



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:19 PM UTC

PDB ID : 8PEH / pdb_00008peh
Title : Crystal structure of Lotus japonicus SYMRK kinase domain D738N
Authors : Noergaard, M.M.M.; Gysel, K.; Hansen, S.B.; Andersen, K.R.
Deposited on : 2023-06-14
Resolution : 1.95 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

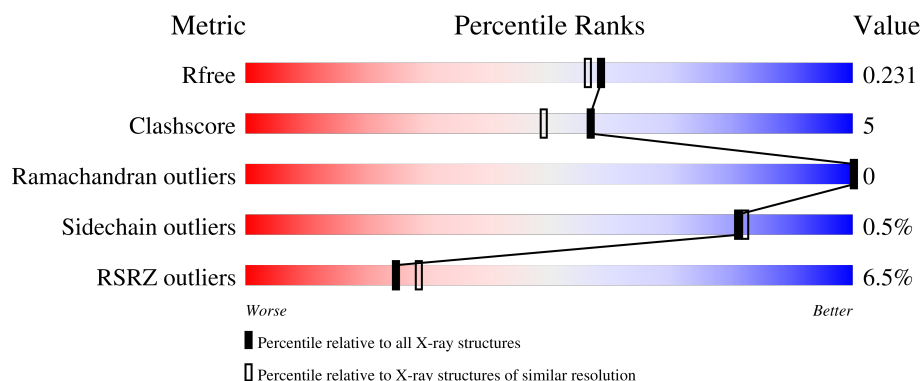
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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.

Mol	Chain	Length	Quality of chain
1	A	300	4% 84% 9% 6%
1	B	300	11% 84% 12% ..
1	C	300	4% 89% 7% .

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	903	-	-	X	-
2	SO4	B	908	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7477 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.

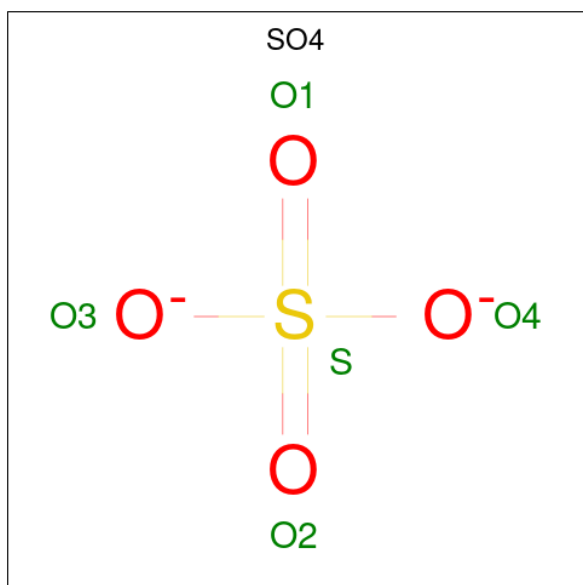
- Molecule 1 is a protein called Receptor-like kinase SYMRK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	290	Total	C	N	O	S	0	4	0
			2327	1477	400	442	8			
1	C	287	Total	C	N	O	S	0	1	0
			2282	1453	389	432	8			
1	A	282	Total	C	N	O	S	0	2	0
			2246	1427	385	426	8			

There are 3 discrepancies between the modelled and reference sequences:

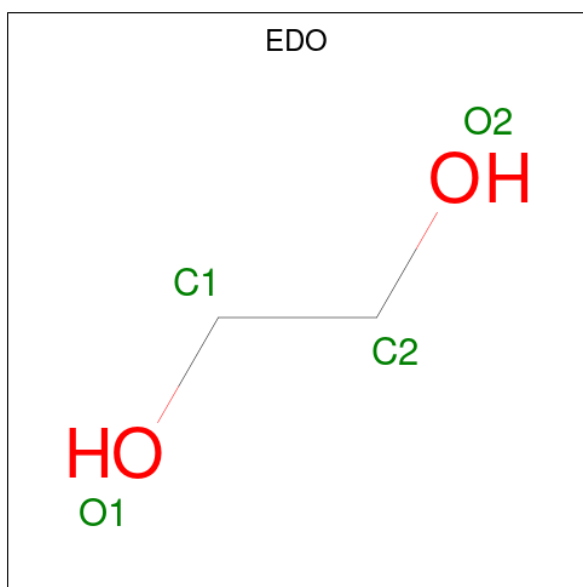
Chain	Residue	Modelled	Actual	Comment	Reference
B	738	ASN	ASP	engineered mutation	UNP Q8LKX1
C	738	ASN	ASP	engineered mutation	UNP Q8LKX1
A	738	ASN	ASP	engineered mutation	UNP Q8LKX1

