W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:08 PM GMT

PDB ID	:	4KNH
Title	:	Structure of the Chaetomium thermophilum adaptor nucleoporin Nup192 N-terminal domain
Authors	:	Stuwe, T.; Lin, D.H.; Collins, L.N.; Hoelz, A.
Deposited on	:	2013-05-09
Resolution	:	2.70 Å(reported)

The following versions of software and data (see references ⓘ) 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 2.70 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.
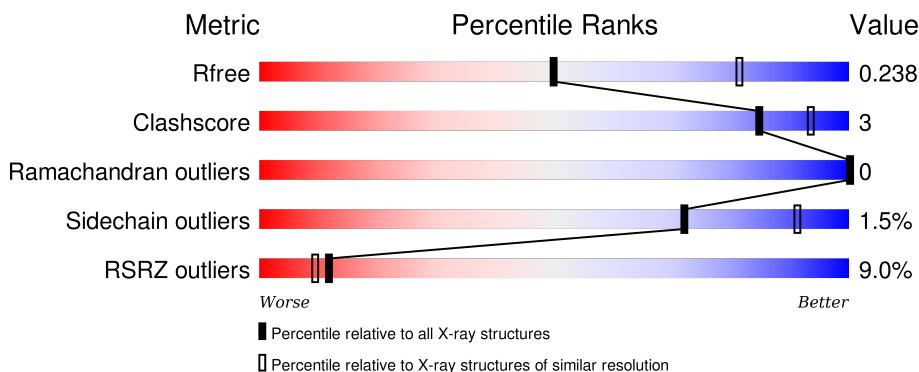
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	961	11% 86% 9% 5%
1	B	961	6% 83% 6% 11%
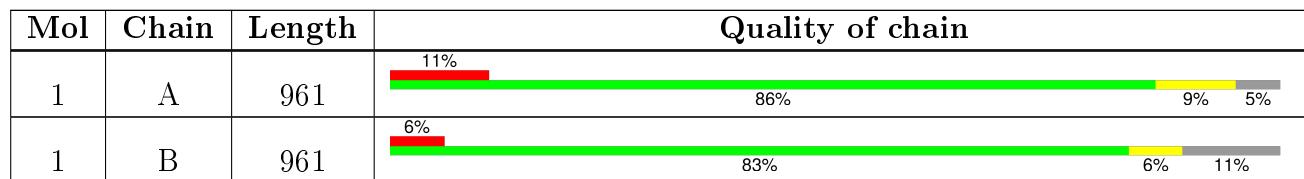
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	1001	-	-	-	X
3	EDO	A	1002	-	-	-	X
3	EDO	A	1003	-	-	-	X
3	EDO	A	1005	-	-	-	X
3	EDO	A	1006	-	-	-	X
3	EDO	A	1008	-	-	-	X
3	EDO	A	1009	-	-	-	X
3	EDO	B	1003	-	-	-	X
3	EDO	B	1004	-	-	-	X
3	EDO	B	1006	-	-	-	X
3	EDO	B	1007	-	-	-	X
3	EDO	B	1008	-	-	-	X
3	EDO	B	1009	-	-	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 28868 atoms, of which 14245 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 Nup192p.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	914	Total 14660	C 4670	H 7309	N 1259	O 1377	S 45	0	5	0
1	B	857	Total 13738	C 4393	H 6840	N 1165	O 1298	S 42	0	4	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP G0ZGU6
A	-1	PRO	-	EXPRESSION TAG	UNP G0ZGU6
A	0	HIS	-	EXPRESSION TAG	UNP G0ZGU6
B	-2	GLY	-	EXPRESSION TAG	UNP G0ZGU6
B	-1	PRO	-	EXPRESSION TAG	UNP G0ZGU6
B	0	HIS	-	EXPRESSION TAG	UNP G0ZGU6

