Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:10 PM GMT

PDB ID	:	4NPA
Title	:	Scrystal structure of protein with unknown function from Vibrio cholerae at P22121 spacegroup
Authors	:	Boyko, K.M.; Gorbacheva, M.A.; Rakitina, T.V.; Korgenevsky, D.A.; Dorovatovsky, P.V.; Lipkin, A.V.; Minor, W.; Shumilin, I.A.; Popov, V.O.
Deposited on	:	2013-11-21
Resolution	:	2.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

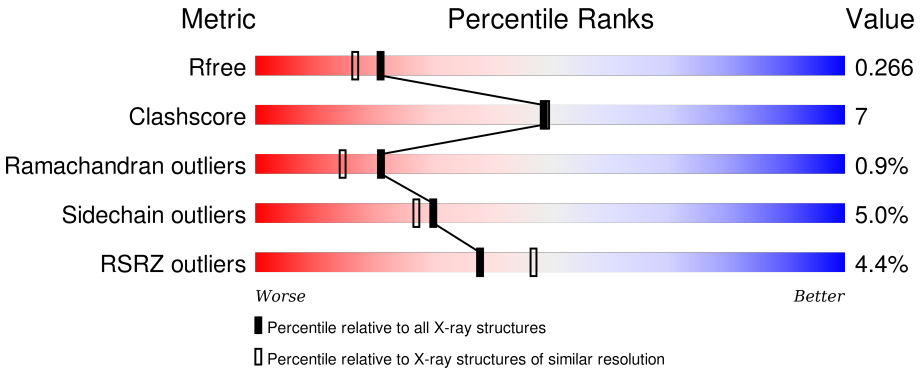
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.10 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 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	456	2% 75% 15% • 8%
1	B	456	3% 74% 15% • 8%
1	C	456	5% 74% 16% • 8%
1	D	456	5% 72% 17% • 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12881 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.

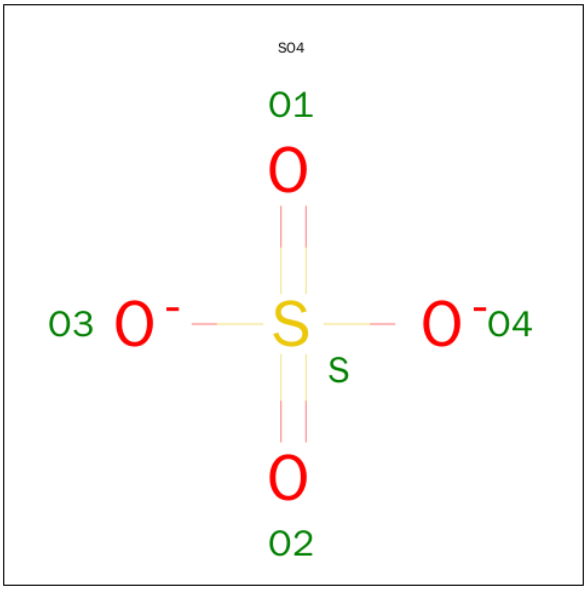
- Molecule 1 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3173	2017	557	578	21			
1	B	420	Total	C	N	O	S	0	1	0
			3175	2013	556	585	21			
1	C	418	Total	C	N	O	S	0	1	0
			3164	2011	553	579	21			
1	D	413	Total	C	N	O	S	0	2	0
			3041	1923	537	562	19			

There are 20 discrepancies between the modelled and reference sequences:

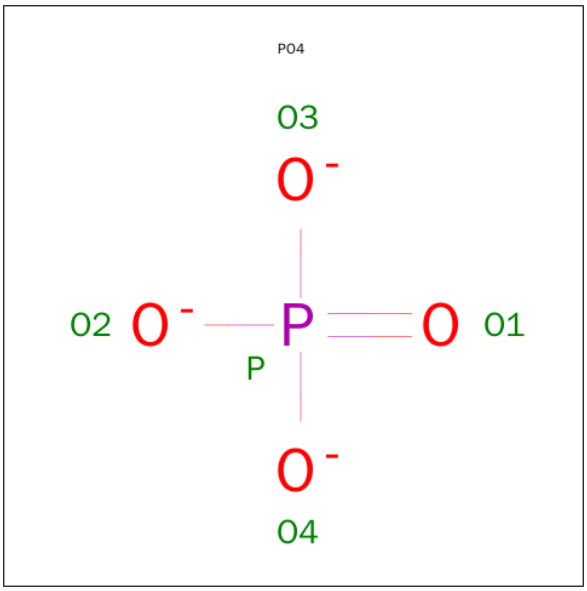
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	EXPRESSION TAG	UNP Q9KTK3
A	5	SER	-	EXPRESSION TAG	UNP Q9KTK3
A	6	LEU	-	EXPRESSION TAG	UNP Q9KTK3
A	458	GLU	-	EXPRESSION TAG	UNP Q9KTK3
A	459	GLY	-	EXPRESSION TAG	UNP Q9KTK3
B	4	MET	-	EXPRESSION TAG	UNP Q9KTK3
B	5	SER	-	EXPRESSION TAG	UNP Q9KTK3
B	6	LEU	-	EXPRESSION TAG	UNP Q9KTK3
B	458	GLU	-	EXPRESSION TAG	UNP Q9KTK3
B	459	GLY	-	EXPRESSION TAG	UNP Q9KTK3
C	4	MET	-	EXPRESSION TAG	UNP Q9KTK3
C	5	SER	-	EXPRESSION TAG	UNP Q9KTK3
C	6	LEU	-	EXPRESSION TAG	UNP Q9KTK3
C	458	GLU	-	EXPRESSION TAG	UNP Q9KTK3
C	459	GLY	-	EXPRESSION TAG	UNP Q9KTK3
D	4	MET	-	EXPRESSION TAG	UNP Q9KTK3
D	5	SER	-	EXPRESSION TAG	UNP Q9KTK3
D	6	LEU	-	EXPRESSION TAG	UNP Q9KTK3
D	458	GLU	-	EXPRESSION TAG	UNP Q9KTK3
D	459	GLY	-	EXPRESSION TAG	UNP Q9KTK3