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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	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	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

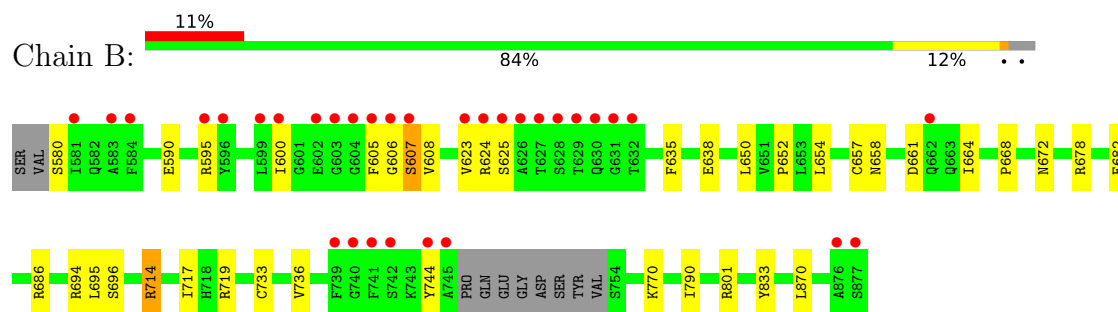
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	170	Total O 170 170	0	0
4	C	162	Total O 162 162	0	0
4	A	179	Total O 179 179	0	0

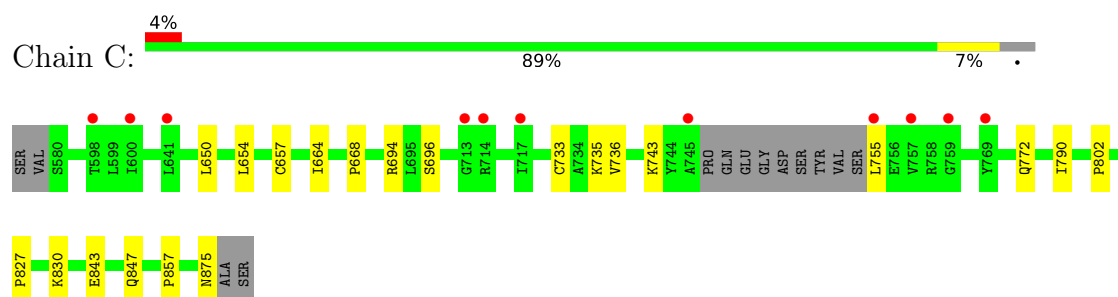
3 Residue-property plots [i](#)

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.

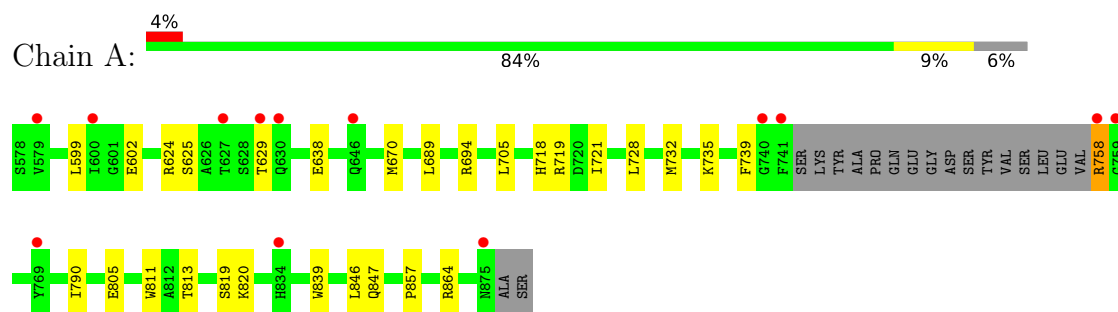
• Molecule 1: Receptor-like kinase SYMRK