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
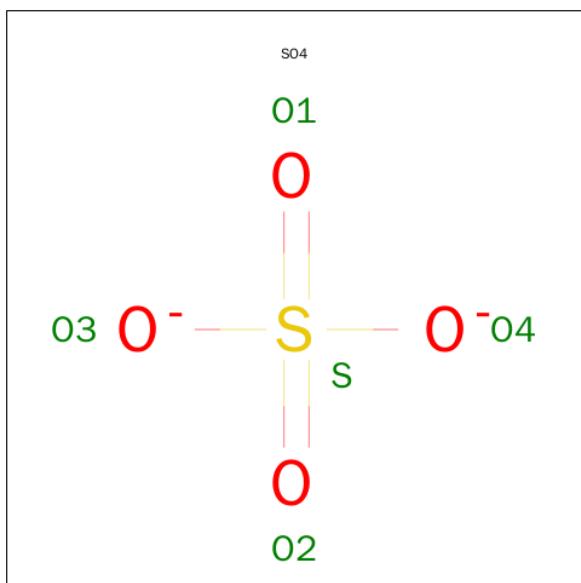
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
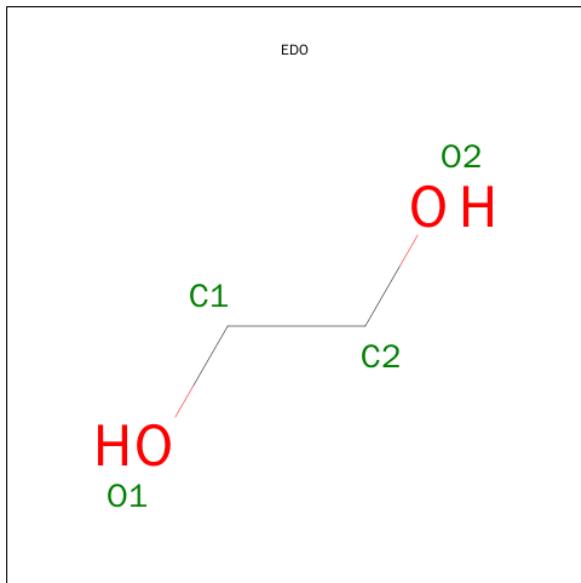
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 10	C 2	H 6	O 2	0	0
3	A	1	Total 10	C 2	H 6	O 2	0	0
3	A	1	Total 10	C 2	H 6	O 2	0	0
3	A	1	Total 10	C 2	H 6	O 2	0	0
3	A	1	Total 10	C 2	H 6	O 2	0	0
3	A	1	Total 10	C 2	H 6	O 2	0	0
3	A	1	Total 10	C 2	H 6	O 2	0	0
3	A	1	Total 10	C 2	H 6	O 2	0	0
3	B	1	Total 10	C 2	H 6	O 2	0	0
3	B	1	Total 10	C 2	H 6	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 10	C 2	H 6	O 2	0	0
3	B	1	Total 10	C 2	H 6	O 2	0	0
3	B	1	Total 10	C 2	H 6	O 2	0	0
3	B	1	Total 10	C 2	H 6	O 2	0	0
3	B	1	Total 10	C 2	H 6	O 2	0	0
3	B	1	Total 10	C 2	H 6	O 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	132	Total 132	O 132	0	0
5	B	165	Total 167	O 167	0	2