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



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0

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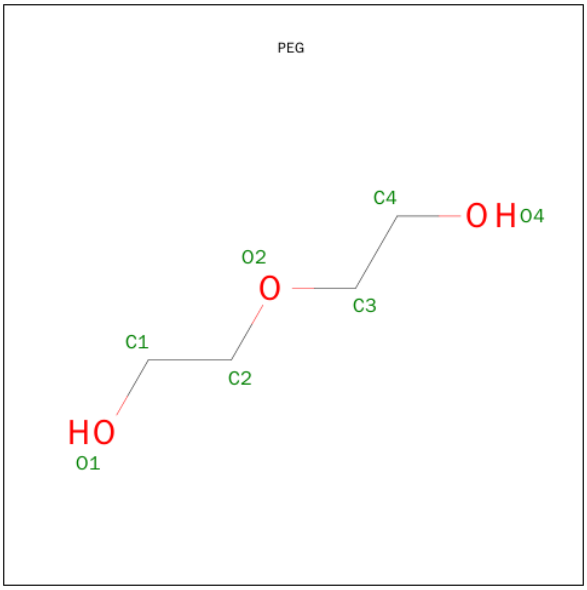
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O P 5 4 1	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 7 4 3	0	0

- Molecule 5 is water.

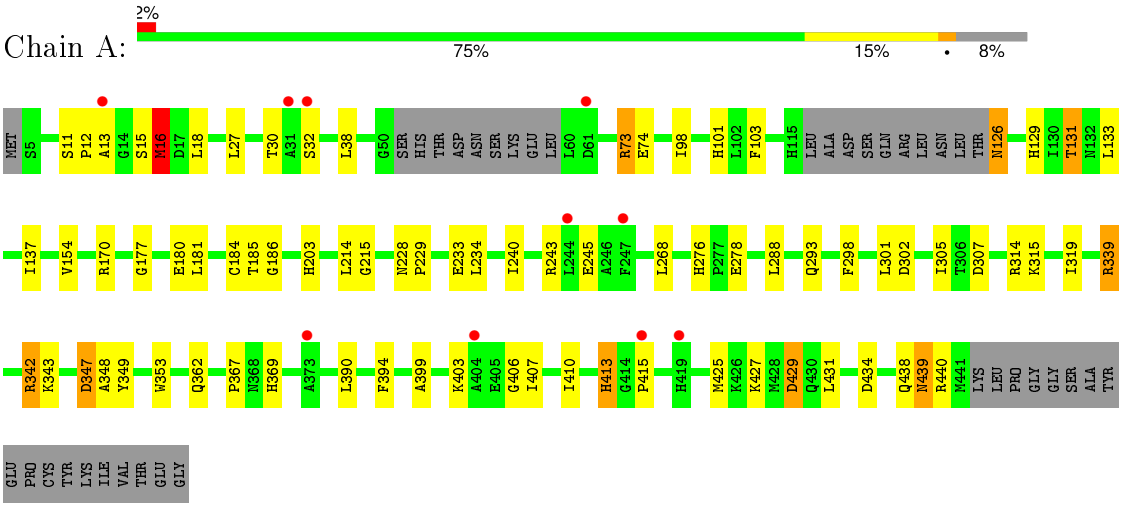
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	93	Total O 93 93	0	0
5	B	91	Total O 91 91	0	0
5	C	78	Total O 78 78	0	0
5	D	39	Total O 39 39	0	0

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.