• Molecule 1: Receptor-like kinase SYMRK



• Molecule 1: Receptor-like kinase SYMRK



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.87Å 77.96Å 101.40Å 90.00° 90.15° 90.00°	Depositor
Resolution (Å)	41.59 – 1.95 41.59 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.4 (41.59-1.95) 97.4 (41.59-1.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.195 , 0.231 0.195 , 0.231	Depositor DCC
R_{free} test set	3738 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.599	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7477	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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: EDO, SO4, CME

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	0.28	0/2284	0.45	0/3094
1	B	0.29	0/2366	0.44	0/3201
1	C	0.27	0/2318	0.44	0/3140
All	All	0.28	0/6968	0.44	0/9435

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	2246	0	2227	22	0
1	B	2327	0	2310	28	0
1	C	2282	0	2265	14	0
2	A	20	0	0	0	0
2	B	40	0	0	4	0
2	C	15	0	0	0	0
3	A	8	0	12	1	0
3	B	8	0	12	1	0
3	C	20	0	30	1	0
4	A	179	0	0	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	170	0	0	4	1
4	C	162	0	0	2	0
All	All	7477	0	6856	64	1

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 (64) 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:606:GLY:HA2	1:B:625:SER:HB2	1.75	0.68
1:B:682:GLU:OE1	1:B:686:ARG:NH1	2.26	0.68
1:A:689:LEU:HD11	1:A:732:MET:HE2	1.76	0.66
1:B:624:ARG:NH1	1:B:661:ASP:O	2.29	0.64
1:A:719:ARG:NH2	4:A:1003:HOH:O	2.32	0.63
1:A:624:ARG:NH2	1:A:638:GLU:OE2	2.31	0.60
1:C:650:LEU:HD23	1:C:736:VAL:HB	1.84	0.59
1:C:654:LEU:HG	1:C:668:PRO:HD3	1.84	0.58
1:A:758:ARG:HA	1:A:758:ARG:NH1	2.20	0.56
1:B:657:CYS:HB3	1:B:664:ILE:HB	1.88	0.56
1:C:802:PRO:HB3	3:C:906:EDO:H22	1.87	0.56
1:A:599:LEU:HD21	1:A:602:GLU:HG3	1.87	0.55
1:A:805:GLU:HG2	1:A:811:TRP:CD1	2.42	0.55
1:B:833:TYR:OH	4:B:1002:HOH:O	2.19	0.54
1:A:670:MET:HE1	1:A:735:LYS:HD2	1.90	0.54
1:B:686:ARG:NH2	2:B:908:SO4:O2	2.39	0.54
1:C:694:ARG:HB3	1:C:790:ILE:HG23	1.91	0.52
1:A:813:THR:HG23	1:A:846:LEU:HD21	1.93	0.49
1:B:694:ARG:HB3	1:B:790:ILE:HG23	1.95	0.49
1:B:714:ARG:HD2	1:B:744:TYR:HB3	1.94	0.49
1:A:819:SER:HA	1:A:839:TRP:CH2	2.47	0.49
1:B:650:LEU:HD23	1:B:736:VAL:HB	1.95	0.48
1:A:820:LYS:NZ	4:A:1011:HOH:O	2.45	0.48
1:B:580:SER:N	4:B:1014:HOH:O	2.46	0.48
