



Full wwPDB X-ray Structure Validation Report i

Feb 19, 2024 – 11:30 AM EST

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)

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 types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) i) 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 : 2.36
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) : 2.36

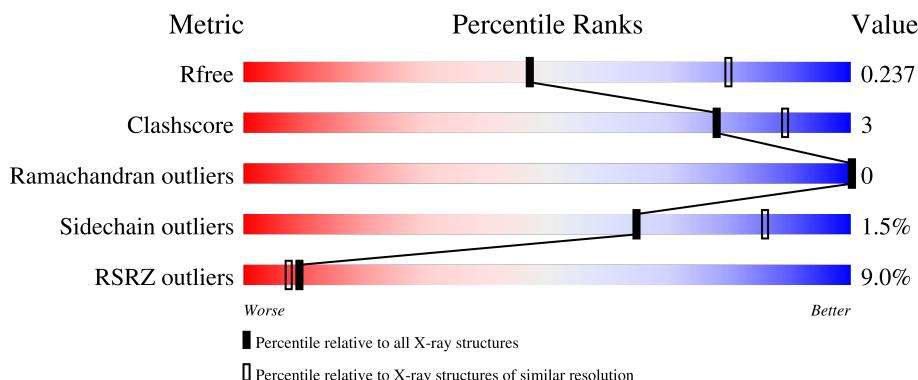
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

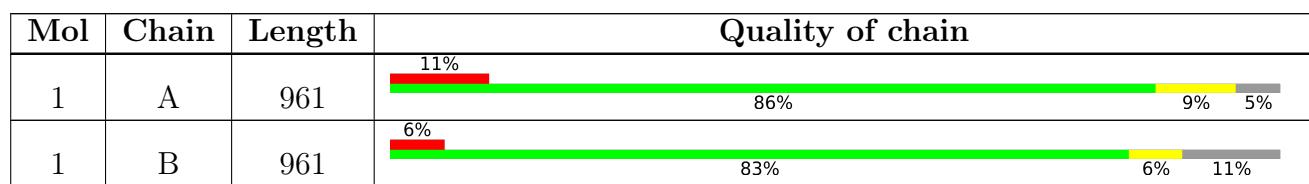
The reported resolution of this entry is 2.70 Å.

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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.



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
3	EDO	A	1003	-	-	-	X
3	EDO	A	1006	-	-	-	X
3	EDO	A	1009	-	-	-	X
3	EDO	B	1009	-	-	-	X

2 Entry composition [\(i\)](#)

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.

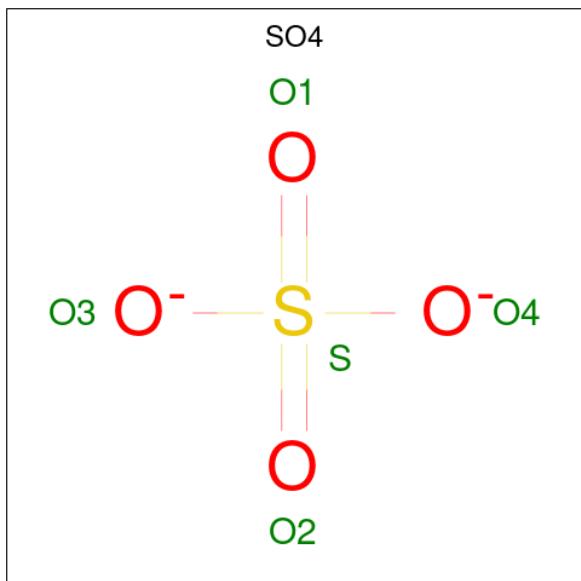
- Molecule 1 is a protein called Nup192p.

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

There are 6 discrepancies between the modelled and reference sequences:

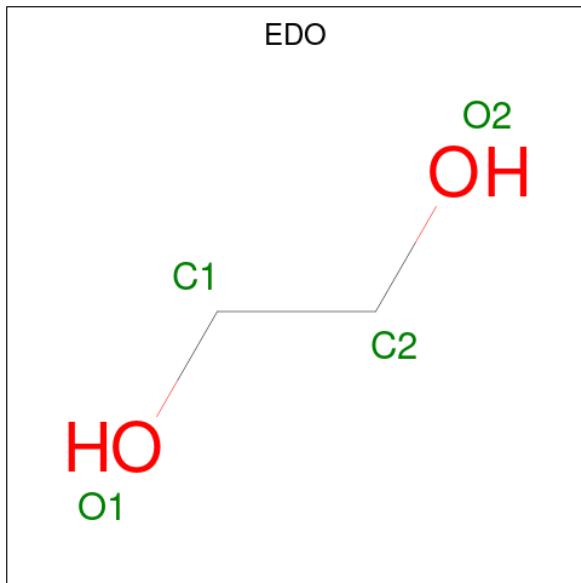
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP G0ZGU6
A	-1	PRO	-	expression tag	UNP G0ZGU6
A	0	HIS	-	expression tag	UNP G0ZGU6
B	-2	GLY	-	expression tag	UNP G0ZGU6
B	-1	PRO	-	expression tag	UNP G0ZGU6
B	0	HIS	-	expression tag	UNP G0ZGU6