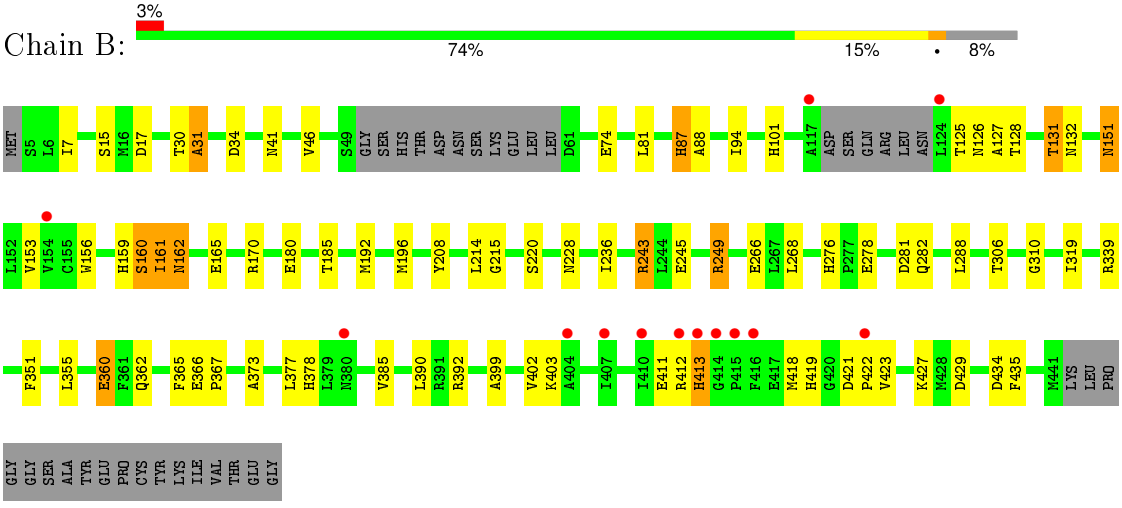
- Molecule 1: Putative uncharacterized protein

Chain A:



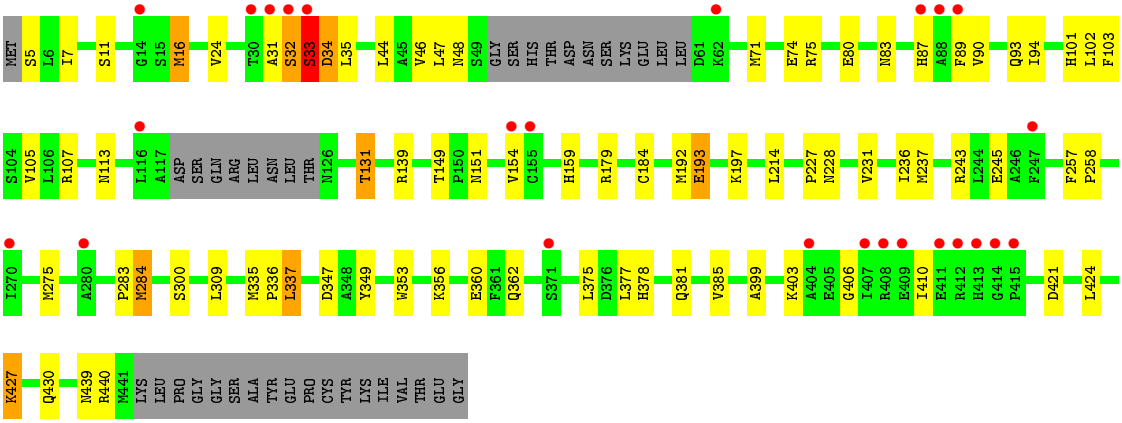
- Molecule 1: Putative uncharacterized protein

Chain B:



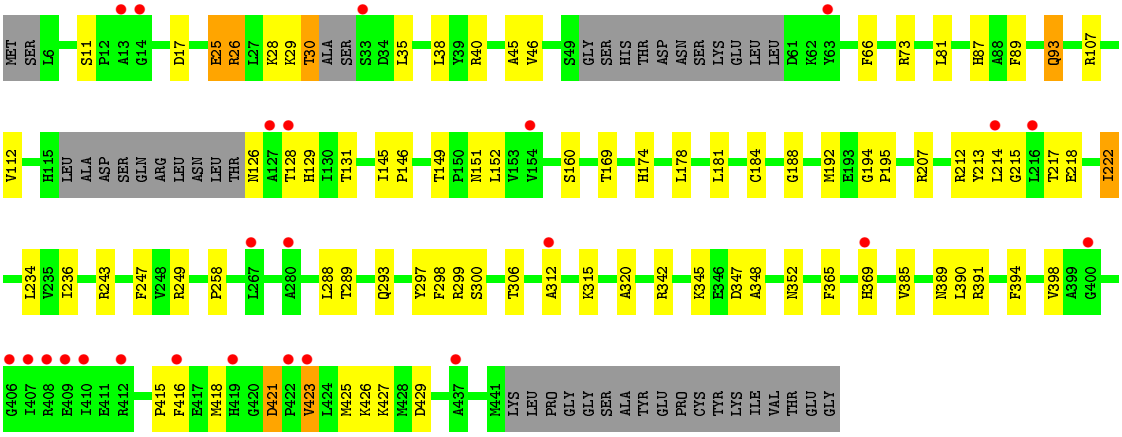
- Molecule 1: Putative uncharacterized protein

Chain C:



- Molecule 1: Putative uncharacterized protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.33Å 96.34Å 333.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.74 – 2.10 29.74 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.74-2.10) 99.7 (29.74-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.206 , 0.267 0.206 , 0.266	Depositor DCC
R_{free} test set	5550 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 111183 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12881	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: PO4, PEG, 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	1.06	1/3241 (0.0%)	1.14	14/4397 (0.3%)
1	B	1.09	1/3246 (0.0%)	1.11	12/4404 (0.3%)
1	C	0.99	1/3238 (0.0%)	1.07	8/4398 (0.2%)
1	D	0.92	1/3115 (0.0%)	1.00	4/4241 (0.1%)
All	All	1.02	4/12840 (0.0%)	1.08	38/17440 (0.2%)

