



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:53 AM UTC

PDB ID : 5AK6 / pdb_00005ak6
Title : ligand complex structure of soluble epoxide hydrolase
Authors : Oster, L.; Tapani, S.; Xue, Y.; Kack, H.
Deposited on : 2015-03-02
Resolution : 2.15 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

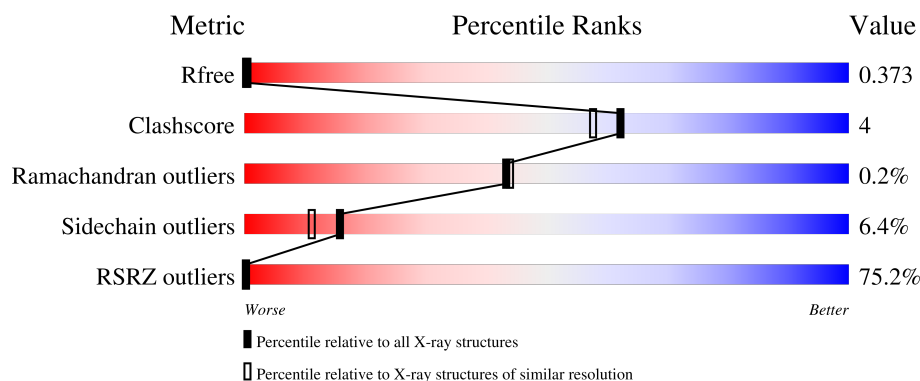
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	549	74% 81% 15% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4683 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 BIFUNCTIONAL EPOXIDE HYDROLASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	541	4286	2748	722	780	36	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P34913

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



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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

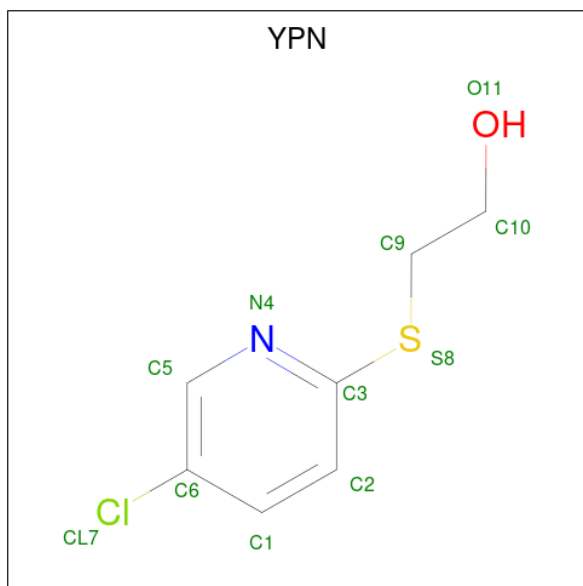
- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2-[(5-CHLORO-2-PYRIDYL)SULFANYL]ETHANOL (CCD ID: YPN)

(formula: C₇H₈ClNOS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	S	
			11	7	1	1	1	1	0
5	A	1	Total	C	Cl	N	O	S	
			11	7	1	1	1	1	0
5	A	1	Total	C	Cl	N	O	S	
			11	7	1	1	1	1	0