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

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

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

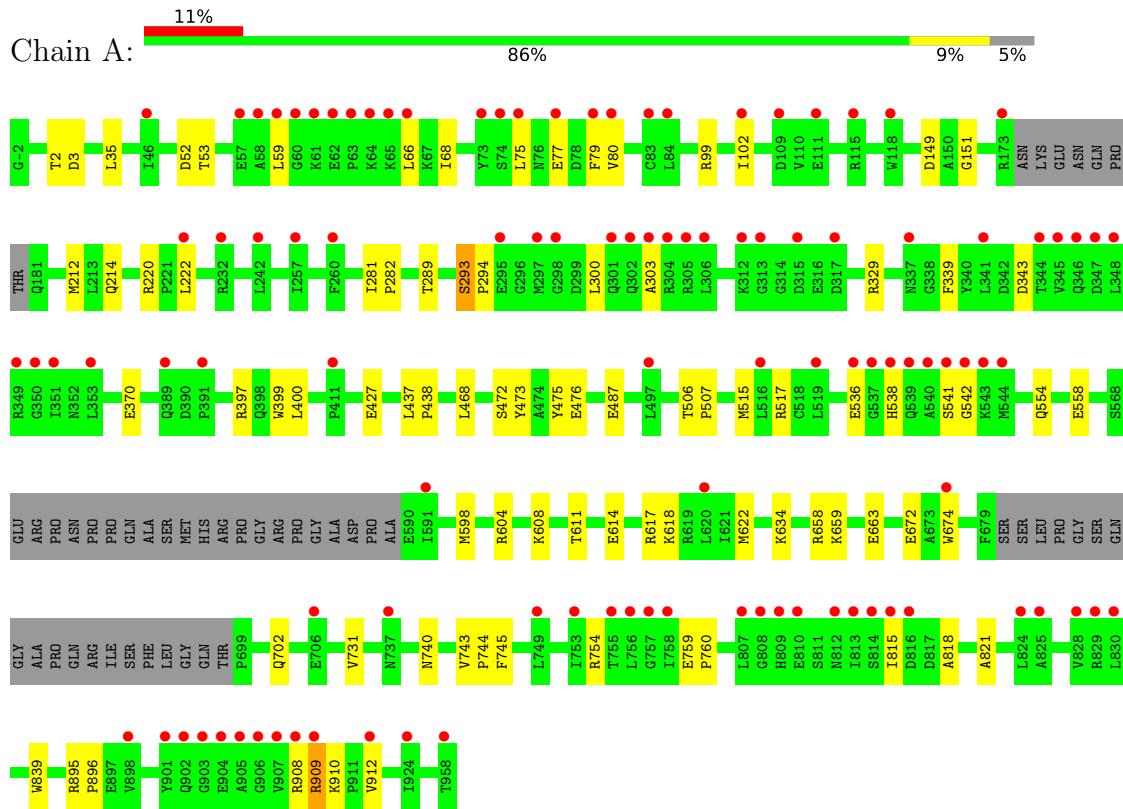
- Molecule 5 is water.