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	1
1	B	0	1
1	C	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	GLU	CD-OE2	-5.80	1.19	1.25
1	C	74	GLU	CG-CD	5.50	1.60	1.51
1	B	153	VAL	C-O	5.49	1.33	1.23
1	D	213	TYR	CG-CD2	5.08	1.45	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	339	ARG	NE-CZ-NH2	-16.27	112.16	120.30
1	B	339	ARG	NE-CZ-NH2	-12.10	114.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	339	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	C	107	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	B	339	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	B	214	LEU	CB-CG-CD1	-8.18	97.09	111.00
1	C	107	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	302	ASP	CB-CG-OD1	7.59	125.13	118.30
1	A	302	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	A	170	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	A	342	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	A	214	LEU	CB-CG-CD1	-6.91	99.26	111.00
1	B	170	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	D	212	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	18	LEU	CB-CG-CD1	-6.39	100.13	111.00
1	D	214	LEU	CB-CG-CD1	-6.25	100.38	111.00
1	A	16	MET	CG-SD-CE	6.06	109.90	100.20
1	B	249	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	233	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	B	243	ARG	CB-CG-CD	-5.85	96.39	111.60
1	A	73	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	C	139	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	170	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	B	385	VAL	CB-CA-C	5.56	121.97	111.40
1	D	107	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	C	214	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	C	440	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	B	34	ASP	CB-CG-OD1	5.42	123.17	118.30
1	A	347	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	281	ASP	CB-CG-OD1	5.39	123.15	118.30
1	C	75	ARG	CG-CD-NE	-5.37	100.53	111.80
1	B	162	ASN	N-CA-C	-5.32	96.63	111.00
1	A	440	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	C	179	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	11	SER	C-N-CD	5.08	139.06	128.40
1	D	81	LEU	CB-CG-CD1	-5.03	102.44	111.00
1	C	337	LEU	CA-CB-CG	5.01	126.83	115.30
1	B	215	GLY	N-CA-C	-5.01	100.58	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	SER	Peptide

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Mol	Chain	Res	Type	Group
1	B	15	SER	Peptide
1	C	33	SER	Peptide

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	3173	0	3086	43	0
1	B	3175	0	3057	50	0
1	C	3164	0	3058	47	0
1	D	3041	0	2831	43	0
2	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	D	7	0	10	1	0
5	A	93	0	0	3	0
5	B	91	0	0	2	0
5	C	78	0	0	3	0
5	D	39	0	0	1	0
All	All	12881	0	12042	178	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 7.