1:C:735:LYS:NZ	4:C:1006:HOH:O	2.47	0.47
1:A:735:LYS:HE3	4:A:1072:HOH:O	2.14	0.47
1:A:728:LEU:HD13	1:A:732:MET:HE1	1.97	0.47
1:B:719:ARG:NH2	2:B:903:SO4:O1	2.38	0.46
1:C:743:LYS:HB3	1:C:743:LYS:HE3	1.75	0.46
1:A:694:ARG:HB3	1:A:790:ILE:HG23	1.97	0.46
1:B:654:LEU:HD21	1:B:668:PRO:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:672:ASN:OD1	1:B:678:ARG:NH2	2.49	0.45
1:B:606:GLY:CA	1:B:625:SER:HB2	2.44	0.45
1:A:847[B]:GLN:HG2	1:A:857:PRO:HD3	1.99	0.45
1:A:625:SER:O	1:A:629:THR:HG23	2.17	0.45
1:C:847:GLN:HG2	1:C:857:PRO:HD3	1.99	0.44
1:B:695:LEU:HD21	1:B:870:LEU:HA	1.98	0.44
1:A:718:HIS:CD2	1:A:739:PHE:HB3	2.51	0.44
1:A:624:ARG:HH22	1:A:638:GLU:CD	2.24	0.44
1:B:600:ILE:HB	1:B:608:VAL:HG13	2.00	0.44
1:C:694:ARG:HB3	1:C:790:ILE:CG2	2.47	0.44
1:A:819:SER:HA	1:A:839:TRP:HH2	1.83	0.44
1:A:864:ARG:HH22	3:A:905:EDO:C2	2.30	0.44
1:B:605:PHE:O	1:B:625:SER:N	2.50	0.43
1:C:827:PRO:HA	1:C:830:LYS:HG3	2.00	0.43
1:A:694:ARG:HB3	1:A:790:ILE:CG2	2.48	0.43
1:B:717:ILE:HG22	1:B:719:ARG:HG3	2.00	0.43
1:C:755[A]:LEU:HD13	1:C:772:GLN:HB3	2.01	0.43
1:A:721:ILE:HD13	1:A:721:ILE:HA	1.81	0.43
1:C:875:ASN:OD1	4:C:1001:HOH:O	2.21	0.42
1:A:705:LEU:HD23	1:A:705:LEU:HA	1.93	0.42
1:B:696:SER:OG	1:B:733:CME:HZ3	2.20	0.42
1:B:770[B]:LYS:HE2	3:B:909:EDO:H11	2.01	0.42
1:B:719:ARG:NH2	2:B:903:SO4:O3	2.52	0.41
1:C:657:CYS:HB3	1:C:664:ILE:HB	2.03	0.41
1:B:590:GLU:OE2	1:B:595:ARG:NH1	2.52	0.41
1:B:652:PRO:O	1:B:668:PRO:HD3	2.20	0.41
1:B:801:ARG:NH1	4:B:1001:HOH:O	2.18	0.41
1:B:638:GLU:HB3	4:B:1054:HOH:O	2.21	0.41
1:C:755[B]:LEU:HD13	1:C:772:GLN:HB3	2.01	0.41
1:B:607:SER:O	1:B:623:VAL:HG22	2.21	0.41
1:B:635:PHE:HD2	1:B:658:ASN:HD22	1.68	0.41
1:C:696:SER:OG	1:C:733:CME:OH	2.25	0.41
1:B:686:ARG:NH2	2:B:908:SO4:S	2.91	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1039:HOH:O	4:A:1061:HOH:O[4_456]	2.19	0.01

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	279/300 (93%)	273 (98%)	6 (2%)	0	100	100
1	B	289/300 (96%)	281 (97%)	8 (3%)	0	100	100
1	C	282/300 (94%)	274 (97%)	8 (3%)	0	100	100
All	All	850/900 (94%)	828 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	242/255 (95%)	241 (100%)	1 (0%)	84	85
1	B	250/255 (98%)	248 (99%)	2 (1%)	73	74
1	C	245/255 (96%)	244 (100%)	1 (0%)	84	85
All	All	737/765 (96%)	733 (100%)	4 (0%)	81	82