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

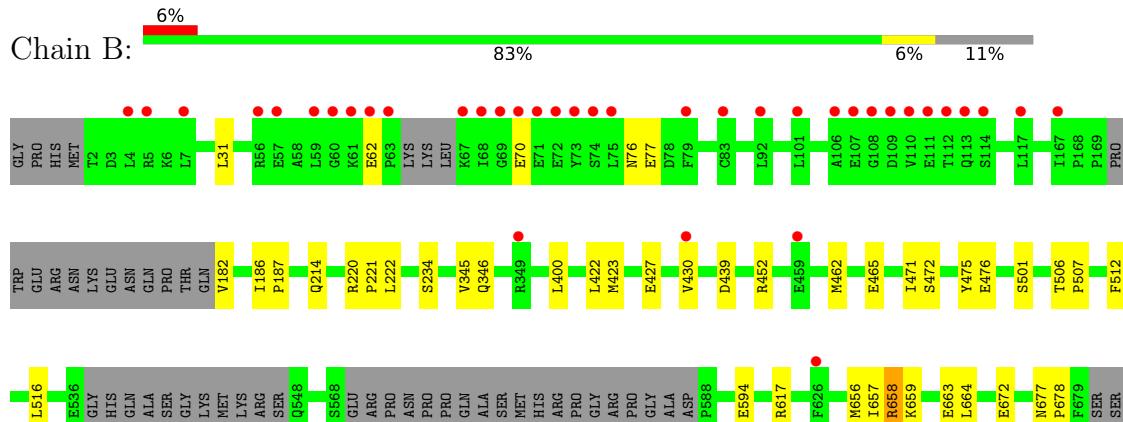
3 Residue-property plots

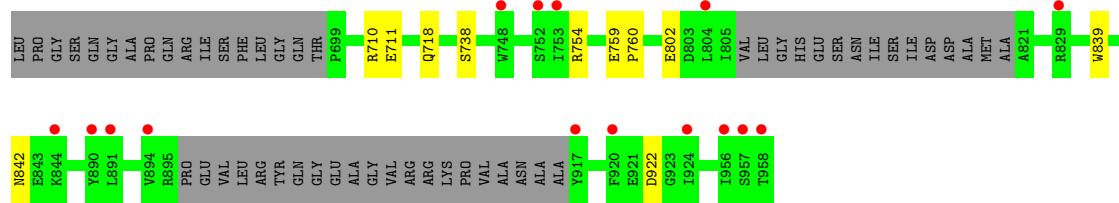
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 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
$\langle I/\sigma(I) \rangle^1$	2.95 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R , R_{free}	0.192 , 0.231 0.199 , 0.237	Depositor DCC
R_{free} test set	3390 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	74.7	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28868	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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, EDO, 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	0.22	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:HG12	1:B:182:VAL:O	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:472:SER:O	1:B:476:GLU:HB2	2.14	0.47
1:B:759:GLU:N	1:B:760:PRO:CD	2.78	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:A:839:TRP:CZ2	1:A:912:VAL:HG11	2.53	0.44
1:B:214:GLN:HG3	1:B:222:LEU:CD2	2.47	0.44
1:A:212:MET:HG2	1:B:400:LEU:O	2.17	0.44
1:A:818:ALA:HB1	1:A:821:ALA:HB2	1.98	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:C	1:B:31:LEU:HD23	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:66:LEU:HD23	1:A:102:ILE:HD11	2.01	0.43
1:A:909:ARG:O	1:A:910:LYS:C	2.57	0.43
1:A:214:GLN:HG3	1:A:222:LEU:HD23	2.00	0.43
1:A:468:LEU:HD22	1:A:515:MET:CE	2.48	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:659:LYS:HE2	1:A:731:VAL:O	2.21	0.41
1:A:743:VAL:HG22	1:A:744:PRO:HD2	2.02	0.41
1:A:472:SER:O	1:A:476:GLU:HB2	2.21	0.41
1:A:506:THR:HG23	1:A:598:MET:HE3	2.01	0.41
1:A:99:ARG:C	1:A:99:ARG:HD2	2.41	0.41
1:A:281:ILE:HB	1:A:282:PRO:HD3	2.03	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:517:ARG:HG2	1:A:608:LYS:HG3	2.03	0.40
1:A:622:MET:CG	1:A:622:MET:O	2.70	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%)	60 84
1	B	756/835 (90%)	746 (99%)	10 (1%)	69 87
All	All	1558/1670 (93%)	1534 (98%)	24 (2%)	65 86