All (178) 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:B:30:THR:O	1:B:31:ALA:CB	2.08	0.97
1:B:30:THR:O	1:B:31:ALA:HB2	1.64	0.97
1:C:283:PRO:O	1:C:284:MET:CB	2.11	0.94
1:D:28:LYS:O	1:D:30:THR:HG22	1.70	0.90
1:D:415:PRO:HB3	4:D:502:PEG:H31	1.58	0.86
1:B:276:HIS:CE1	1:B:278:GLU:HG3	2.15	0.82
1:C:283:PRO:O	1:C:284:MET:HB2	1.78	0.82
1:C:33:SER:C	1:C:35:LEU:H	1.90	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:425:MET:O	1:D:429:ASP:HB2	1.88	0.74
1:A:399:ALA:HA	1:A:403:LYS:HD3	1.70	0.74
1:B:161[B]:ILE:HG13	1:B:165:GLU:OE1	1.88	0.73
1:A:185:THR:HG23	1:A:186:GLY:O	1.87	0.72
1:A:307:ASP:OD2	1:A:427:LYS:HE2	1.90	0.70
1:A:131:THR:HB	1:A:245:GLU:OE2	1.91	0.70
1:C:131:THR:HB	1:C:245:GLU:OE2	1.91	0.70
1:B:276:HIS:HE1	1:B:278:GLU:HG3	1.57	0.69
1:B:243:ARG:HD3	5:B:621:HOH:O	1.92	0.69
1:C:105:VAL:HA	1:C:236:ILE:HD13	1.73	0.69
1:D:25:GLU:HG2	1:D:26:ARG:N	2.05	0.69
1:C:283:PRO:O	1:C:284:MET:HB3	1.94	0.67
1:A:314:ARG:NH1	1:A:319:ILE:HD12	2.10	0.67
1:C:89:PHE:HA	1:C:93:GLN:O	1.95	0.67
1:A:126:ASN:HA	1:A:129:HIS:HB3	1.76	0.67
1:C:131:THR:HG22	1:C:362:GLN:HE22	1.60	0.66
1:D:243:ARG:HD3	1:D:247:PHE:CE2	2.31	0.66
1:B:131:THR:HG22	1:B:362:GLN:NE2	2.10	0.66
1:B:131:THR:HB	1:B:245:GLU:OE2	1.96	0.65
1:C:16:MET:HE3	5:C:636:HOH:O	1.97	0.64
1:B:125:THR:O	1:B:127:ALA:N	2.31	0.63
1:D:421:ASP:OD1	1:D:423:VAL:HG23	1.97	0.63
1:B:236:ILE:HD12	1:B:236:ILE:N	2.12	0.63
1:C:275:MET:HE1	1:C:309:LEU:HD13	1.81	0.62
1:D:217:THR:HG21	1:D:222:ILE:HG13	1.82	0.61
1:C:16:MET:HG3	1:C:103:PHE:HB3	1.82	0.61
1:C:159[B]:HIS:CE1	1:C:192:MET:HG3	2.36	0.60
1:D:288:LEU:HB3	1:D:298:PHE:CE1	2.36	0.60
1:A:438:GLN:O	1:A:439:ASN:HB2	2.01	0.60
1:A:425:MET:O	1:A:429:ASP:HB2	2.00	0.60
1:B:360:GLU:CD	1:B:360:GLU:H	2.04	0.60
1:A:154:VAL:HA	1:A:184:CYS:O	2.02	0.59
1:C:16:MET:CE	5:C:636:HOH:O	2.49	0.59
1:A:369:HIS:CE1	1:A:413:HIS:HB3	2.38	0.58
1:C:275:MET:CE	1:C:309:LEU:HD13	2.33	0.58
1:C:44:LEU:O	1:C:48:ASN:HB2	2.03	0.58
1:A:268:LEU:HD13	1:A:390:LEU:HB3	1.85	0.57
1:B:159:HIS:ND1	3:B:501:PO4:O2	2.26	0.57
1:B:161[B]:ILE:CG1	1:B:165:GLU:OE1	2.53	0.56
1:C:399:ALA:HA	1:C:403:LYS:HD3	1.88	0.56
1:B:131:THR:HG22	1:B:362:GLN:HE22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ALA:O	1:B:94:ILE:HA	2.06	0.56
1:B:30:THR:O	1:B:31:ALA:HB3	2.05	0.55
1:B:192:MET:HE2	1:B:192:MET:HA	1.89	0.55
1:C:33:SER:C	1:C:35:LEU:N	2.60	0.53
1:A:131:THR:HG22	1:A:362:GLN:HE22	1.74	0.53
1:D:87:HIS:H	1:D:87:HIS:CD2	2.25	0.53
1:A:98:ILE:HD13	5:A:665:HOH:O	2.09	0.53
1:D:421:ASP:OD1	1:D:421:ASP:C	2.47	0.52
1:D:347:ASP:OD1	1:D:348:ALA:N	2.43	0.52
1:A:12:PRO:O	1:A:12:PRO:CD	2.57	0.52
1:C:378:HIS:HA	1:C:421:ASP:HB2	1.92	0.52
1:B:423:VAL:HG12	1:B:427:LYS:HE2	1.91	0.52
1:D:152:LEU:HD11	1:D:184:CYS:HB2	1.91	0.52
1:D:369:HIS:CD2	1:D:416:PHE:HA	2.44	0.51
1:C:47:LEU:HD21	1:C:102:LEU:HD11	1.91	0.51
1:A:12:PRO:HD2	1:A:12:PRO:O	2.10	0.51
1:C:5:SER:HB2	1:C:83:ASN:OD1	2.10	0.51
1:C:378:HIS:H	1:C:381:GLN:HE21	1.57	0.51
1:D:385:VAL:O	1:D:389:ASN:ND2	2.43	0.51
1:B:399:ALA:HA	1:B:403:LYS:HD3	1.92	0.51
1:A:16:MET:HG3	1:A:103:PHE:HB3	1.93	0.51
1:B:74:GLU:HG3	1:C:349:TYR:CZ	2.46	0.51
1:A:399:ALA:O	1:A:406:GLY:HA3	2.12	0.50
1:C:335:MET:N	1:C:336:PRO:CD	2.75	0.50
1:B:365:PHE:CD1	1:B:392:ARG:HD3	2.47	0.50
1:C:237:MET:HG3	1:C:243:ARG:HA	1.94	0.50
1:D:89:PHE:HA	1:D:93:GLN:O	2.12	0.50
1:D:426:LYS:O	1:D:429:ASP:HB3	2.11	0.50
1:C:46:VAL:HG22	1:C:227:PRO:HG2	1.94	0.50
1:B:249:ARG:HD2	1:B:351:PHE:CZ	2.47	0.50
1:D:194:GLY:N	1:D:195:PRO:CD	2.74	0.49
1:B:412:ARG:O	1:B:413:HIS:ND1	2.46	0.49
1:B:127:ALA:O	1:B:131:THR:HG23	2.12	0.49
1:A:415:PRO:HB3	5:A:669:HOH:O	2.12	0.49
1:C:231:VAL:O	1:D:207:ARG:NH2	2.46	0.49
1:B:282:GLN:HG3	1:B:355:LEU:HD12	1.94	0.48
1:B:288:LEU:O	1:B:319:ILE:HA	2.13	0.48
1:C:406:GLY:O	1:C:410:ILE:HG12	2.14	0.48
1:B:74:GLU:HB2	1:C:349:TYR:CD1	2.49	0.48
1:B:276:HIS:CE1	1:B:278:GLU:CG	2.92	0.48
1:B:360:GLU:CD	1:B:360:GLU:N	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:THR:HB	1:D:195:PRO:HG3	1.95	0.47
