2	SO4	A	707	-	-	-	X
2	SO4	A	709	-	-	X	-
2	SO4	B	806	-	-	-	X
2	SO4	B	812	-	-	X	X

2 Entry composition

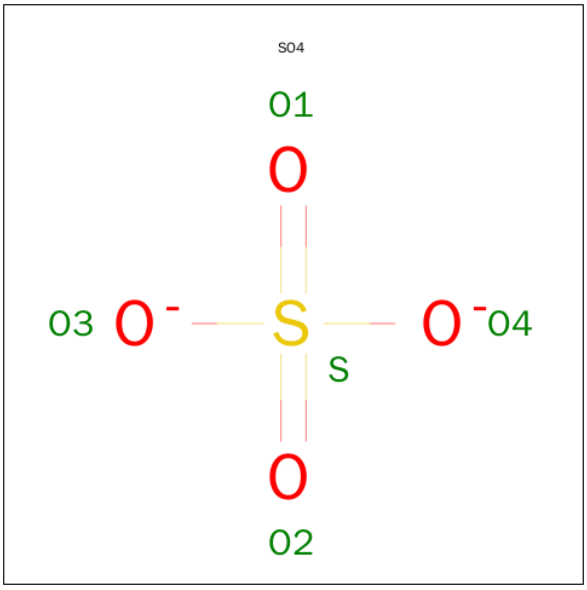
There are 3 unique types of molecules in this entry. The entry contains 8984 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Exopolyphosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	37	0
			4127	2625	734	744	24			
1	B	500	Total	C	N	O	S	0	25	0
			4078	2586	723	747	22			

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



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

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

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

- Molecule 3 is water.

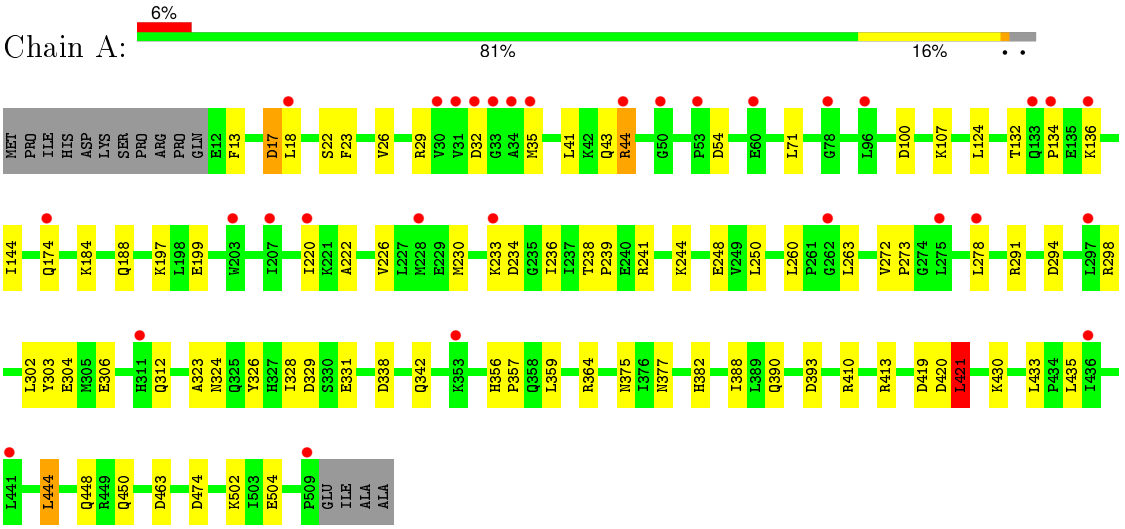
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	313	Total O 313 313	0	0
3	B	321	Total O 321 321	0	0

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.