3 Residue-property plots ⓘ

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: Nup192p

- Molecule 1: Nup192p
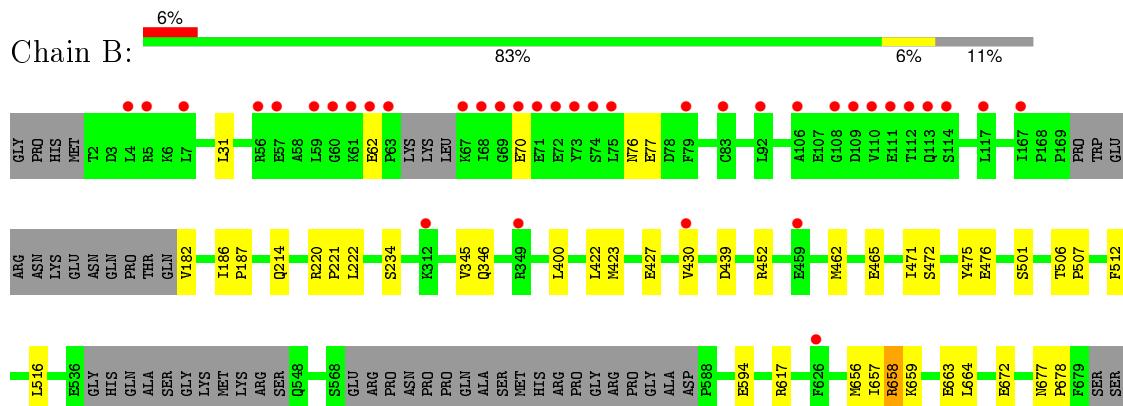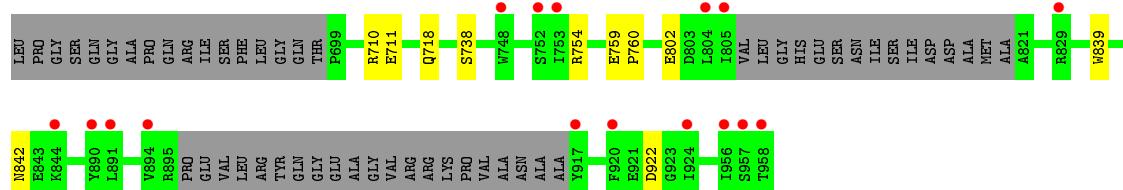
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	102.87Å 102.87Å 443.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.77 – 2.70 48.77 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.77-2.70) 100.0 (48.77-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.192 , 0.231 0.202 , 0.238	Depositor DCC
R_{free} test set	3390 reflections (5.37%)	DCC
Wilson B-factor (Å²)	74.7	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.36 , 47.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 66567 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	28868	wwPDB-VP
Average B, all atoms (Å²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, EDO

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	0.22	0/7527	0.37	0/10189
1	B	0.22	0/7054	0.36	0/9545
All	All	0.22	0/14581	0.37	0/19734

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	A	7351	7309	7268	55	0
1	B	6898	6840	6806	28	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	32	48	48	0	0
3	B	32	48	48	0	0
4	B	1	0	0	0	0
5	A	132	0	0	2	0
5	B	167	0	0	1	0
All	All	14623	14245	14170	82	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 3.