1:D:188:GLY:O	1:D:192:MET:HB2	2.13	0.47
1:A:133:LEU:O	1:A:137:ILE:HG13	2.13	0.47
1:D:345:LYS:N	1:D:345:LYS:CD	2.77	0.47
1:D:45:ALA:HB3	1:D:222:ILE:HD13	1.96	0.47
1:D:249:ARG:HD3	1:D:352:ASN:O	2.14	0.47
1:A:243:ARG:HB3	5:A:653:HOH:O	2.15	0.47
1:B:74:GLU:HB2	1:C:349:TYR:CE1	2.50	0.47
1:A:301:LEU:O	1:A:305:ILE:HG12	2.15	0.47
1:C:87:HIS:CD2	5:C:671:HOH:O	2.68	0.46
1:B:180:GLU:HB3	1:B:208:TYR:CD1	2.50	0.46
1:C:101:HIS:HE1	1:C:228:ASN:O	1.96	0.46
1:D:217:THR:CG2	1:D:236:ILE:HD13	2.46	0.46
1:C:105:VAL:HG22	1:C:236:ILE:HD11	1.97	0.46
1:B:399:ALA:HA	1:B:403:LYS:CD	2.46	0.46
1:C:427:LYS:HE3	1:C:427:LYS:HB3	1.39	0.46
1:B:412:ARG:O	1:B:413:HIS:CG	2.69	0.46
1:B:378:HIS:HA	1:B:421:ASP:HB2	1.97	0.45
1:A:215:GLY:O	1:A:234:LEU:HD12	2.16	0.45
1:D:174:HIS:CE1	1:D:178:LEU:HD11	2.51	0.45
1:B:160:SER:HA	5:B:626:HOH:O	2.16	0.45
1:D:312:ALA:O	1:D:315:LYS:HG2	2.17	0.45
1:D:215:GLY:O	1:D:234:LEU:HD12	2.16	0.45
1:A:240:ILE:HA	1:A:240:ILE:HD13	1.87	0.45
1:B:434:ASP:O	1:B:435:PHE:C	2.55	0.45
1:A:177:GLY:HA2	1:A:203:HIS:CD2	2.52	0.44
1:D:194:GLY:N	1:D:195:PRO:HD3	2.31	0.44
1:D:394:PHE:O	1:D:398:VAL:HG23	2.17	0.44
1:C:90:VAL:N	1:C:93:GLN:O	2.41	0.44
1:C:131:THR:HG22	1:C:362:GLN:NE2	2.32	0.44
1:A:98:ILE:HG13	1:A:229:PRO:HB3	2.00	0.44
1:A:276:HIS:ND1	1:A:278:GLU:HB2	2.32	0.44
1:A:131:THR:HG22	1:A:362:GLN:NE2	2.33	0.44
1:D:390:LEU:O	1:D:391:ARG:C	2.56	0.44
1:B:185:THR:HG22	1:B:196:MET:CE	2.48	0.44
1:B:399:ALA:CB	1:B:403:LYS:HD3	2.47	0.43
1:D:421:ASP:OD1	1:D:423:VAL:CG2	2.65	0.43
1:B:87:HIS:H	1:B:87:HIS:CD2	2.33	0.43
1:A:101:HIS:HE1	1:A:228:ASN:O	2.00	0.43
1:D:40:ARG:NH1	1:D:66:PHE:O	2.49	0.43
1:A:288:LEU:HB3	1:A:298:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ILE:HG23	1:C:80:GLU:HG2	2.00	0.43
1:C:257:PHE:HB3	1:C:258:PRO:CD	2.49	0.43
1:C:35:LEU:HA	1:C:35:LEU:HD12	1.73	0.43
1:B:101:HIS:HE1	1:B:228:ASN:O	2.02	0.43
1:D:390:LEU:HD23	1:D:390:LEU:HA	1.82	0.43
1:C:154:VAL:HA	1:C:184:CYS:O	2.18	0.43
1:B:306:THR:O	1:B:310:GLY:HA2	2.19	0.43
1:D:145:ILE:HA	1:D:146:PRO:HD3	1.86	0.43
1:C:32:SER:C	1:C:34:ASP:N	2.71	0.42
1:C:360:GLU:OE1	1:C:360:GLU:HA	2.18	0.42
1:B:377:LEU:HA	1:B:377:LEU:HD23	1.85	0.42
1:A:342:ARG:HD2	1:A:348:ALA:O	2.19	0.42
1:B:421:ASP:HA	1:B:422:PRO:HD3	1.77	0.42
1:B:128:THR:O	1:B:132:ASN:ND2	2.52	0.42
1:D:128:THR:HG22	1:D:129:HIS:N	2.34	0.42
1:C:347:ASP:OD1	1:C:353:TRP:HB2	2.19	0.42
1:C:375:LEU:HD23	1:C:375:LEU:HA	1.86	0.42
1:B:366:GLU:HA	1:B:367:PRO:HD2	1.91	0.42
1:D:195:PRO:HD2	5:D:615:HOH:O	2.19	0.42
1:B:7:ILE:HA	1:B:81:LEU:O	2.19	0.42
1:C:71:MET:CE	1:C:80:GLU:HB2	2.49	0.41
1:A:73:ARG:HA	1:A:73:ARG:HD3	1.86	0.41
1:D:35:LEU:HD12	1:D:35:LEU:HA	1.73	0.41
1:A:343:LYS:HD3	1:A:349:TYR:OH	2.20	0.41
1:C:193:GLU:HG3	1:C:197:LYS:HE3	2.02	0.41
1:D:151:ASN:HB2	1:D:181:LEU:HD23	2.02	0.41
1:D:258:PRO:HA	1:D:297:TYR:CE2	2.55	0.41
1:A:347:ASP:OD1	1:A:353:TRP:HB2	2.20	0.41
1:A:268:LEU:CD1	1:A:394:PHE:CE2	3.04	0.41
1:A:268:LEU:CD1	1:A:394:PHE:HE2	2.33	0.41
1:A:407:ILE:O	1:A:410:ILE:N	2.54	0.41
1:B:268:LEU:HD13	1:B:390:LEU:HB3	2.03	0.41
1:C:377:LEU:HB3	1:C:424:LEU:HD23	2.03	0.41
1:C:356:LYS:HA	1:C:356:LYS:HD2	1.93	0.41
1:D:289:THR:HA	1:D:320:ALA:O	2.20	0.41
1:B:373:ALA:O	1:B:419:HIS:CE1	2.74	0.41
1:D:342:ARG:HD2	1:D:348:ALA:O	2.21	0.41
1:A:410:ILE:HD12	1:A:415:PRO:HA	2.02	0.41
1:D:73:ARG:HA	1:D:73:ARG:HD3	1.83	0.40
1:A:367:PRO:HG2	1:A:399:ALA:CB	2.51	0.40
1:A:399:ALA:O	1:A:403:LYS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLU:HA	1:D:347:ASP:O	2.21	0.40
1:B:180:GLU:HB3	1:B:208:TYR:CE1	2.56	0.40
1:A:126:ASN:C	1:A:126:ASN:HD22	2.25	0.40
1:A:431:LEU:O	1:A:434:ASP:HB2	2.22	0.40
1:B:156:TRP:CE3	1:B:266:GLU:HB3	2.56	0.40
1:A:181:LEU:HD23	1:A:181:LEU:HA	1.90	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	412/456 (90%)	397 (96%)	13 (3%)	2 (0%)	34 30
1	B	415/456 (91%)	387 (93%)	22 (5%)	6 (1%)	14 7
1	C	413/456 (91%)	384 (93%)	24 (6%)	5 (1%)	16 10
1	D	407/456 (89%)	376 (92%)	29 (7%)	2 (0%)	34 30
All	All	1647/1824 (90%)	1544 (94%)	88 (5%)	15 (1%)	21 15