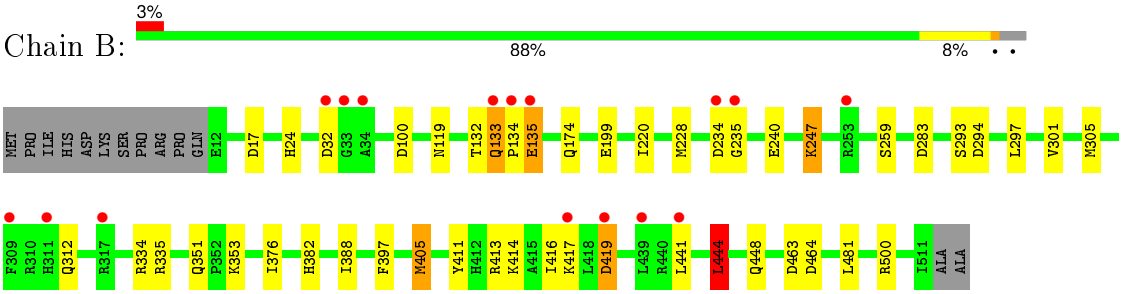
- Molecule 1: Exopolyphosphatase

Chain A:



- Molecule 1: Exopolyphosphatase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	89.14Å 89.14Å 350.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.74 – 1.90 27.56 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.8 (27.74-1.90) 92.8 (27.56-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.39 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.204 , 0.242 0.208 , 0.245	Depositor DCC
R_{free} test set	10531 reflections (11.23%)	DCC
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 104324 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8984	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: 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	0.60	0/4362	0.82	17/5889 (0.3%)
1	B	0.63	0/4261	0.82	9/5754 (0.2%)
All	All	0.61	0/8623	0.82	26/11643 (0.2%)

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	329	ASP	CB-CG-OD2	8.82	126.24	118.30
1	A	17	ASP	CB-CG-OD2	8.57	126.02	118.30
1	B	444	LEU	CA-CB-CG	8.19	134.15	115.30
1	A	393	ASP	CB-CG-OD2	6.96	124.57	118.30
1	A	54	ASP	CB-CG-OD2	6.78	124.40	118.30
1	B	464	ASP	CB-CG-OD2	6.71	124.34	118.30
1	B	100	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	463	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	32	ASP	CB-CG-OD2	6.46	124.11	118.30
1	B	234	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	444	LEU	CA-CB-CG	6.30	129.79	115.30
1	A	420	ASP	CB-CG-OD2	6.19	123.87	118.30
1	B	419	ASP	CB-CG-OD2	6.16	123.85	118.30
1	B	335	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	234	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	100	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	338	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	294[A]	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	294[B]	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	419	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	32	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	474	ASP	CB-CG-OD2	5.38	123.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	421	LEU	CA-CB-CG	5.31	127.52	115.30
1	B	283	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	444	LEU	CB-CG-CD1	-5.23	102.10	111.00
1	B	463	ASP	CB-CG-OD2	5.08	122.87	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4127	0	4156	64	0
1	B	4078	0	4088	29	0
2	A	65	0	0	5	0
2	B	80	0	0	3	0
3	A	313	0	0	4	0
3	B	321	0	0	2	0
All	All	8984	0	8244	89	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 5.