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

Sometimes 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 monosaccharides 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
3	EDO	A	1005	-	3,3,3	0.48	0	2,2,2	0.29	0
3	EDO	B	1002	-	3,3,3	0.46	0	2,2,2	0.31	0
2	SO4	B	1001	-	4,4,4	0.14	0	6,6,6	0.05	0
3	EDO	B	1003	-	3,3,3	0.44	0	2,2,2	0.33	0
3	EDO	B	1004	-	3,3,3	0.45	0	2,2,2	0.32	0
3	EDO	A	1009	-	3,3,3	0.48	0	2,2,2	0.27	0
3	EDO	A	1002	-	3,3,3	0.46	0	2,2,2	0.25	0
3	EDO	A	1006	-	3,3,3	0.46	0	2,2,2	0.23	0
3	EDO	A	1008	-	3,3,3	0.44	0	2,2,2	0.33	0
3	EDO	B	1006	-	3,3,3	0.47	0	2,2,2	0.28	0
2	SO4	A	1001	-	4,4,4	0.14	0	6,6,6	0.05	0
3	EDO	A	1003	-	3,3,3	0.47	0	2,2,2	0.29	0
3	EDO	A	1004	-	3,3,3	0.42	0	2,2,2	0.29	0
3	EDO	B	1005	-	3,3,3	0.44	0	2,2,2	0.31	0
3	EDO	B	1009	-	3,3,3	0.49	0	2,2,2	0.22	0
3	EDO	A	1007	-	3,3,3	0.45	0	2,2,2	0.30	0
3	EDO	B	1008	-	3,3,3	0.46	0	2,2,2	0.30	0
3	EDO	B	1007	-	3,3,3	0.47	0	2,2,2	0.28	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
3	EDO	A	1005	-	-	0/1/1/1	-
3	EDO	B	1002	-	-	0/1/1/1	-
3	EDO	B	1003	-	-	1/1/1/1	-
3	EDO	B	1004	-	-	0/1/1/1	-
3	EDO	A	1009	-	-	0/1/1/1	-
3	EDO	A	1002	-	-	0/1/1/1	-
3	EDO	A	1006	-	-	1/1/1/1	-
3	EDO	A	1008	-	-	0/1/1/1	-
3	EDO	B	1006	-	-	0/1/1/1	-
3	EDO	A	1003	-	-	0/1/1/1	-
3	EDO	A	1004	-	-	0/1/1/1	-
3	EDO	B	1005	-	-	0/1/1/1	-
3	EDO	B	1009	-	-	0/1/1/1	-
3	EDO	A	1007	-	-	0/1/1/1	-
3	EDO	B	1008	-	-	0/1/1/1	-
3	EDO	B	1007	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1003	EDO	O1-C1-C2-O2
3	A	1006	EDO	O1-C1-C2-O2