All (82) 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:452:ARG:NH2	1:B:594:GLU:OE2	2.23	0.71
1:A:77:GLU:N	1:A:77:GLU:OE2	2.30	0.65
1:B:76:ASN:OD1	1:B:77:GLU:N	2.32	0.62
1:A:617:ARG:NH2	1:A:663:GLU:OE1	2.32	0.62
1:B:711:GLU:O	1:B:718:GLN:NE2	2.34	0.60
1:A:289:THR:HA	1:A:293:SER:HB2	1.85	0.56
1:A:634:LYS:HG2	1:A:674:TRP:CH2	2.39	0.56
1:A:604:ARG:NH2	5:A:1103:HOH:O	2.38	0.56
1:A:437:LEU:N	1:A:438:PRO:HD3	2.22	0.55
1:B:182:VAL:O	1:B:182:VAL:HG12	2.06	0.55
1:A:538:HIS:CD2	1:A:542:GLY:HA2	2.42	0.54
1:A:759:GLU:N	1:A:760:PRO:CD	2.72	0.53
1:B:501:SER:HB3	1:B:512:PHE:CZ	2.43	0.53
1:A:554:GLN:NE2	5:A:1199:HOH:O	2.43	0.52
1:B:617:ARG:NH2	1:B:663:GLU:OE1	2.41	0.51
1:B:186:ILE:HB	1:B:187:PRO:HD3	1.93	0.51
1:B:617:ARG:NE	1:B:658:ARG:O	2.44	0.51
1:A:672:GLU:OE2	1:A:754:ARG:NH2	2.43	0.50
1:A:743:VAL:HG22	1:A:745:PHE:CE1	2.47	0.50
1:A:895:ARG:N	1:A:896:PRO:HD2	2.27	0.50
1:A:289:THR:O	1:A:293:SER:HB2	2.12	0.49
1:B:738:SER:OG	1:B:802:GLU:OE2	2.22	0.49
1:A:2:THR:HG23	1:A:3:ASP:N	2.28	0.49
1:B:657:ILE:HD12	1:B:658:ARG:N	2.28	0.49
1:A:300:LEU:HA	1:A:303:ALA:HB3	1.94	0.48
1:A:468:LEU:HB3	1:A:515:MET:HE2	1.95	0.48
1:A:52:ASP:OD1	1:A:53:THR:N	2.47	0.48
1:B:220:ARG:HG2	1:B:221:PRO:HD2	1.96	0.47
1:A:75:LEU:CD2	1:A:79:PHE:CD1	2.97	0.47
1:B:506:THR:HB	1:B:507:PRO:HD3	1.96	0.47
1:A:614:GLU:OE2	1:A:617:ARG:NH1	2.48	0.47
1:B:672:GLU:OE2	1:B:754:ARG:NH1	2.48	0.47
1:B:759:GLU:N	1:B:760:PRO:CD	2.78	0.47
1:B:472:SER:O	1:B:476:GLU:HB2	2.14	0.47
1:A:908:ARG:O	1:A:909:ARG:C	2.53	0.47
1:B:214:GLN:HG3	1:B:222:LEU:HD23	1.95	0.47
1:A:149:ASP:OD1	1:A:151:GLY:N	2.48	0.46
1:A:300:LEU:HD22	1:A:339:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:THR:HB	1:A:507:PRO:HD3	1.97	0.46
1:A:214:GLN:HG3	1:A:222:LEU:CD2	2.46	0.46
1:A:300:LEU:HD23	1:A:300:LEU:N	2.31	0.46
1:B:439:ASP:N	1:B:439:ASP:OD1	2.48	0.45
1:A:743:VAL:CG2	1:A:745:PHE:CE1	3.00	0.45
1:A:611:THR:O	1:A:658:ARG:NH2	2.50	0.45
1:A:59:LEU:HG	1:A:80:VAL:HG23	1.97	0.45
1:A:659:LYS:CE	1:A:731:VAL:O	2.66	0.44
1:B:214:GLN:HG3	1:B:222:LEU:CD2	2.47	0.44
1:A:839:TRP:CZ2	1:A:912:VAL:HG11	2.53	0.44
1:A:818:ALA:HB1	1:A:821:ALA:HB2	1.98	0.44
1:A:212:MET:HG2	1:B:400:LEU:O	2.17	0.44
1:A:329:ARG:NH2	1:A:370:GLU:OE2	2.50	0.44
1:B:594:GLU:HB2	5:B:1111:HOH:O	2.16	0.44
1:B:839:TRP:O	1:B:842:ASN:HB3	2.18	0.44
1:B:31:LEU:HD23	1:B:31:LEU:C	2.38	0.44
1:A:397:ARG:NH2	1:A:473:TYR:CD1	2.86	0.43
1:B:677:ASN:N	1:B:678:PRO:CD	2.81	0.43
1:B:422:LEU:HD12	1:B:423:MET:HE2	1.99	0.43
1:A:399:TRP:CD2	1:A:400:LEU:HD12	2.53	0.43
1:A:909:ARG:O	1:A:910:LYS:C	2.57	0.43
1:A:66:LEU:HD23	1:A:102:ILE:HD11	2.01	0.43
1:A:468:LEU:HD22	1:A:515:MET:CE	2.48	0.43
1:A:214:GLN:HG3	1:A:222:LEU:HD23	2.00	0.43
1:B:656:MET:CE	1:B:664:LEU:HD13	2.50	0.42
1:A:618:LYS:O	1:A:622:MET:HG2	2.20	0.42
1:B:430:VAL:HG11	1:B:471:ILE:HG12	2.01	0.42
1:A:75:LEU:HD22	1:A:79:PHE:CD1	2.55	0.41
1:A:759:GLU:OE2	1:A:909:ARG:NH2	2.54	0.41
1:A:743:VAL:HG22	1:A:744:PRO:HD2	2.02	0.41
1:A:659:LYS:HE2	1:A:731:VAL:O	2.21	0.41
1:A:506:THR:HG23	1:A:598:MET:HE3	2.01	0.41
1:A:472:SER:O	1:A:476:GLU:HB2	2.21	0.41
1:A:293:SER:CB	1:A:294:PRO:HD2	2.51	0.41
1:A:759:GLU:OE2	1:A:909:ARG:CZ	2.68	0.41
1:A:281:ILE:HB	1:A:282:PRO:HD3	2.03	0.41
1:A:99:ARG:HD2	1:A:99:ARG:C	2.41	0.41
1:A:622:MET:CG	1:A:622:MET:O	2.70	0.40
1:A:517:ARG:HG2	1:A:608:LYS:HG3	2.03	0.40
1:A:427:GLU:HG3	1:A:475:TYR:CZ	2.57	0.40
1:B:462:MET:SD	1:B:465:GLU:HG3	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:PRO:HA	1:A:339:PHE:CE1	2.57	0.40
1:A:634:LYS:CG	1:A:674:TRP:CH2	3.05	0.40
1:B:427:GLU:HG3	1:B:475:TYR:CZ	2.57	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	911/961 (95%)	868 (95%)	43 (5%)	0	100	100
1	B	845/961 (88%)	820 (97%)	25 (3%)	0	100	100
All	All	1756/1922 (91%)	1688 (96%)	68 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	802/835 (96%)	788 (98%)	14 (2%)	68	90
1	B	756/835 (90%)	746 (99%)	10 (1%)	76	92
All	All	1558/1670 (93%)	1534 (98%)	24 (2%)	72	91