All (89) 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:260[B]:LEU:HB2	1:A:263[B]:LEU:CD1	1.83	1.09
1:A:260[B]:LEU:HB2	1:A:263[B]:LEU:HD13	1.15	1.05
1:A:13[B]:PHE:CE2	1:A:306[B]:GLU:OE1	2.09	1.05
1:A:260[B]:LEU:CB	1:A:263[B]:LEU:HD13	1.88	1.03
1:A:184[B]:LYS:HD2	1:A:188[B]:GLN:NE2	1.76	0.99
1:A:260[B]:LEU:CB	1:A:263[B]:LEU:CD1	2.43	0.93
1:A:304[B]:GLU:HG2	3:A:993:HOH:O	1.72	0.89
1:B:132:THR:O	1:B:134:PRO:HD3	1.74	0.86
1:A:13[B]:PHE:CE2	1:A:306[B]:GLU:CD	2.49	0.86
1:A:184[B]:LYS:HD2	1:A:188[B]:GLN:HE22	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119[B]:ASN:ND2	3:B:1046:HOH:O	2.09	0.77
1:A:410[B]:ARG:NH1	3:A:948:HOH:O	2.18	0.76
1:A:13[B]:PHE:CZ	1:A:306[B]:GLU:OE1	2.39	0.74
1:A:364[B]:ARG:NH1	2:A:711:SO4:O3	2.22	0.72
1:A:13[B]:PHE:CD2	1:A:306[B]:GLU:OE1	2.44	0.70
1:A:260[B]:LEU:HB3	1:A:263[B]:LEU:CD1	2.22	0.69
1:A:13[B]:PHE:CZ	1:A:306[B]:GLU:CD	2.67	0.68
1:A:390:GLN:OE1	1:A:410[B]:ARG:NH2	2.26	0.68
1:A:35[B]:MET:HG2	1:A:303:TYR:CE2	2.29	0.67
1:A:199[A]:GLU:HG2	1:B:448:GLN:HG2	1.78	0.64
1:B:133:GLN:NE2	1:B:293:SER:OG	2.32	0.63
1:A:144:ILE:HD12	1:A:220[B]:ILE:HD11	1.81	0.62
1:B:500:ARG:NH2	2:B:812:SO4:O4	2.30	0.59
1:A:260[B]:LEU:CB	1:A:263[B]:LEU:HD11	2.29	0.59
1:B:132:THR:C	1:B:134:PRO:HD3	2.24	0.58
1:A:132:THR:O	1:A:134:PRO:HD3	2.04	0.57
1:B:133:GLN:O	1:B:135:GLU:N	2.38	0.56
1:A:448:GLN:HG2	1:B:199[B]:GLU:HB2	1.86	0.56
1:A:199[A]:GLU:HG2	1:B:448:GLN:CG	2.35	0.56
1:B:228:MET:SD	1:B:235:GLY:HA2	2.45	0.56
1:A:230:MET:SD	1:A:248:GLU:HG3	2.46	0.55
1:A:430[A]:LYS:HE3	2:A:709:SO4:O2	2.06	0.55
1:A:356:HIS:HB3	2:A:710:SO4:O2	2.07	0.54
1:A:124:LEU:CD2	1:A:304[B]:GLU:HG3	2.38	0.54
1:A:41:LEU:HD12	3:A:1065:HOH:O	2.07	0.53
1:A:184[B]:LYS:CD	1:A:188[B]:GLN:NE2	2.63	0.53
1:A:226:VAL:O	1:A:230:MET:HG3	2.09	0.52
1:A:382:HIS:CD2	1:A:382:HIS:H	2.27	0.52
1:A:222:ALA:O	1:A:226:VAL:HG23	2.10	0.52
1:B:301:VAL:O	1:B:305:MET:HG3	2.10	0.51
1:B:376:ILE:HD11	1:B:388[B]:ILE:HD11	1.93	0.51
1:A:26:VAL:HB	1:A:298:ARG:HD2	1.92	0.50
1:B:382:HIS:CD2	1:B:382:HIS:H	2.29	0.50
1:B:382:HIS:HD2	1:B:413:ARG:HH11	1.60	0.50
1:A:421:LEU:HD11	1:A:433:LEU:HD21	1.93	0.50
1:A:382:HIS:HD2	1:A:413:ARG:HH11	1.60	0.48
1:A:260[B]:LEU:HB2	1:A:263[B]:LEU:HD11	1.85	0.47
1:A:323:ALA:HA	1:A:328:ILE:HD12	1.96	0.47
1:A:502:LYS:NZ	1:A:504:GLU:OE1	2.40	0.47
1:B:17:ASP:OD2	1:B:24:HIS:HB2	2.13	0.47
1:A:184[B]:LYS:HG2	1:A:250:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LEU:HB3	1:A:435:LEU:HD11	1.97	0.47
1:B:441:LEU:HA	1:B:444:LEU:HD13	1.97	0.47
1:B:397:PHE:HE2	1:B:405[A]:MET:HE3	1.80	0.47
1:A:26:VAL:HG13	1:A:302:LEU:HD13	1.97	0.46
1:B:413:ARG:NE	2:B:805:SO4:O4	2.45	0.46
1:A:132:THR:C	1:A:134:PRO:HD3	2.36	0.46
1:A:197:LYS:HD3	2:A:706:SO4:O1	2.15	0.45
1:B:382:HIS:CD2	1:B:413:ARG:HH11	2.34	0.45
1:A:236:ILE:HD11	1:A:291[A]:ARG:HH21	1.82	0.44
1:A:241:ARG:HA	1:A:244:LYS:HD2	2.00	0.44
1:B:500:ARG:HB2	1:B:500:ARG:HE	1.64	0.43
1:A:272:VAL:N	1:A:273:PRO:HD2	2.33	0.43
1:A:326:TYR:O	1:A:375:ASN:ND2	2.51	0.43
1:A:35[B]:MET:HG2	1:A:303:TYR:HE2	1.80	0.43
1:A:238:THR:HB	1:A:239:PRO:HD2	2.00	0.42
1:A:390:GLN:HG3	3:A:1206:HOH:O	2.19	0.42
1:A:382:HIS:CD2	1:A:413:ARG:HH11	2.37	0.42
1:B:500:ARG:NH2	2:B:812:SO4:S	2.92	0.42
1:A:430[A]:LYS:CE	2:A:709:SO4:O2	2.68	0.42
1:B:411:TYR:HD2	1:B:416:ILE:HG13	1.85	0.41
1:B:220[B]:ILE:HG12	3:B:1043:HOH:O	2.20	0.41
1:A:331:GLU:OE1	1:A:450:GLN:HG2	2.19	0.41
1:A:18:LEU:HD22	1:A:23:PHE:CD2	2.56	0.41
1:A:199[B]:GLU:OE1	1:B:481:LEU:HB3	2.20	0.41
1:A:356:HIS:HA	1:A:357:PRO:HD3	1.85	0.40
1:A:220[B]:ILE:HD12	1:A:278:LEU:HD22	2.02	0.40
1:B:240:GLU:H	1:B:240:GLU:CD	2.25	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	534/513 (104%)	521 (98%)	13 (2%)	0	100	100
1	B	524/513 (102%)	510 (97%)	13 (2%)	1 (0%)	52	42
All	All	1058/1026 (103%)	1031 (97%)	26 (2%)	1 (0%)	56	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	133	GLN

