



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:03 PM GMT

PDB ID : 3SL4
Title : Crystal structure of the catalytic domain of PDE4D2 with compound 10D
Authors : Feil, S.F.
Deposited on : 2011-06-24
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

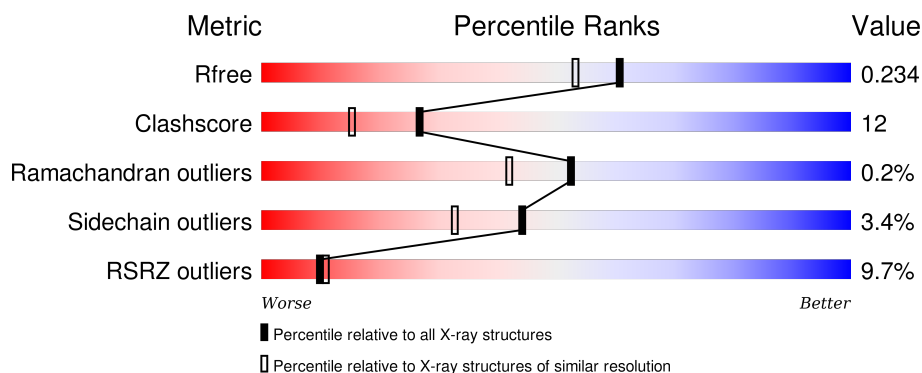
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 $\leq 5\%$. 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	361	<div> <div>10%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>• 9%</div> </div> </div>
1	B	361	<div> <div>8%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>• 10%</div> </div> </div>
1	C	361	<div> <div>11%</div> <div> <div></div> <div>71%</div> <div>18%</div> <div>• 10%</div> </div> </div>
1	D	361	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>• 10%</div> </div> </div>

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	10	-	-	-	X
3	EDO	A	11	-	-	-	X
3	EDO	A	15	-	-	-	X
3	EDO	A	16	-	-	-	X
3	EDO	A	17	-	-	-	X
3	EDO	A	21	-	-	X	X
3	EDO	A	443	-	-	X	X
3	EDO	A	9	-	-	-	X
3	EDO	B	11	-	-	-	X
3	EDO	B	13	-	-	-	X
3	EDO	B	15	-	-	X	X
3	EDO	B	16	-	-	X	X
3	EDO	B	18	-	-	X	X
3	EDO	B	19	-	-	-	X
3	EDO	C	12	-	-	-	X
3	EDO	C	13	-	-	-	X
3	EDO	C	14	-	-	-	X
3	EDO	C	15	-	-	-	X
3	EDO	C	4	-	-	-	X
3	EDO	D	14	-	-	-	X
3	EDO	D	15	-	-	-	X
3	EDO	D	17	-	-	-	X
3	EDO	D	20	-	-	-	X
3	EDO	D	21	-	-	X	X
3	EDO	D	22	-	-	-	X
3	EDO	D	5	-	-	X	X
3	EDO	D	6	-	-	-	X
4	DMS	B	7	-	-	-	X
4	DMS	D	13	-	-	-	X
4	DMS	D	23	-	-	X	-
4	DMS	D	8	-	-	X	-
4	DMS	D	9	-	-	-	X
5	PEG	A	440	-	-	-	X
5	PEG	D	12	-	-	X	X
5	PEG	D	16	-	-	X	X
5	PEG	D	19	-	-	-	X
5	PEG	D	441	-	-	X	X
6	PO4	A	20	-	-	X	-
6	PO4	B	20	-	-	-	X
6	PO4	C	17	-	-	-	X
8	EPE	B	6	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	EPE	C	7	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11484 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2658	1681	454	509	14			
1	B	325	Total	C	N	O	S	0	0	0
			2631	1664	450	503	14			
1	C	325	Total	C	N	O	S	0	2	0
			2647	1672	452	508	15			
1	D	324	Total	C	N	O	S	0	2	0
			2636	1666	450	506	14			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