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	126	ASN
1	B	162	ASN
1	B	411	GLU
1	C	31	ALA
1	C	34	ASP
1	C	284	MET
1	B	31	ALA
1	B	413	HIS
1	C	32	SER

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Mol	Chain	Res	Type
1	D	26	ARG
1	D	29	LYS
1	A	13	ALA
1	B	151	ASN
1	C	151	ASN
1	A	32	SER

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	322/385 (84%)	310 (96%)	12 (4%)	41	41
1	B	322/385 (84%)	308 (96%)	14 (4%)	35	34
1	C	322/385 (84%)	307 (95%)	15 (5%)	32	30
1	D	291/385 (76%)	268 (92%)	23 (8%)	15	11
All	All	1257/1540 (82%)	1193 (95%)	64 (5%)	30	26

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	MET
1	A	27	LEU
1	A	30	THR
1	A	38	LEU
1	A	126	ASN
1	A	131	THR
1	A	293	GLN
1	A	315	LYS
1	A	339	ARG
1	A	413	HIS
1	A	429	ASP
1	A	439	ASN
1	B	17	ASP
1	B	41	ASN
1	B	46	VAL

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Mol	Chain	Res	Type
1	B	87	HIS
1	B	131	THR
1	B	151	ASN
1	B	160	SER
1	B	161[A]	ILE
1	B	161[B]	ILE
1	B	220	SER
1	B	360	GLU
1	B	402	VAL
1	B	418	MET
1	B	429	ASP
1	C	11	SER
1	C	16	MET
1	C	24	VAL
1	C	33	SER
1	C	94	ILE
1	C	113	ASN
1	C	131	THR
1	C	149	THR
1	C	193	GLU
1	C	300	SER
1	C	337	LEU
1	C	385	VAL
1	C	427	LYS
1	C	430	GLN
1	C	439	ASN
1	D	11	SER
1	D	17	ASP
1	D	25	GLU
1	D	30	THR
1	D	38	LEU
1	D	46	VAL
1	D	93	GLN
1	D	112	VAL
1	D	126	ASN
1	D	131	THR
1	D	149	THR
1	D	160	SER
1	D	218	GLU
1	D	222	ILE
1	D	293	GLN
1	D	299	ARG