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	68	ILE
1	A	220[A]	ARG
1	A	220[B]	ARG
1	A	293	SER
1	A	343	ASP
1	A	487	GLU
1	A	536	GLU
1	A	541	SER
1	A	558	GLU
1	A	702	GLN
1	A	740	ASN
1	A	815	ILE
1	A	909	ARG
1	B	62	GLU
1	B	70	GLU
1	B	234	SER
1	B	345	VAL
1	B	346	GLN
1	B	516	LEU
1	B	658	ARG
1	B	659	LYS
1	B	710	ARG
1	B	922	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	346	GLN
1	A	425	HIS
1	B	113	GLN
1	B	275	HIS
1	B	677	ASN
1	B	887	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	SO4	A	1001	-	4,4,4	0.24	0	6,6,6	0.08	0
3	EDO	A	1002	-	3,3,3	0.47	0	2,2,2	0.34	0
3	EDO	A	1003	-	3,3,3	0.48	0	2,2,2	0.37	0
3	EDO	A	1004	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	A	1005	-	3,3,3	0.49	0	2,2,2	0.38	0
3	EDO	A	1006	-	3,3,3	0.47	0	2,2,2	0.32	0
3	EDO	A	1007	-	3,3,3	0.47	0	2,2,2	0.39	0
3	EDO	A	1008	-	3,3,3	0.45	0	2,2,2	0.42	0
3	EDO	A	1009	-	3,3,3	0.49	0	2,2,2	0.35	0
2	SO4	B	1001	-	4,4,4	0.22	0	6,6,6	0.09	0
3	EDO	B	1002	-	3,3,3	0.47	0	2,2,2	0.40	0
3	EDO	B	1003	-	3,3,3	0.45	0	2,2,2	0.42	0
3	EDO	B	1004	-	3,3,3	0.46	0	2,2,2	0.41	0
3	EDO	B	1005	-	3,3,3	0.46	0	2,2,2	0.40	0
3	EDO	B	1006	-	3,3,3	0.48	0	2,2,2	0.37	0
3	EDO	B	1007	-	3,3,3	0.48	0	2,2,2	0.37	0
3	EDO	B	1008	-	3,3,3	0.47	0	2,2,2	0.38	0
3	EDO	B	1009	-	3,3,3	0.50	0	2,2,2	0.30	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

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no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
3	EDO	A	1002	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1003	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1004	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1005	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1006	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1007	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1008	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1009	-	-	0/1/1/1	0/0/0/0
2	SO4	B	1001	-	-	0/0/0/0	0/0/0/0
3	EDO	B	1002	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1003	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1004	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1005	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1006	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1007	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1008	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1009	-	-	0/1/1/1	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.