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



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

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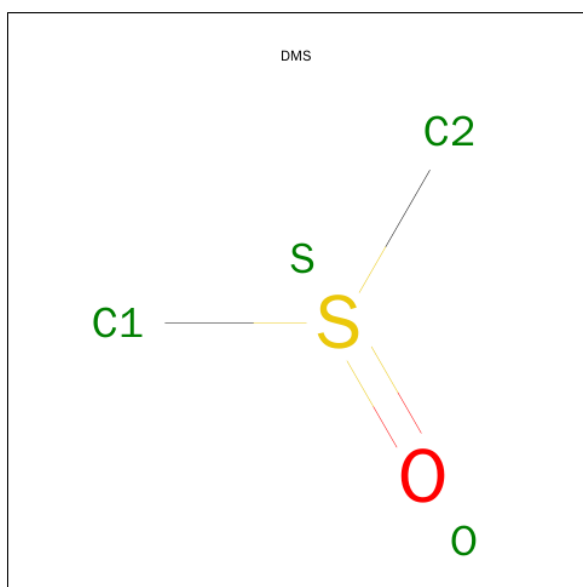
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0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

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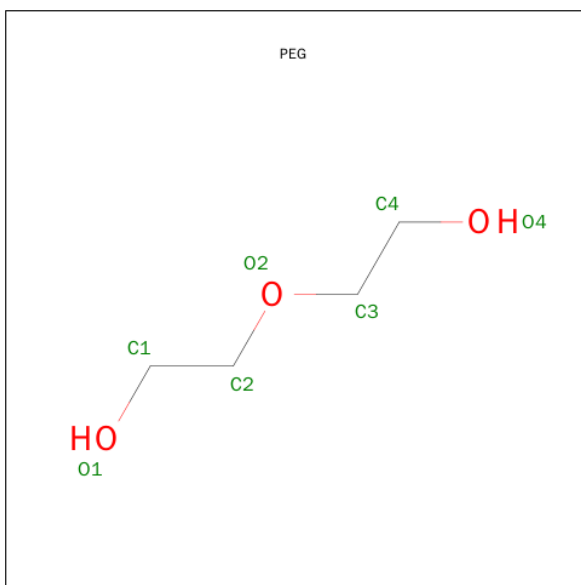
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total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

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



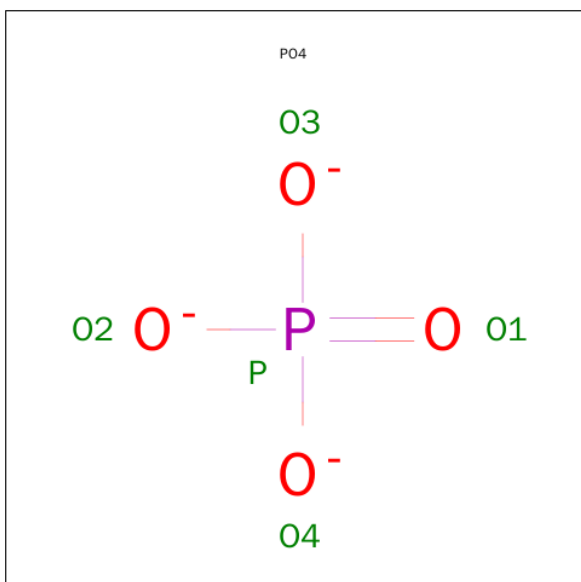
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



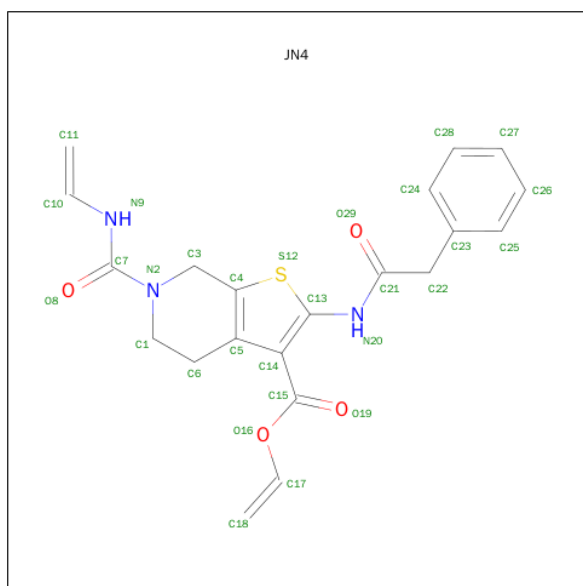
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	D	1	Total O P 5 4 1	0	0