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	460/437 (105%)	444 (96%)	16 (4%)	43	31
1	B	450/437 (103%)	433 (96%)	17 (4%)	40	28
All	All	910/874 (104%)	877 (96%)	33 (4%)	44	30

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	22	SER
1	A	29	ARG
1	A	43	GLN
1	A	44[A]	ARG
1	A	44[B]	ARG
1	A	71	LEU
1	A	107	LYS
1	A	136	LYS
1	A	174	GLN
1	A	233	LYS
1	A	312	GLN
1	A	342	GLN
1	A	377	ASN
1	A	421	LEU

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Mol	Chain	Res	Type
1	A	444	LEU
1	B	135	GLU
1	B	174	GLN
1	B	247[A]	LYS
1	B	247[B]	LYS
1	B	259[A]	SER
1	B	259[B]	SER
1	B	297	LEU
1	B	312	GLN
1	B	334	ARG
1	B	351	GLN
1	B	353	LYS
1	B	405[A]	MET
1	B	405[B]	MET
1	B	414	LYS
1	B	417	LYS
1	B	419	ASP
1	B	444	LEU

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	21	ASN
1	A	67	ASN
1	A	94	GLN
1	A	325	GLN
1	A	342	GLN
1	A	375	ASN
1	A	382	HIS
1	A	478	GLN
1	B	133	GLN
1	B	325	GLN
1	B	382	HIS
1	B	478	GLN

5.3.3 RNA

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)