No monomer is involved in short contacts.

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, 95th 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(Å²)	Q<0.9
1	A	914/961 (95%)	0.89	106 (11%)	6	5	35, 67, 134, 204	0
1	B	857/961 (89%)	0.64	53 (6%)	24	23	34, 59, 110, 170	0
All	All	1771/1922 (92%)	0.77	159 (8%)	12	9	34, 63, 124, 204	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	756	LEU	14.8
1	A	344	THR	9.4
1	A	540	ALA	8.9
1	A	59	LEU	8.5
1	A	539	GLN	8.2
1	A	349	ARG	8.1
1	A	812	ASN	7.9
1	A	345	VAL	7.9
1	A	908	ARG	7.6
1	A	351	ILE	7.5
1	A	544	MET	7.4
1	A	757	GLY	7.3
1	A	348	LEU	6.8
1	B	75	LEU	6.7
1	A	904	GLU	6.6
1	A	543	LYS	5.8
1	B	110	VAL	5.6
1	A	350	GLY	5.6
1	A	173	ARG	5.4
1	B	68	ILE	5.4
1	A	907	VAL	5.4
1	A	346	GLN	5.3
1	A	542	GLY	5.1
1	A	815	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	66	LEU	5.1
1	A	905	ALA	5.0
1	B	73	TYR	5.0
1	A	901	TYR	4.9
1	A	75	LEU	4.9
1	A	80	VAL	4.9
1	A	906	GLY	4.9
1	A	538	HIS	4.7
1	A	541	SER	4.6
1	B	59	LEU	4.5
1	B	459	GLU	4.5
1	B	63	PRO	4.4
1	A	813	ILE	4.4
1	B	67	LYS	4.4
1	B	958	THR	4.3
1	A	814	SER	4.3
1	B	60	GLY	4.3
1	B	748	TRP	4.2
1	A	61	LYS	4.2
1	B	753	ILE	4.1
1	B	72	GLU	4.1
1	B	894	VAL	3.9
1	A	755	THR	3.9
1	A	824	LEU	3.8
1	B	61	LYS	3.8
1	A	65	LYS	3.8
1	B	74	SER	3.7
1	A	816	ASP	3.7
1	A	301	GLN	3.7
1	B	626	PHE	3.7
1	B	109	ASP	3.7
1	B	70	GLU	3.6
1	A	909	ARG	3.6
1	A	674	TRP	3.6
1	A	341	LEU	3.6
1	B	56	ARG	3.6
1	B	917	TYR	3.5
1	A	347	ASP	3.5
1	B	108	GLY	3.4
1	A	79	PHE	3.4
1	A	830	LEU	3.4
1	B	111	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	58	ALA	3.4
1	B	891	LEU	3.4
1	A	295	GLU	3.3
1	B	79	PHE	3.3
1	A	902	GLN	3.3
1	A	64	LYS	3.3
1	A	57	GLU	3.2
1	A	297	MET	3.2
1	A	537	GLY	3.2
1	B	62	GLU	3.2
1	B	114	SER	3.2
1	A	810	GLU	3.2
1	A	302	GLN	3.1
1	A	411	PRO	3.1
1	A	912	VAL	3.1
1	B	4	LEU	3.1
1	A	809	HIS	3.1
1	A	46	ILE	3.0
1	A	536	GLU	3.0
1	A	312	LYS	3.0
1	A	84	LEU	2.9
1	A	306	LEU	2.9
1	B	117	LEU	2.8
1	A	73	TYR	2.8
1	B	924	ILE	2.8
1	A	313	GLY	2.8
1	A	389[A]	GLN	2.8
1	B	113	GLN	2.7
1	A	63	PRO	2.7
1	A	305	ARG	2.7
1	A	109	ASP	2.7
1	B	167	ILE	2.6
1	A	337	ASN	2.6
1	A	737	ASN	2.6
1	B	7	LEU	2.6
1	B	844	LYS	2.6