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	607	SER
1	B	714	ARG
1	C	843	GLU
1	A	758	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	617	GLN
1	A	663	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CME	A	733	1	8,9,10	0.95	0	6,9,11	0.95	0
1	CME	C	733	1	8,9,10	0.94	0	6,9,11	0.89	0
1	CME	B	733	1	8,9,10	0.94	0	6,9,11	0.66	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
1	CME	A	733	1	-	0/5/8/10	-
1	CME	C	733	1	-	2/5/8/10	-
1	CME	B	733	1	-	0/5/8/10	-

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
1	C	733	CME	CZ-CE-SD-SG
1	C	733	CME	CA-CB-SG-SD

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	733	CME	1	0
1	B	733	CME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
3	EDO	A	906	-	3,3,3	0.44	0	2,2,2	0.40	0
2	SO4	A	902	-	4,4,4	0.23	0	6,6,6	0.08	0
3	EDO	C	905	-	3,3,3	0.42	0	2,2,2	0.40	0
3	EDO	A	905	-	3,3,3	0.42	0	2,2,2	0.51	0
2	SO4	B	905	-	4,4,4	0.23	0	6,6,6	0.19	0
3	EDO	C	908	-	3,3,3	0.47	0	2,2,2	0.38	0
3	EDO	C	904	-	3,3,3	0.36	0	2,2,2	0.57	0
2	SO4	B	908	-	4,4,4	0.23	0	6,6,6	0.10	0
2	SO4	A	903	-	4,4,4	0.24	0	6,6,6	0.17	0
2	SO4	B	904	-	4,4,4	0.23	0	6,6,6	0.24	0
3	EDO	C	906	-	3,3,3	0.39	0	2,2,2	0.60	0
2	SO4	A	904	-	4,4,4	0.30	0	6,6,6	0.14	0
2	SO4	B	907	-	4,4,4	0.17	0	6,6,6	0.29	0
3	EDO	B	910	-	3,3,3	0.41	0	2,2,2	0.45	0
2	SO4	B	901	-	4,4,4	0.25	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	909	-	3,3,3	0.39	0	2,2,2	0.49	0
2	SO4	C	901	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	B	903	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	C	903	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	A	901	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	B	906	-	4,4,4	0.24	0	6,6,6	0.10	0
3	EDO	C	907	-	3,3,3	0.44	0	2,2,2	0.43	0
2	SO4	B	902	-	4,4,4	0.26	0	6,6,6	0.09	0
2	SO4	C	902	-	4,4,4	0.23	0	6,6,6	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	906	-	-	0/1/1/1	-
3	EDO	C	905	-	-	0/1/1/1	-
3	EDO	B	910	-	-	0/1/1/1	-
3	EDO	C	907	-	-	1/1/1/1	-
3	EDO	B	909	-	-	1/1/1/1	-
3	EDO	A	905	-	-	1/1/1/1	-
3	EDO	C	908	-	-	0/1/1/1	-
3	EDO	C	904	-	-	1/1/1/1	-
3	EDO	C	906	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	904	EDO	O1-C1-C2-O2
3	B	909	EDO	O1-C1-C2-O2
3	C	906	EDO	O1-C1-C2-O2
3	C	907	EDO	O1-C1-C2-O2
3	A	905	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	905	EDO	1	0
2	B	908	SO4	2	0
3	C	906	EDO	1	0
3	B	909	EDO	1	0
2	B	903	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, 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	281/300 (93%)	0.33	13 (4%)	37	43	19, 43, 73, 120	2 (0%)
1	B	289/300 (96%)	0.60	32 (11%)	10	12	19, 42, 89, 126	4 (1%)
1	C	286/300 (95%)	0.39	11 (3%)	44	50	26, 44, 76, 103	1 (0%)
All	All	856/900 (95%)	0.44	56 (6%)	25	28	19, 43, 83, 126	7 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	741	PHE	5.7
1	B	629	THR	5.6
1	B	605	PHE	5.3
1	B	583	ALA	4.9
1	B	627	THR	4.9
1	B	604	GLY	4.4
1	B	628	SER	4.2
1	B	624	ARG	4.2
1	C	755[A]	LEU	4.0
1	B	741	PHE	4.0
1	C	757	VAL	3.8
1	B	626	ALA	3.8
1	B	745	ALA	3.8
1	A	630	GLN	3.5
1	A	579	VAL	3.5
1	B	600	ILE	3.4
1	B	606	GLY	3.3
1	B	739	PHE	3.2
1	B	623	VAL	3.2
1	B	599	LEU	3.1
1	C	600	ILE	2.9
1	A	646[A]	GLN	2.9
1	B	602	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	877	SER	2.8
1	C	759	GLY	2.8
1	A	875	ASN	2.8
1	B	625	SER	2.7
1	B	630	GLN	2.7
1	B	876	ALA	2.7
1	A	769	TYR	2.7
1	C	713	GLY	2.7
1	A	740	GLY	2.7
1	C	598	THR	2.7
1	B	603	GLY	2.6
1	B	584	PHE	2.6
1	C	745	ALA	2.6
1	B	581	ILE	2.6
1	A	627	THR	2.6
1	A	759	GLY	2.5
1	A	629	THR	2.5
1	B	740	GLY	2.5
1	B	632	THR	2.5
1	C	769	TYR	2.4
1	A	758	ARG	2.3
1	A	600	ILE	2.3
1	B	742	SER	2.2
1	A	834	HIS	2.2
1	C	717	ILE	2.2
1	B	662	GLN	2.1
1	B	631	GLY	2.1
1	C	641	LEU	2.1
1	B	744	TYR	2.1
1	C	714	ARG	2.1
1	B	595	ARG	2.1
1	B	607	SER	2.0
1	B	596	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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($\text{\AA}^2$)	Q<0.9
1	CME	C	733	10/11	0.81	0.14	41,46,70,71	10
1	CME	A	733	10/11	0.85	0.16	42,50,70,103	0
1	CME	B	733	10/11	0.91	0.12	40,50,66,68	3