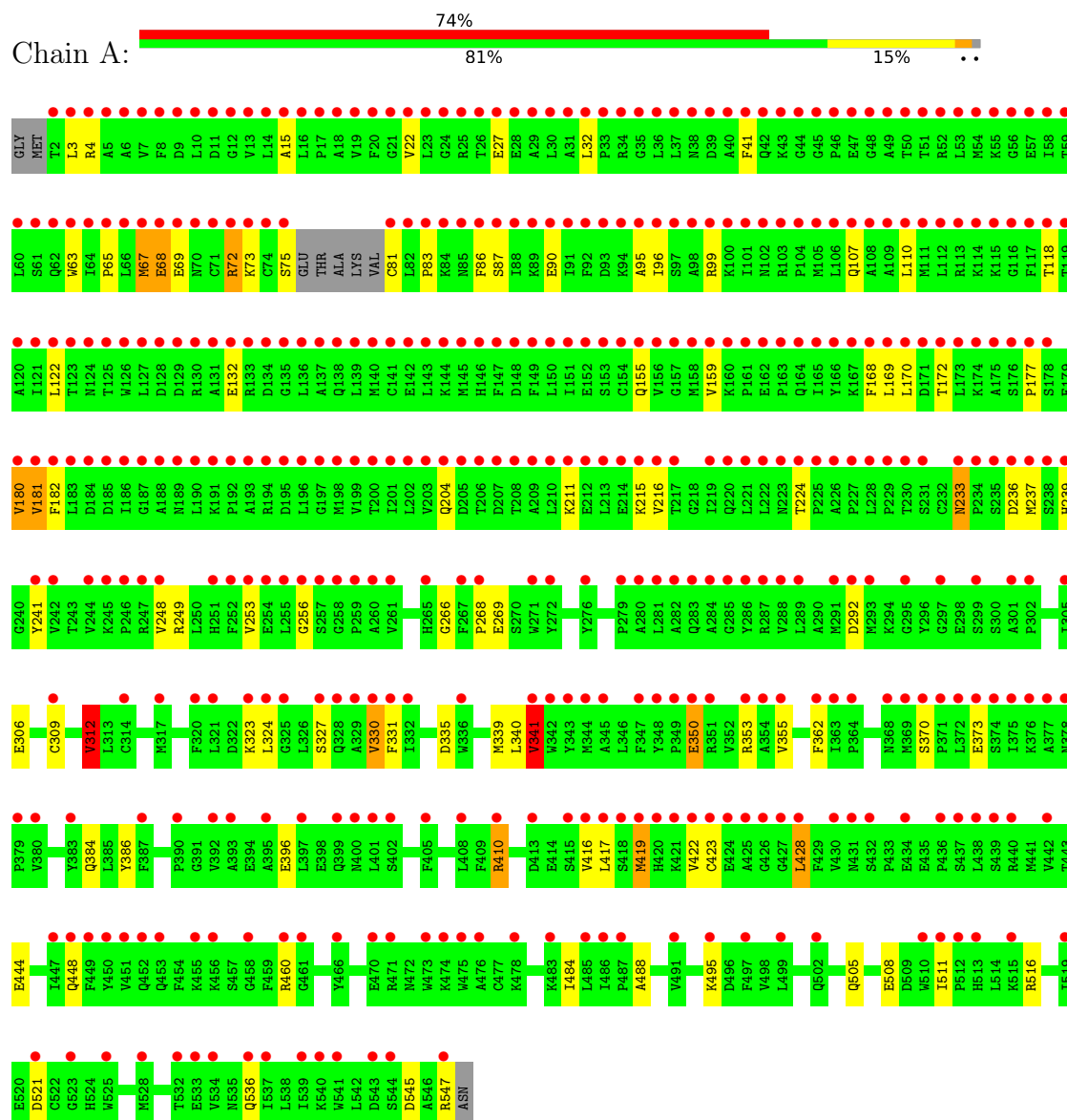
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	334	Total	O		
			334	334	0	0