1	A	516	LEU	2.6
1	B	57	GLU	2.6
1	B	69	GLY	2.6
1	B	5	ARG	2.6
1	A	749	LEU	2.6
1	A	353	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	115	ARG	2.5
1	A	758	ILE	2.5
1	B	920	PHE	2.5
1	A	828	VAL	2.5
1	A	391	PRO	2.4
1	B	890	TYR	2.4
1	A	83	CYS	2.4
1	B	83	CYS	2.4
1	A	60	GLY	2.4
1	B	752	SER	2.4
1	A	753	ILE	2.4
1	B	430	VAL	2.4
1	A	298	GLY	2.3
1	A	825	ALA	2.3
1	A	260	PHE	2.3
1	A	497	LEU	2.3
1	A	118	TRP	2.3
1	B	829	ARG	2.3
1	A	62	GLU	2.3
1	A	303	ALA	2.3
1	A	591	ILE	2.3
1	A	924	ILE	2.3
1	A	257	ILE	2.3
1	B	112	THR	2.2
1	A	222	LEU	2.2
1	A	940	LEU	2.2
1	B	92	LEU	2.2
1	A	74	SER	2.2
1	B	71	GLU	2.2
1	A	620	LEU	2.2
1	B	805	ILE	2.2
1	A	412	PHE	2.2
1	A	111	GLU	2.2
1	A	242	LEU	2.2
1	A	317	ASP	2.1
1	A	68	ILE	2.1
1	A	77	GLU	2.1
1	B	106	ALA	2.1
1	A	808	GLY	2.1
1	A	568	SER	2.1
1	A	102	ILE	2.1
1	B	349	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	748	TRP	2.1
1	A	232	ARG	2.1
1	B	956	ILE	2.1
1	A	898	VAL	2.0
1	B	312	LYS	2.0
1	B	957	SER	2.0
1	A	829	ARG	2.0
1	A	557	LYS	2.0
1	B	804	LEU	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, 95th 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
3	EDO	B	1009	4/4	0.71	0.61	8.36	64,77,90,90	0
3	EDO	A	1003	4/4	0.71	0.45	8.07	47,63,76,76	0
3	EDO	B	1003	4/4	0.96	0.39	6.99	45,54,66,72	0
3	EDO	A	1008	4/4	0.83	0.60	6.57	80,96,104,104	0
2	SO4	B	1001	5/5	0.90	0.42	6.03	85,88,96,100	0
3	EDO	B	1006	4/4	0.83	0.35	5.45	60,72,80,80	0
3	EDO	B	1007	4/4	0.76	0.34	4.10	60,75,90,90	0
3	EDO	B	1004	4/4	0.85	0.39	3.83	60,75,81,93	0
3	EDO	A	1005	4/4	0.77	0.31	3.77	77,92,102,102	0
3	EDO	A	1009	4/4	0.15	0.47	3.28	88,105,113,114	0
3	EDO	A	1002	4/4	0.92	0.27	2.44	55,66,69,69	0
3	EDO	B	1008	4/4	0.88	0.39	2.38	81,97,101,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
3	EDO	A	1006	4/4	0.62	0.40	2.14	65,78,82,88	0
3	EDO	A	1004	4/4	0.90	0.32	1.15	61,74,84,88	0
3	EDO	B	1002	4/4	0.84	0.23	0.87	48,60,74,74	0
3	EDO	B	1005	4/4	0.91	0.22	0.29	52,62,70,70	0
2	SO4	A	1001	5/5	0.92	0.23	0.09	108,112,115,119	0
3	EDO	A	1007	4/4	0.86	0.23	-0.09	63,75,80,85	0
4	MG	B	1010	1/1	0.93	0.24	-	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.