29 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	701	-	4,4,4	0.37	0	6,6,6	0.25	0
2	SO4	A	702	-	4,4,4	0.22	0	6,6,6	0.17	0
2	SO4	A	703	-	4,4,4	0.23	0	6,6,6	0.90	0
2	SO4	A	704	-	4,4,4	0.31	0	6,6,6	0.23	0
2	SO4	A	705	-	4,4,4	0.41	0	6,6,6	0.20	0
2	SO4	A	706	-	4,4,4	0.38	0	6,6,6	0.66	0
2	SO4	A	707	-	4,4,4	0.24	0	6,6,6	0.45	0
2	SO4	A	708	-	4,4,4	0.40	0	6,6,6	0.41	0
2	SO4	A	709	-	4,4,4	0.21	0	6,6,6	0.28	0
2	SO4	A	710	-	4,4,4	0.46	0	6,6,6	0.31	0
2	SO4	A	711	-	4,4,4	0.19	0	6,6,6	0.21	0
2	SO4	A	712	-	4,4,4	0.19	0	6,6,6	0.18	0
2	SO4	A	901	-	4,4,4	0.67	0	6,6,6	0.41	0
2	SO4	B	801	-	4,4,4	0.84	0	6,6,6	0.72	0
2	SO4	B	802	-	4,4,4	0.54	0	6,6,6	0.35	0
2	SO4	B	803	-	4,4,4	0.54	0	6,6,6	0.38	0
2	SO4	B	804	-	4,4,4	0.28	0	6,6,6	0.20	0
2	SO4	B	805	-	4,4,4	0.25	0	6,6,6	0.32	0
2	SO4	B	806	-	4,4,4	0.21	0	6,6,6	0.60	0
2	SO4	B	807	-	4,4,4	0.26	0	6,6,6	0.33	0
2	SO4	B	808	-	4,4,4	0.19	0	6,6,6	0.45	0
2	SO4	B	809	-	4,4,4	0.26	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	B	810	-	4,4,4	0.39	0	6,6,6	0.15	0
2	SO4	B	811	-	4,4,4	0.09	0	6,6,6	0.26	0
2	SO4	B	812	-	4,4,4	0.23	0	6,6,6	0.16	0
2	SO4	B	813	-	4,4,4	0.33	0	6,6,6	0.40	0
2	SO4	B	814	-	4,4,4	0.25	0	6,6,6	0.32	0
2	SO4	B	815	-	4,4,4	0.34	0	6,6,6	0.42	0
2	SO4	B	816	-	4,4,4	0.21	0	6,6,6	0.29	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	SO4	A	701	-	-	0/0/0/0	0/0/0/0
2	SO4	A	702	-	-	0/0/0/0	0/0/0/0
2	SO4	A	703	-	-	0/0/0/0	0/0/0/0
2	SO4	A	704	-	-	0/0/0/0	0/0/0/0
2	SO4	A	705	-	-	0/0/0/0	0/0/0/0
2	SO4	A	706	-	-	0/0/0/0	0/0/0/0
2	SO4	A	707	-	-	0/0/0/0	0/0/0/0
2	SO4	A	708	-	-	0/0/0/0	0/0/0/0
2	SO4	A	709	-	-	0/0/0/0	0/0/0/0
2	SO4	A	710	-	-	0/0/0/0	0/0/0/0
2	SO4	A	711	-	-	0/0/0/0	0/0/0/0
2	SO4	A	712	-	-	0/0/0/0	0/0/0/0
2	SO4	A	901	-	-	0/0/0/0	0/0/0/0
2	SO4	B	801	-	-	0/0/0/0	0/0/0/0
2	SO4	B	802	-	-	0/0/0/0	0/0/0/0
2	SO4	B	803	-	-	0/0/0/0	0/0/0/0
2	SO4	B	804	-	-	0/0/0/0	0/0/0/0
2	SO4	B	805	-	-	0/0/0/0	0/0/0/0
2	SO4	B	806	-	-	0/0/0/0	0/0/0/0
2	SO4	B	807	-	-	0/0/0/0	0/0/0/0
2	SO4	B	808	-	-	0/0/0/0	0/0/0/0
2	SO4	B	809	-	-	0/0/0/0	0/0/0/0
2	SO4	B	810	-	-	0/0/0/0	0/0/0/0
2	SO4	B	811	-	-	0/0/0/0	0/0/0/0
2	SO4	B	812	-	-	0/0/0/0	0/0/0/0
2	SO4	B	813	-	-	0/0/0/0	0/0/0/0
2	SO4	B	814	-	-	0/0/0/0	0/0/0/0
2	SO4	B	815	-	-	0/0/0/0	0/0/0/0
2	SO4	B	816	-	-	0/0/0/0	0/0/0/0