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: BIFUNCTIONAL EPOXIDE HYDROLASE 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	91.74Å 91.74Å 245.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.48 – 2.15 79.45 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (80.48-2.15) 99.9 (79.45-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.12Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.204 , 0.248 0.356 , 0.373	Depositor DCC
R_{free} test set	1774 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	4683	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, YPN, 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	0.91	0/4390	1.32	27/5947 (0.5%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	VAL	N-CA-CB	9.82	121.23	110.53
1	A	516	ARG	CA-C-N	8.03	127.79	121.61
1	A	516	ARG	C-N-CA	8.03	127.79	121.61
1	A	292	ASP	N-CA-C	-7.13	95.36	107.99
1	A	269	GLU	N-CA-C	7.10	119.30	109.29
1	A	180	VAL	N-CA-C	6.69	117.48	108.11
1	A	118	THR	N-CA-C	-6.18	99.17	109.24
1	A	444	GLU	CA-C-N	6.16	128.54	120.28
1	A	444	GLU	C-N-CA	6.16	128.54	120.28
1	A	341	VAL	N-CA-CB	-5.78	102.67	110.54
1	A	341	VAL	CB-CA-C	5.76	119.91	112.14
1	A	248	VAL	N-CA-C	5.58	115.89	107.75
1	A	419	MET	N-CA-C	5.47	119.64	112.92
1	A	96	ILE	CA-C-N	5.46	127.60	120.28
1	A	96	ILE	C-N-CA	5.46	127.60	120.28
1	A	505	GLN	N-CA-C	5.31	118.55	111.75
1	A	312	VAL	N-CA-CB	5.20	119.25	110.56
1	A	182	PHE	CA-CB-CG	5.17	118.97	113.80
1	A	204	GLN	N-CA-C	-5.17	100.23	108.30
1	A	417	LEU	N-CA-C	5.16	117.31	108.90
1	A	545	ASP	N-CA-C	5.13	120.54	113.97
1	A	340	LEU	CA-C-N	5.12	127.48	120.46
1	A	340	LEU	C-N-CA	5.12	127.48	120.46
1	A	362	PHE	CA-CB-CG	-5.10	108.70	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	LYS	N-CA-C	-5.04	105.87	111.36
1	A	423	CYS	CA-C-N	5.01	127.25	120.38
1	A	423	CYS	C-N-CA	5.01	127.25	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4286	0	4288	34	13
2	A	10	0	0	0	0
3	A	14	0	20	3	0
4	A	6	0	8	0	0
5	A	33	0	24	2	0
6	A	334	0	0	4	8
All	All	4683	0	4340	36	16

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 4.

All (36) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:PHE:HB3	1:A:341:VAL:HG22	1.52	0.91
1:A:41:PHE:HA	1:A:67:MET:HE1	1.56	0.86
1:A:384:GLN:HE22	5:A:1553:YPN:H5	1.54	0.72
1:A:69:GLU:HG3	1:A:73:LYS:HZ2	1.53	0.71
1:A:422:VAL:HG11	1:A:428:LEU:HD22	1.78	0.65
1:A:309:CYS:SG	1:A:312:VAL:HG13	2.41	0.60
1:A:67:MET:HA	1:A:67:MET:HE2	1.84	0.59
1:A:350:GLU:HG3	6:A:2204:HOH:O	2.03	0.57
1:A:266:GLY:HA3	1:A:335:ASP:HB3	1.84	0.57
1:A:22:VAL:HG11	1:A:95:ALA:HB2	1.88	0.55
1:A:233:ASN:ND2	6:A:2133:HOH:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:PHE:HA	1:A:67:MET:CE	2.34	0.55
3:A:1550:PEG:H31	6:A:2333:HOH:O	2.07	0.54
3:A:1551:PEG:H21	5:A:1555:YPN:N4	2.23	0.53
1:A:341:VAL:HG13	1:A:355:VAL:HG23	1.90	0.51
1:A:339:MET:HE3	1:A:339:MET:HA	1.93	0.51
1:A:27:GLU:HA	1:A:32:LEU:HD12	1.94	0.50
1:A:341:VAL:HG13	1:A:355:VAL:CG2	2.42	0.49
1:A:3:LEU:HD13	1:A:181:VAL:HG22	1.95	0.48
1:A:83:PRO:HG2	1:A:86:PHE:HB2	1.95	0.48
1:A:495:LYS:HD2	1:A:521:ASP:HA	1.96	0.48
1:A:484:ILE:HB	1:A:511:ILE:HG12	1.97	0.46
1:A:410:ARG:HD2	1:A:416:VAL:HG22	1.98	0.46
1:A:355:VAL:O	1:A:488:ALA:HA	2.16	0.46
1:A:168:PHE:O	1:A:172:THR:HG23	2.17	0.44
1:A:41:PHE:CA	1:A:67:MET:HE1	2.39	0.44
1:A:170:LEU:HD13	1:A:177:PRO:HD3	2.00	0.43
1:A:107:GLN:HG2	6:A:2053:HOH:O	2.17	0.43
1:A:63:TRP:CZ2	1:A:67:MET:HE3	2.54	0.42
1:A:15:ALA:HB1	1:A:99:ARG:HG2	2.02	0.42
1:A:122:LEU:HD22	1:A:169:LEU:HD22	2.00	0.42
1:A:370:SER:HB2	1:A:373:GLU:HG3	2.02	0.41
1:A:69:GLU:HG3	1:A:73:LYS:NZ	2.31	0.40
1:A:87:SER:HB3	1:A:90:GLU:HB2	2.03	0.40
1:A:386:TYR:OH	1:A:396:GLU:OE1	2.36	0.40
1:A:536:GLN:HB2	3:A:1550:PEG:H41	2.03	0.40