- Molecule 7 is ETHENYL 6-(ETHENYLCARBAMOYL)-2-[(PHENYLACETYL)AMINO]-4,5,6,7-TETRAHYDROTHIENO[2,3-C]PYRIDINE-3-CARBOXYLATE (three-letter code: JN4) (formula: C₂₁H₂₁N₃O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O S 29 21 3 4 1	0	0
7	B	1	Total C N O S 29 21 3 4 1	0	0
7	C	1	Total C N O S 29 21 3 4 1	0	0
7	D	1	Total C N O S 29 21 3 4 1	0	0

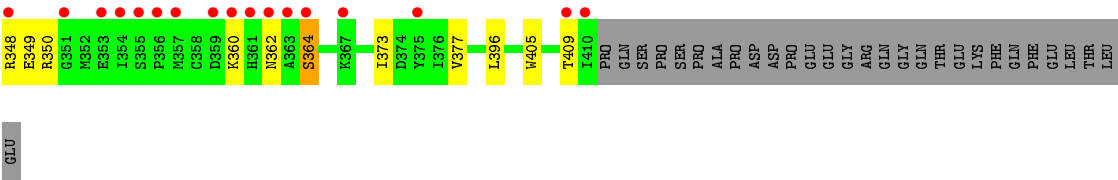
- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



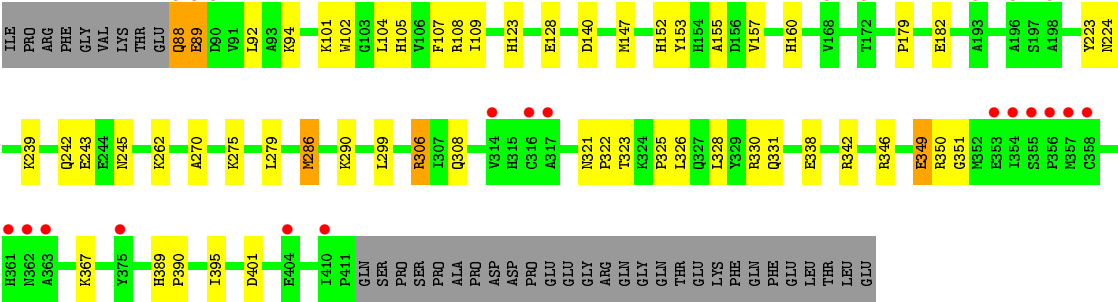
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	119	Total	O	0	0
			119	119		
9	B	121	Total	O	0	0
			121	121		
9	C	87	Total	O	0	0
			87	87		
9	D	140	Total	O	0	0
			140	140		



● Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.38Å 111.09Å 161.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.62 – 1.90 32.62 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.5 (32.62-1.90) 98.6 (32.62-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.194 , 0.227 0.203 , 0.234	Depositor DCC
R_{free} test set	6980 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 138715 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11484	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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, 0.375 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: ZN, EPE, JN4, PO4, EDO, DMS, PEG

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	0.38	0/2712	0.51	0/3684
1	B	0.34	0/2685	0.48	0/3648
1	C	0.34	0/2700	0.48	0/3668
1	D	0.40	0/2690	0.52	1/3655 (0.0%)
All	All	0.36	0/10787	0.50	1/14655 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	306	ARG	NE-CZ-NH2	-5.11	117.75	120.30

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	2658	0	2616	67	0
1	B	2631	0	2586	47	0
1	C	2647	0	2598	59	0
1	D	2636	0	2585	87	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	64	0	96	22	0
3	B	44	0	66	19	0
3	C	40	0	60	13	0
3	D	56	0	84	23	0
4	A	8	0	12	1	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	16	0	24	16	0
5	A	7	0	10	1	0
5	D	28	0	40	20	0
6	A	5	0	0	3	0
6	B	5	0	0	1	0
6	C	5	0	0	1	0
6	D	5	0	0	1	0
7	A	29	0	21	2	0
7	B	29	0	21	2	0
7	C	29	0	21	4	0
7	D	29	0	21	3	0
8	B	15	0	17	0	0
8	C	15	0	17	2	0
9	A	119	0	0	6	0
9	B	121	0	0	10	0
9	C	87	0	0	5	0
9	D	140	0	0	9	0
All	All	11484	0	10907	265	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 12.