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	SO4	B	901	5/5	0.59	0.13	82,84,98,105	5
2	SO4	B	906	5/5	0.66	0.11	67,82,108,110	0
2	SO4	A	902	5/5	0.67	0.10	91,91,126,136	0
3	EDO	A	906	4/4	0.68	0.18	59,60,61,63	0
3	EDO	C	907	4/4	0.70	0.17	53,55,59,70	0
3	EDO	A	905	4/4	0.74	0.15	51,58,60,61	0
3	EDO	B	910	4/4	0.74	0.15	58,60,60,67	0
2	SO4	C	901	5/5	0.75	0.09	97,100,110,114	0
3	EDO	B	909	4/4	0.75	0.16	52,57,57,58	0
2	SO4	A	901	5/5	0.76	0.09	93,95,112,112	0
2	SO4	B	902	5/5	0.78	0.14	49,55,61,65	5
3	EDO	C	906	4/4	0.82	0.13	60,61,62,63	0
3	EDO	C	908	4/4	0.83	0.13	47,55,60,60	0
2	SO4	B	908	5/5	0.83	0.09	96,99,110,111	0
2	SO4	B	905	5/5	0.83	0.12	74,75,85,88	0
2	SO4	A	903	5/5	0.85	0.10	55,66,72,91	0
2	SO4	A	904	5/5	0.85	0.10	54,55,84,88	0
2	SO4	B	903	5/5	0.85	0.13	51,57,62,66	5
3	EDO	C	905	4/4	0.87	0.14	56,58,61,68	0
3	EDO	C	904	4/4	0.87	0.12	58,62,65,66	0
2	SO4	B	907	5/5	0.90	0.17	29,31,37,43	5
2	SO4	C	903	5/5	0.91	0.08	58,61,69,81	0
2	SO4	B	904	5/5	0.94	0.09	39,41,46,55	5
2	SO4	C	902	5/5	0.97	0.13	39,42,46,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.