All (16) 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)
1:A:68:GLU:OE1	1:A:72:ARG:NH2[8_435]	1.28	0.92
6:A:2093:HOH:O	6:A:2312:HOH:O[8_545]	1.64	0.56
1:A:327:SER:OG	6:A:2071:HOH:O[12_544]	1.65	0.55
1:A:239:HIS:O	1:A:241:TYR:N[12_544]	1.69	0.51
1:A:68:GLU:OE1	1:A:72:ARG:CZ[8_435]	1.73	0.47
1:A:239:HIS:N	1:A:241:TYR:O[12_544]	1.84	0.36
1:A:155:GLN:NE2	6:A:2290:HOH:O[12_544]	1.92	0.28
1:A:327:SER:N	6:A:2151:HOH:O[12_544]	1.94	0.26
1:A:237:MET:O	6:A:2140:HOH:O[12_544]	1.96	0.24
1:A:236:ASP:OD1	1:A:323:LYS:NZ[12_544]	2.04	0.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLY:N	1:A:324:LEU:O[12_544]	2.06	0.14
1:A:65:PRO:O	1:A:69:GLU:OE2[8_435]	2.08	0.12
1:A:236:ASP:O	1:A:323:LYS:CD[12_544]	2.10	0.10
6:A:2077:HOH:O	6:A:2205:HOH:O[12_544]	2.12	0.08
1:A:324:LEU:O	6:A:2147:HOH:O[12_544]	2.15	0.05
6:A:2134:HOH:O	6:A:2196:HOH:O[12_544]	2.15	0.05

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	537/549 (98%)	523 (97%)	13 (2%)	1 (0%)	43 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	PRO

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	468/474 (99%)	438 (94%)	30 (6%)	16 11