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(Å ²)	Q<0.9
1	A	914/961 (95%)	0.88	107 (11%) 4 3	35, 67, 134, 204	0
1	B	857/961 (89%)	0.62	53 (6%) 20 19	34, 59, 110, 170	0
All	All	1771/1922 (92%)	0.75	160 (9%) 9 7	34, 63, 124, 204	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	756	LEU	14.8
1	A	344	THR	10.3
1	A	540	ALA	9.2
1	A	59	LEU	8.9
1	A	812	ASN	8.1
1	A	539	GLN	8.0
1	A	351	ILE	8.0
1	A	349	ARG	8.0
1	A	345	VAL	7.9
1	A	544	MET	7.7
1	A	757	GLY	7.2
1	A	348	LEU	7.1
1	A	908	ARG	7.1
1	B	75	LEU	6.8
1	A	543	LYS	6.2
1	B	110	VAL	6.2
1	A	904	GLU	6.0
1	A	907	VAL	5.9
1	A	350	GLY	5.7
1	A	346	GLN	5.6
1	A	542	GLY	5.4
1	A	815	ILE	5.2
1	A	905	ALA	5.1
1	A	906	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	68	ILE	5.1
1	A	901	TYR	5.0
1	A	66	LEU	5.0
1	B	73	TYR	4.9
1	A	75	LEU	4.8
1	B	958	THR	4.7
1	A	80	VAL	4.7
1	A	813	ILE	4.6
1	A	173	ARG	4.5
1	A	541	SER	4.4
1	B	63	PRO	4.4
1	B	59	LEU	4.4
1	B	459	GLU	4.3
1	B	753	ILE	4.3
1	A	538	HIS	4.3
1	B	60	GLY	4.2
1	A	824	LEU	4.2
1	B	67	LYS	4.2
1	B	748	TRP	4.1
1	A	814	SER	4.1
1	A	755	THR	4.1
1	A	830	LEU	4.0
1	B	894	VAL	4.0
1	B	108	GLY	3.9
1	A	61	LYS	3.9
1	B	61	LYS	3.9
1	B	72	GLU	3.8
1	A	301	GLN	3.8
1	A	341	LEU	3.7
1	B	917	TYR	3.7
1	A	816	ASP	3.7
1	B	109	ASP	3.6
1	B	56	ARG	3.5
1	B	626	PHE	3.5
1	B	111	GLU	3.5
1	A	909	ARG	3.5
1	A	674	TRP	3.5
1	B	891	LEU	3.5
1	B	4	LEU	3.5
1	A	79	PHE	3.4
1	B	70	GLU	3.4
1	A	347	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	79	PHE	3.3
1	B	74	SER	3.3
1	A	58	ALA	3.3
1	A	64	LYS	3.3
1	A	295	GLU	3.3
1	A	537	GLY	3.2
1	A	57	GLU	3.2
1	A	302	GLN	3.2
1	A	810	GLU	3.1
1	B	62	GLU	3.1
1	A	46	ILE	3.1
1	B	114	SER	3.1
1	A	65	LYS	3.0
1	A	809	HIS	3.0
1	B	924	ILE	3.0
1	A	902	GLN	2.9
1	A	306	LEU	2.9
1	A	758	ILE	2.9
1	B	113	GLN	2.9
1	A	305	ARG	2.9
1	A	84	LEU	2.9
1	A	912	VAL	2.9
1	A	109	ASP	2.9
1	A	297	MET	2.9
1	B	117	LEU	2.8
1	A	353	LEU	2.8
1	A	313	GLY	2.7
1	B	69	GLY	2.7
1	A	389[A]	GLN	2.7
1	A	411	PRO	2.7
1	B	7	LEU	2.7
1	B	5	ARG	2.7
1	A	737	ASN	2.7
1	A	73	TYR	2.7
1	A	312	LYS	2.7
1	A	516	LEU	2.6
1	A	749	LEU	2.6
1	A	115	ARG	2.6
1	A	825	ALA	2.6
1	A	337	ASN	2.6
1	B	957	SER	2.5
1	A	753	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	106	ALA	2.5
1	B	844	LYS	2.5
1	B	890	TYR	2.5
1	A	536	GLU	2.5
1	A	303	ALA	2.5
1	A	63	PRO	2.5
1	B	57	GLU	2.5
1	B	167	ILE	2.5
1	A	620	LEU	2.5
1	A	74	SER	2.4
1	B	107	GLU	2.4
1	A	828	VAL	2.4
1	B	920	PHE	2.4
1	A	118	TRP	2.4
1	A	298	GLY	2.4
1	A	497	LEU	2.3
1	B	71	GLU	2.3
1	A	391	PRO	2.3
1	A	62	GLU	2.3
1	B	829	ARG	2.3
1	A	257	ILE	2.3
1	A	924	ILE	2.3
1	B	430	VAL	2.3
1	A	829	ARG	2.3
1	A	222	LEU	2.3
1	B	752	SER	2.2
1	A	102	ILE	2.2
1	B	83	CYS	2.2
1	A	317	ASP	2.2
1	A	77	GLU	2.2
1	A	111	GLU	2.2
1	A	260	PHE	2.2
1	A	591	ILE	2.2
1	B	101	LEU	2.2
1	A	898	VAL	2.2
1	B	112	THR	2.2
1	A	808	GLY	2.1
1	A	903	GLY	2.1
1	A	83	CYS	2.1
1	A	232	ARG	2.1
1	A	304	ARG	2.1
1	B	92	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	315	ASP	2.1
1	A	242	LEU	2.1
1	A	519	LEU	2.1
1	B	349	ARG	2.1
1	A	706	GLU	2.1
1	A	60	GLY	2.1
1	B	956	ILE	2.0
1	A	807	LEU	2.0
1	A	958	THR	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 monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å ²)	Q<0.9
3	EDO	A	1009	4/4	0.10	0.48	88,105,113,114	0
3	EDO	A	1006	4/4	0.59	0.41	65,78,82,88	0
3	EDO	A	1003	4/4	0.69	0.45	47,63,76,76	0
3	EDO	B	1009	4/4	0.69	0.58	64,77,90,90	0
3	EDO	B	1007	4/4	0.77	0.32	60,75,90,90	0
3	EDO	A	1005	4/4	0.77	0.32	77,92,102,102	0
3	EDO	B	1006	4/4	0.83	0.35	60,72,80,80	0
3	EDO	A	1007	4/4	0.83	0.25	63,75,80,85	0
3	EDO	B	1004	4/4	0.83	0.42	60,75,81,93	0
3	EDO	A	1008	4/4	0.84	0.58	80,96,104,104	0
3	EDO	B	1002	4/4	0.85	0.23	48,60,74,74	0
3	EDO	B	1008	4/4	0.90	0.37	81,97,101,102	0
3	EDO	A	1004	4/4	0.91	0.30	61,74,84,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	1001	5/5	0.92	0.23	108,112,115,119	0
3	EDO	B	1005	4/4	0.92	0.21	52,62,70,70	0
2	SO4	B	1001	5/5	0.92	0.41	85,88,96,100	0
3	EDO	A	1002	4/4	0.93	0.27	55,66,69,69	0
4	MG	B	1010	1/1	0.94	0.24	65,65,65,65	0
3	EDO	B	1003	4/4	0.96	0.36	45,54,66,72	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.