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Mol	Chain	Res	Type
1	D	300	SER
1	D	306	THR
1	D	365	PHE
1	D	418	MET
1	D	421	ASP
1	D	423	VAL
1	D	427	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	101	HIS
1	A	126	ASN
1	A	167	GLN
1	A	333	ASN
1	A	362	GLN
1	A	381	GLN
1	A	430	GLN
1	B	87	HIS
1	B	101	HIS
1	B	115	HIS
1	B	151	ASN
1	B	333	ASN
1	B	362	GLN
1	B	419	HIS
1	C	101	HIS
1	C	167	GLN
1	C	333	ASN
1	C	362	GLN
1	C	413	HIS
1	D	101	HIS
1	D	126	ASN
1	D	293	GLN
1	D	316	HIS

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)

5 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	501	-	4,4,4	1.16	1 (25%)	6,6,6	0.98	1 (16%)
3	PO4	B	501	-	4,4,4	0.51	0	6,6,6	0.28	0
3	PO4	C	501	-	4,4,4	0.36	0	6,6,6	0.32	0
3	PO4	D	501	-	4,4,4	0.42	0	6,6,6	0.33	0
4	PEG	D	502	-	6,6,6	0.56	0	5,5,5	0.58	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	501	-	-	0/0/0/0	0/0/0/0
3	PO4	B	501	-	-	0/0/0/0	0/0/0/0
3	PO4	C	501	-	-	0/0/0/0	0/0/0/0
3	PO4	D	501	-	-	0/0/0/0	0/0/0/0
4	PEG	D	502	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	SO4	O3-S	2.15	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	SO4	O2-S-O1	2.31	116.82	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	PO4	1	0
4	D	502	PEG	1	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	418/456 (91%)	-0.13	10 (2%)	62	68	15, 30, 56, 81	0
1	B	420/456 (92%)	-0.15	13 (3%)	52	61	15, 29, 67, 93	0
1	C	418/456 (91%)	0.03	25 (5%)	25	33	18, 33, 62, 87	0
1	D	413/456 (90%)	0.16	25 (6%)	25	33	20, 39, 72, 94	0
All	All	1669/1824 (91%)	-0.02	73 (4%)	38	47	15, 33, 67, 94	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	410	ILE	8.1
1	D	312	ALA	5.3
1	D	407	ILE	5.0
1	D	422	PRO	4.8
1	B	415	PRO	4.3
1	C	116	LEU	3.9
1	A	13	ALA	3.8
1	D	63	TYR	3.8
1	D	412	ARG	3.7
1	D	409	GLU	3.6
1	B	117	ALA	3.5
1	C	88	ALA	3.5
1	D	408	ARG	3.5
1	C	31	ALA	3.4
1	C	412	ARG	3.2
1	C	411	GLU	3.2
1	A	31	ALA	3.1
1	B	410	ILE	3.1
1	D	416	PHE	3.1
1	B	413	HIS	3.0
1	C	413	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	14	GLY	2.9
1	B	124	LEU	2.9
1	B	404	ALA	2.9
1	C	415	PRO	2.9
1	A	32	SER	2.9
1	C	62	LYS	2.9
1	D	214	LEU	2.8
1	A	415	PRO	2.8
1	C	30	THR	2.8
1	C	33	SER	2.7
1	A	244	LEU	2.7
1	C	407	ILE	2.6
1	D	127	ALA	2.6
1	C	32	SER	2.5
1	B	414	GLY	2.5
1	D	13	ALA	2.5
1	C	371	SER	2.5
1	C	89	PHE	2.4
1	B	380	ASN	2.4
1	C	414	GLY	2.4
1	B	407	ILE	2.4
1	C	14	GLY	2.4
1	D	423	VAL	2.4
1	A	404	ALA	2.4
1	C	247	PHE	2.4
1	D	128	THR	2.3
1	B	422	PRO	2.3
1	D	267	LEU	2.3
1	A	247	PHE	2.3
1	C	155	CYS	2.3
1	C	154	VAL	2.3
1	D	154	VAL	2.3
1	B	416	PHE	2.3
1	C	408	ARG	2.3
1	C	409	GLU	2.3
1	D	280	ALA	2.2
1	C	87	HIS	2.2
1	D	406	GLY	2.2
1	B	412	ARG	2.2
1	D	33	SER	2.2
1	C	280	ALA	2.2
1	D	369	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	373	ALA	2.1
1	A	419	HIS	2.1
1	D	400	GLY	2.1
1	A	61	ASP	2.1
1	D	419	HIS	2.1
1	B	154	VAL	2.1
1	C	404	ALA	2.0
1	D	437	ALA	2.0
1	D	216	LEU	2.0
1	C	270	ILE	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	501	5/5	0.96	0.10	-0.46	31,37,39,44	0
3	PO4	D	501	5/5	0.97	0.10	-1.28	33,36,46,46	0
3	PO4	B	501	5/5	0.97	0.06	-2.03	32,32,35,38	0
3	PO4	C	501	5/5	0.97	0.07	-2.13	32,35,38,42	0
4	PEG	D	502	7/7	0.73	0.17	-	58,65,73,76	0

6.5 Other polymers (i)

There are no such residues in this entry.