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	67	MET
1	A	68	GLU
1	A	72	ARG
1	A	75	SER
1	A	81	CYS
1	A	110	LEU
1	A	132	GLU
1	A	159	VAL
1	A	180	VAL
1	A	181	VAL
1	A	215	LYS
1	A	216	VAL
1	A	224	THR
1	A	233	ASN
1	A	249	ARG
1	A	253	VAL
1	A	306	GLU
1	A	312	VAL
1	A	330	VAL
1	A	341	VAL
1	A	350	GLU
1	A	353	ARG
1	A	410	ARG
1	A	419	MET
1	A	428	LEU
1	A	448	GLN
1	A	460	ARG
1	A	508	GLU
1	A	547	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	GLN
1	A	138	GLN
1	A	233	ASN
1	A	384	GLN
1	A	452	GLN
1	A	453	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
5	YPN	A	1553	-	11,11,11	0.49	0	13,13,13	0.95	0
3	PEG	A	1550	-	6,6,6	0.71	0	5,5,5	1.07	0
5	YPN	A	1554	-	11,11,11	0.34	0	13,13,13	0.77	0
5	YPN	A	1555	-	11,11,11	0.73	0	13,13,13	0.85	0
3	PEG	A	1551	-	6,6,6	0.52	0	5,5,5	1.08	0
2	SO4	A	1548	-	4,4,4	0.35	0	6,6,6	0.19	0
2	SO4	A	1549	-	4,4,4	0.40	0	6,6,6	0.25	0
4	GOL	A	1552	-	5,5,5	0.75	0	5,5,5	0.62	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	YPN	A	1553	-	-	0/4/4/4	0/1/1/1
5	YPN	A	1554	-	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	1550	-	-	3/4/4/4	-
5	YPN	A	1555	-	-	3/4/4/4	0/1/1/1
3	PEG	A	1551	-	-	4/4/4/4	-
4	GOL	A	1552	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1555	YPN	C2-C3-S8-C9
5	A	1555	YPN	N4-C3-S8-C9
5	A	1555	YPN	O11-C10-C9-S8
3	A	1551	PEG	O1-C1-C2-O2
3	A	1550	PEG	O1-C1-C2-O2
3	A	1551	PEG	O2-C3-C4-O4
3	A	1551	PEG	C1-C2-O2-C3
3	A	1550	PEG	C4-C3-O2-C2
3	A	1550	PEG	O2-C3-C4-O4
3	A	1551	PEG	C4-C3-O2-C2
4	A	1552	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1553	YPN	1	0
3	A	1550	PEG	2	0
5	A	1555	YPN	1	0
3	A	1551	PEG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	541/549 (98%)	3.26	407 (75%) 0 0	12, 30, 67, 98	0