All (265) 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:214:ASN:HD22	3:B:15:EDO:H21	1.01	1.14
1:B:214:ASN:ND2	3:B:15:EDO:H21	1.78	0.96
1:C:157:VAL:HA	3:C:13:EDO:H11	1.52	0.89
7:D:442:JN4:C10	7:D:442:JN4:H1	2.03	0.86
1:D:102:TRP:H	5:D:12:PEG:C4	1.89	0.86
1:B:221:LEU:HG	9:B:483:HOH:O	1.75	0.85
1:A:132:LEU:HD22	1:A:139:VAL:HG12	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:5:EDO:H11	9:D:495:HOH:O	1.80	0.82
1:A:366:GLU:HG2	1:A:409:THR:HG23	1.63	0.81
1:D:102:TRP:H	5:D:12:PEG:H42	1.46	0.81
1:D:243:GLU:OE1	3:D:5:EDO:H21	1.82	0.79
1:D:275:LYS:HE2	9:D:443:HOH:O	1.81	0.79
1:D:152:HIS:HE1	3:D:5:EDO:H22	1.46	0.79
1:A:148:THR:HG23	3:A:443:EDO:H22	1.65	0.79
1:B:352:MET:HE2	3:B:15:EDO:H22	1.63	0.79
1:D:401:ASP:HB2	5:D:16:PEG:H41	1.64	0.78
1:D:331:GLN:HE22	4:D:23:DMS:H21	1.48	0.78
1:D:108:ARG:H	4:D:23:DMS:C1	1.97	0.77
1:C:151:ASP:HA	3:C:14:EDO:H21	1.65	0.76
1:A:239:LYS:HZ2	1:D:239:LYS:HZ1	1.30	0.76
1:A:362:ASN:H	1:A:362:ASN:HD22	1.32	0.74
1:D:286:MET:HG3	3:D:15:EDO:H11	1.69	0.74
1:C:345:ASP:O	1:C:349:GLU:HG3	1.87	0.73
1:D:306:ARG:NH2	9:D:508:HOH:O	2.19	0.72
1:B:177:SER:HA	3:B:16:EDO:H21	1.70	0.72
1:B:214:ASN:HD22	3:B:15:EDO:C2	1.92	0.72
1:C:111:GLU:OE1	8:C:7:EPE:H52	1.90	0.71
1:A:148:THR:HG23	3:A:443:EDO:C2	2.19	0.71
1:A:406:TYR:O	1:A:409:THR:HG22	1.89	0.70
1:D:223:TYR:HD1	3:D:21:EDO:H11	1.56	0.70
1:A:239:LYS:HZ2	1:D:239:LYS:NZ	1.89	0.70
1:D:346:ARG:HH21	1:D:350:ARG:HH22	1.37	0.69
1:B:412:GLN:HA	1:B:412:GLN:OE1	1.91	0.69
7:C:18:JN4:H18A	9:C:482:HOH:O	1.91	0.69
1:A:239:LYS:NZ	1:D:239:LYS:NZ	2.41	0.69
1:D:123:HIS:HD2	3:D:10:EDO:H22	1.58	0.69
1:C:321[B]:ASN:HD22	7:C:18:JN4:C24	2.06	0.68
1:C:116:ARG:NE	1:C:147[A]:MET:HE1	2.09	0.68
1:B:130:ASP:OD2	1:B:133:LYS:HB2	1.94	0.67
1:A:278:ASN:HD22	1:A:278:ASN:H	1.42	0.66
1:B:290:LYS:NZ	3:B:18:EDO:H21	2.09	0.66
1:D:108:ARG:H	4:D:23:DMS:H13	1.58	0.66
1:D:105:HIS:HB3	4:D:23:DMS:H12	1.76	0.66