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.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	706	SO4	1	0
2	A	709	SO4	2	0
2	A	710	SO4	1	0
2	A	711	SO4	1	0
2	B	805	SO4	1	0
2	B	812	SO4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	498/513 (97%)	0.24	31 (6%)	24	27	9, 14, 19, 23	0
1	B	500/513 (97%)	0.07	16 (3%)	51	54	9, 14, 19, 23	0
All	All	998/1026 (97%)	0.16	47 (4%)	35	38	9, 14, 19, 23	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	PRO	6.0
1	B	311	HIS	4.3
1	A	233	LYS	4.3
1	A	311	HIS	4.1
1	B	32	ASP	3.9
1	A	34	ALA	3.5
1	B	33	GLY	3.4
1	A	33	GLY	3.4
1	A	32	ASP	3.1
1	A	136	LYS	3.0
1	A	78	GLY	3.0
1	B	235	GLY	3.0
1	A	262	GLY	3.0
1	A	18	LEU	2.9
1	A	353	LYS	2.9
1	A	278	LEU	2.9
1	B	441	LEU	2.8
1	A	44[A]	ARG	2.8
1	A	35[A]	MET	2.8
1	A	203[A]	TRP	2.8
1	B	234	ASP	2.7
1	B	253[A]	ARG	2.7
1	A	207	ILE	2.7
1	A	133	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	96	LEU	2.6
1	A	297	LEU	2.6
1	A	53	PRO	2.5
1	B	419	ASP	2.4
1	B	135	GLU	2.4
1	A	441	LEU	2.4
1	B	309	PHE	2.4
1	A	50	GLY	2.4
1	A	509	PRO	2.4
1	A	436[A]	ILE	2.4
1	A	60	GLU	2.3
1	A	174	GLN	2.3
1	A	275	LEU	2.3
1	A	134	PRO	2.3
1	B	417	LYS	2.3
1	A	31	VAL	2.2
1	B	317	ARG	2.2
1	A	30	VAL	2.2
1	B	133	GLN	2.1
1	A	220[A]	ILE	2.1
1	A	228	MET	2.1
1	B	439	LEU	2.1
1	B	34	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. 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	701	5/5	0.84	0.32	8.22	34,35,35,35	5
2	SO4	A	707	5/5	0.91	0.18	3.47	42,43,44,44	0
2	SO4	B	806	5/5	0.93	0.19	2.92	47,49,49,49	0
2	SO4	B	812	5/5	0.98	0.26	2.18	55,55,55,55	0
2	SO4	B	807	5/5	0.96	0.16	1.22	46,46,46,46	0
2	SO4	A	712	5/5	0.97	0.14	1.17	53,53,53,54	0
2	SO4	B	801	5/5	0.98	0.10	0.50	30,31,32,34	0
2	SO4	B	809	5/5	0.89	0.15	0.20	43,43,43,43	5
2	SO4	B	813	5/5	0.98	0.09	0.15	32,33,34,34	0
2	SO4	A	702	5/5	0.95	0.12	0.04	52,52,52,53	0
2	SO4	A	708	5/5	0.97	0.16	-0.03	48,49,49,50	0
2	SO4	A	704	5/5	0.94	0.12	-0.24	32,32,32,33	5
2	SO4	B	804	5/5	0.99	0.10	-0.51	40,41,42,42	0
2	SO4	B	802	5/5	0.99	0.08	-0.75	29,29,30,30	0
2	SO4	A	705	5/5	0.99	0.09	-0.77	37,38,38,38	0
2	SO4	A	901	5/5	0.98	0.10	-0.84	43,44,44,45	0
2	SO4	B	803	5/5	0.99	0.06	-2.06	32,32,33,33	0
2	SO4	A	703	5/5	0.90	0.14	-	50,50,50,50	0
2	SO4	B	808	5/5	0.97	0.13	-	50,50,50,50	0
2	SO4	B	805	5/5	0.94	0.18	-	35,36,36,37	5
2	SO4	A	709	5/5	0.92	0.17	-	36,36,37,37	5
2	SO4	A	711	5/5	0.95	0.13	-	34,34,34,34	5
2	SO4	B	810	5/5	0.98	0.14	-	46,46,47,47	0
2	SO4	A	706	5/5	0.97	0.17	-	48,49,49,50	0
2	SO4	B	814	5/5	0.93	0.13	-	36,36,36,37	5
2	SO4	B	816	5/5	0.97	0.18	-	49,49,49,50	0
2	SO4	A	710	5/5	0.98	0.09	-	40,40,40,41	0
2	SO4	B	815	5/5	0.95	0.16	-	49,49,49,49	0
2	SO4	B	811	5/5	0.94	0.26	-	55,56,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.