All (407) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	LEU	8.9
1	A	20	PHE	8.5
1	A	92	PHE	8.2
1	A	37	LEU	7.8
1	A	416	VAL	7.5
1	A	19	VAL	7.5
1	A	63	TRP	7.4
1	A	59	THR	7.2
1	A	44	GLY	7.2
1	A	82	LEU	7.1
1	A	3	LEU	6.9
1	A	188	ALA	6.8
1	A	154	CYS	6.8
1	A	209	ALA	6.7
1	A	151	ILE	6.7
1	A	167	LYS	6.6
1	A	58	ILE	6.6
1	A	202	LEU	6.6
1	A	23	LEU	6.6
1	A	161	PRO	6.5
1	A	159	VAL	6.5
1	A	168	PHE	6.5
1	A	66	LEU	6.5
1	A	136	LEU	6.5
1	A	175	ALA	6.4
1	A	88	ILE	6.4
1	A	84	LYS	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	73	LYS	6.4
1	A	201	ILE	6.3
1	A	47	GLU	6.3
1	A	83	PRO	6.2
1	A	40	ALA	6.2
1	A	182	PHE	6.2
1	A	178	SER	6.1
1	A	547	ARG	6.1
1	A	149	PHE	6.1
1	A	86	PHE	6.1
1	A	203	VAL	6.1
1	A	51	THR	6.1
1	A	49	ALA	6.0
1	A	43	LYS	6.0
1	A	22	VAL	6.0
1	A	30	LEU	6.0
1	A	75	SER	5.9
1	A	67	MET	5.8
1	A	192	PRO	5.8
1	A	127	LEU	5.8
1	A	190	LEU	5.7
1	A	72	ARG	5.7
1	A	139	LEU	5.7
1	A	64	ILE	5.7
1	A	62	GLN	5.6
1	A	101	ILE	5.6
1	A	126	TRP	5.6
1	A	124	ASN	5.6
1	A	415	SER	5.5
1	A	91	ILE	5.5
1	A	46	PRO	5.5
1	A	11	ASP	5.5
1	A	199	VAL	5.5
1	A	189	ASN	5.5
1	A	177	PRO	5.4
1	A	81	CYS	5.4
1	A	193	ALA	5.4
1	A	41	PHE	5.4
1	A	213	LEU	5.4
1	A	116	GLY	5.4
1	A	14	LEU	5.3
1	A	53	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	143	LEU	5.3
1	A	180	VAL	5.3
1	A	60	LEU	5.3
1	A	5	ALA	5.3
1	A	241	TYR	5.2
1	A	71	CYS	5.2
1	A	54	MET	5.2
1	A	39	ASP	5.2
1	A	163	PRO	5.2
1	A	15	ALA	5.2
1	A	131	ALA	5.2
1	A	65	PRO	5.1
1	A	48	GLY	5.1
1	A	219	ILE	5.1
1	A	109	ALA	5.1
1	A	191	LYS	5.1
1	A	2	THR	5.1
1	A	261	VAL	5.1
1	A	7	VAL	5.1
1	A	236	ASP	5.0
1	A	125	THR	5.0
1	A	74	CYS	5.0
1	A	13	VAL	5.0
1	A	216	VAL	5.0
1	A	187	GLY	5.0
1	A	56	GLY	4.9
1	A	256	GLY	4.9
1	A	16	LEU	4.9
1	A	165	ILE	4.9
1	A	162	GLU	4.9
1	A	166	TYR	4.9
1	A	156	VAL	4.9
1	A	181	VAL	4.8
1	A	170	LEU	4.7
1	A	197	GLY	4.7
1	A	34	ARG	4.7
1	A	69	GLU	4.7
1	A	31	ALA	4.7
1	A	186	ILE	4.7
1	A	50	THR	4.6
1	A	55	LYS	4.6
1	A	196	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	510	TRP	4.6
1	A	95	ALA	4.6
1	A	137	ALA	4.6
1	A	150	LEU	4.6
1	A	173	LEU	4.6
1	A	194	ARG	4.6
1	A	85	ASN	4.6
1	A	70	ASN	4.5
1	A	45	GLY	4.5
1	A	155	GLN	4.5
1	A	90	GLU	4.5
1	A	106	LEU	4.5
1	A	145	MET	4.5
1	A	195	ASP	4.5
1	A	115	LYS	4.5
1	A	112	LEU	4.5
1	A	417	LEU	4.5
1	A	121	ILE	4.4
1	A	399	GLN	4.4
1	A	21	GLY	4.4
1	A	419	MET	4.4
1	A	176	SER	4.4
1	A	129	ASP	4.4
1	A	200	THR	4.4
1	A	158	MET	4.4
1	A	6	ALA	4.4
1	A	185	ASP	4.4
1	A	157	GLY	4.3
1	A	198	MET	4.3
1	A	246	PRO	4.3
1	A	215	LYS	4.3
1	A	141	CYS	4.3
1	A	42	GLN	4.3
1	A	120	ALA	4.3
1	A	35	GLY	4.3
1	A	87	SER	4.3
1	A	147	PHE	4.3
1	A	89	LYS	4.2
1	A	61	SER	4.2
1	A	434	GLU	4.2
1	A	26	THR	4.2
1	A	105	MET	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	118	THR	4.1
1	A	420	HIS	4.1
1	A	282	ALA	4.1
1	A	117	PHE	4.1
1	A	144	LYS	4.1
1	A	10	LEU	4.0
1	A	128	ASP	4.0
1	A	421	LYS	4.0
1	A	288	VAL	4.0
1	A	225	PRO	4.0
1	A	122	LEU	4.0
1	A	123	THR	4.0
1	A	93	ASP	4.0
1	A	418	SER	3.9
1	A	172	THR	3.9
1	A	164	GLN	3.9
1	A	4	ARG	3.9
1	A	18	ALA	3.9
1	A	329	ALA	3.9
1	A	174	LYS	3.9
1	A	57	GLU	3.9
1	A	413	ASP	3.9
1	A	138	GLN	3.9
1	A	452	GLN	3.9
1	A	17	PRO	3.9
1	A	238	SER	3.9
1	A	260	ALA	3.9
1	A	96	ILE	3.8
1	A	376	LYS	3.8
1	A	29	ALA	3.8
1	A	205	ASP	3.8
1	A	153	SER	3.8
1	A	114	LYS	3.8
1	A	370	SER	3.8
1	A	372	LEU	3.8
1	A	233	ASN	3.7
1	A	99	ARG	3.7
1	A	108	ALA	3.7
1	A	208	THR	3.7
1	A	133	ARG	3.7
1	A	543	ASP	3.7
1	A	220	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	324	LEU	3.7
1	A	302	PRO	3.7
1	A	119	THR	3.6
1	A	228	LEU	3.6
1	A	38	ASN	3.6
1	A	24	GLY	3.6
1	A	430	VAL	3.6
1	A	171	ASP	3.5
1	A	104	PRO	3.5
1	A	160	LYS	3.5
1	A	184	ASP	3.5
1	A	52	ARG	3.5
1	A	113	ARG	3.5
1	A	255	LEU	3.5
1	A	211	LYS	3.5
1	A	204	GLN	3.5
1	A	450	TYR	3.4
1	A	422	VAL	3.4
1	A	280	ALA	3.4
1	A	27	GLU	3.4
1	A	68	GLU	3.4
1	A	436	PRO	3.4
1	A	331	PHE	3.4
1	A	400	ASN	3.3
1	A	380	VAL	3.3
1	A	132	GLU	3.3
1	A	94	LYS	3.3
1	A	234	PRO	3.3
1	A	97	SER	3.3
1	A	217	THR	3.2
1	A	212	GLU	3.2
1	A	323	LYS	3.2
1	A	438	LEU	3.2
1	A	283	GLN	3.2
1	A	221	LEU	3.1
1	A	375	ILE	3.1
1	A	428	LEU	3.1
1	A	8	PHE	3.1
1	A	456	LYS	3.1
1	A	107	GLN	3.1
1	A	98	ALA	3.1
1	A	355	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	28	GLU	3.1
1	A	12	GLY	3.1
1	A	287	ARG	3.1
1	A	423	CYS	3.1
1	A	135	GLY	3.1
1	A	130	ARG	3.1
1	A	152	GLU	3.1
1	A	214	GLU	3.1
1	A	470	GLU	3.1
1	A	466	TYR	3.0
1	A	497	PHE	3.0
1	A	301	ALA	3.0
1	A	110	LEU	3.0
1	A	244	VAL	3.0
1	A	230	THR	3.0
1	A	252	PHE	3.0
1	A	226	ALA	3.0
1	A	284	ALA	3.0
1	A	345	ALA	3.0
1	A	330	VAL	3.0
1	A	286	TYR	3.0
1	A	402	SER	3.0
1	A	32	LEU	3.0
1	A	183	LEU	3.0
1	A	442	VAL	3.0
1	A	222	LEU	2.9
1	A	297	GLY	2.9
1	A	483	LYS	2.9
1	A	432	SER	2.9
1	A	169	LEU	2.9
1	A	291	MET	2.9
1	A	371	PRO	2.9
1	A	272	TYR	2.9
1	A	387	PHE	2.9
1	A	285	GLY	2.9
1	A	289	LEU	2.9
1	A	309	CYS	2.9
1	A	451	VAL	2.9
1	A	525	TRP	2.9
1	A	521	ASP	2.8
1	A	242	VAL	2.8
1	A	146	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	343	TYR	2.8
1	A	248	VAL	2.8
1	A	336	TRP	2.8
1	A	431	ASN	2.8
1	A	410	ARG	2.8
1	A	100	LYS	2.8
1	A	259	PRO	2.8
1	A	279	PRO	2.8
1	A	392	VAL	2.8
1	A	271	TRP	2.8
1	A	437	SER	2.7
1	A	239	HIS	2.7
1	A	142	GLU	2.7
1	A	207	ASP	2.7
1	A	427	GLY	2.7
1	A	393	ALA	2.7
1	A	540	LYS	2.7
1	A	33	PRO	2.7
1	A	103	ARG	2.7
1	A	305	ILE	2.7
1	A	231	SER	2.7
1	A	541	TRP	2.7
1	A	258	GLY	2.7
1	A	320	PHE	2.7
1	A	440	ARG	2.7
1	A	460	ARG	2.7
1	A	364	PRO	2.7
1	A	448	GLN	2.7
1	A	327	SER	2.7
1	A	148	ASP	2.7
1	A	25	ARG	2.7
1	A	206	THR	2.7
1	A	348	TYR	2.7
1	A	539	ILE	2.7
1	A	369	MET	2.6
1	A	257	SER	2.6
1	A	276	TYR	2.6
1	A	439	SER	2.6
1	A	363	ILE	2.6
1	A	247	ARG	2.6
1	A	461	GLY	2.6
1	A	523	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	254	GLU	2.6
1	A	405	PHE	2.6
1	A	449	PHE	2.6
1	A	453	GLN	2.6
1	A	471	ARG	2.6
1	A	487	PRO	2.6
1	A	267	PHE	2.5
1	A	502	GLN	2.5
1	A	295	GLY	2.5
1	A	325	GLY	2.5
1	A	354	ALA	2.5
1	A	328	GLN	2.5
1	A	408	LEU	2.5
1	A	536	GLN	2.5
1	A	281	LEU	2.5
1	A	485	LEU	2.5
1	A	341	VAL	2.5
1	A	353	ARG	2.5
1	A	447	ILE	2.5
1	A	299	SER	2.5
1	A	377	ALA	2.5
1	A	425	ALA	2.5
1	A	374	SER	2.4
1	A	140	MET	2.4
1	A	397	LEU	2.4
1	A	227	PRO	2.4
1	A	237	MET	2.4
1	A	210	LEU	2.4
1	A	515	LYS	2.4
1	A	401	LEU	2.4
1	A	499	LEU	2.4
1	A	362	PHE	2.4
1	A	528	MET	2.4
1	A	534	VAL	2.4
1	A	251	HIS	2.4
1	A	395	ALA	2.3
1	A	293	MET	2.3
1	A	224	THR	2.3
1	A	473	TRP	2.3
1	A	455	LYS	2.3
1	A	474	LYS	2.3
1	A	332	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	390	PRO	2.3
1	A	532	THR	2.3
1	A	495	LYS	2.3
1	A	235	SER	2.3
1	A	383	TYR	2.3
1	A	342	TRP	2.3
1	A	245	LYS	2.2
1	A	9	ASP	2.2
1	A	111	MET	2.2
1	A	426	GLY	2.2
1	A	476	ALA	2.2
1	A	350	GLU	2.2
1	A	373	GLU	2.2
1	A	513	HIS	2.2
1	A	475	TRP	2.2
1	A	223	ASN	2.2
1	A	349	PRO	2.2
1	A	537	ILE	2.2
1	A	478	LYS	2.2
1	A	317	MET	2.2
1	A	379	PRO	2.2
1	A	486	ILE	2.2
1	A	511	ILE	2.2
1	A	253	VAL	2.2
1	A	458	GLY	2.2
1	A	544	SER	2.2
1	A	344	MET	2.2
1	A	519	ILE	2.1
1	A	533	GLU	2.1
1	A	347	PHE	2.1
1	A	491	VAL	2.1
1	A	321	LEU	2.1
1	A	368	ASN	2.1
1	A	424	GLU	2.1
1	A	134	ASP	2.1
1	A	268	PRO	2.1
1	A	102	ASN	2.1
1	A	378	ASN	2.1
1	A	292	ASP	2.1
1	A	314	CYS	2.0
1	A	351	ARG	2.0
1	A	265	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	229	PRO	2.0
1	A	512	PRO	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 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
4	GOL	A	1552	6/6	0.44	0.30	60,62,62,63	0
3	PEG	A	1551	7/7	0.50	0.36	65,65,66,66	0
2	SO4	A	1549	5/5	0.53	0.30	74,78,79,79	0
3	PEG	A	1550	7/7	0.58	0.29	46,47,48,49	0
5	YPN	A	1555	11/11	0.61	0.30	50,60,69,69	0
2	SO4	A	1548	5/5	0.66	0.20	77,81,82,83	0
5	YPN	A	1554	11/11	0.82	0.18	34,39,51,51	0
5	YPN	A	1553	11/11	0.90	0.12	23,27,29,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.