1:C:153:TYR:O	3:C:14:EDO:H12	1.95	0.66
1:D:102:TRP:H	5:D:12:PEG:H41	1.60	0.66
1:D:262:LYS:HG3	5:D:441:PEG:H32	1.76	0.66
1:C:178:THR:HB	3:C:440:EDO:H21	1.78	0.66
1:A:152:HIS:HE1	3:A:443:EDO:H12	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ARG:CZ	1:C:147[A]:MET:HE1	2.26	0.65
1:A:278:ASN:H	1:A:278:ASN:ND2	1.92	0.65
1:A:372:PHE:CE1	1:A:376:ILE:HD12	2.31	0.65
1:A:132:LEU:CD2	1:A:139:VAL:HG12	2.25	0.65
1:A:366:GLU:HG2	1:A:409:THR:CG2	2.27	0.64
1:D:326:LEU:H	5:D:16:PEG:H21	1.63	0.64
1:A:123:HIS:CE1	1:A:127:GLN:HE21	2.16	0.64
1:A:362:ASN:HD22	1:A:362:ASN:N	1.93	0.63
1:B:178:THR:CG2	1:B:181:LEU:HD12	2.28	0.63
1:D:153:TYR:O	4:D:13:DMS:H23	1.99	0.63
1:C:218:GLU:O	1:C:222:MET:HG2	1.98	0.63
1:D:107:PHE:HB2	4:D:23:DMS:H13	1.79	0.63
1:C:364:SER:HB2	9:C:77:HOH:O	1.99	0.62
1:D:152:HIS:CE1	3:D:5:EDO:H22	2.33	0.62
3:B:18:EDO:H22	9:B:527:HOH:O	2.00	0.62
1:B:178:THR:HG21	1:B:181:LEU:HD12	1.80	0.62
1:D:101:LYS:HA	5:D:12:PEG:H42	1.82	0.61
1:A:350:ARG:HE	3:A:7:EDO:H11	1.64	0.61
1:B:347:GLU:OE2	3:B:15:EDO:H12	2.00	0.61
1:A:152:HIS:HE1	3:A:443:EDO:C1	2.13	0.61
1:A:345:ASP:O	1:A:348:ARG:HG2	2.00	0.61
3:D:21:EDO:H22	9:D:452:HOH:O	1.99	0.61
1:B:290:LYS:HZ3	3:B:18:EDO:H21	1.64	0.61
3:C:13:EDO:H21	9:C:507:HOH:O	2.01	0.61
1:D:102:TRP:N	5:D:12:PEG:H42	2.15	0.60
1:D:401:ASP:CB	5:D:16:PEG:H41	2.31	0.60
1:D:155:ALA:HA	3:D:17:EDO:H12	1.83	0.59
1:C:116:ARG:HG2	1:C:147[A]:MET:HE3	1.84	0.59
1:D:182:GLU:HB2	4:D:8:DMS:H13	1.84	0.59
1:C:262:LYS:NZ	3:C:11:EDO:H22	2.17	0.59
1:D:157:VAL:HA	5:D:19:PEG:H11	1.83	0.59
1:B:182:GLU:HA	3:B:16:EDO:H11	1.83	0.59
1:D:331:GLN:HE22	4:D:23:DMS:C2	2.16	0.59
1:B:139:VAL:HG23	9:B:468:HOH:O	2.02	0.59
1:C:119:THR:OG1	1:C:147[A]:MET:HE2	2.03	0.58
1:D:262:LYS:CG	5:D:441:PEG:H32	2.32	0.58
1:C:302:ASN:ND2	1:C:305:ASP:H	2.02	0.58
1:B:177:SER:CA	3:B:16:EDO:H21	2.33	0.58
1:B:409:THR:O	1:B:409:THR:HG22	2.03	0.58
1:B:352:MET:CE	3:B:15:EDO:H22	2.32	0.58
1:A:152:HIS:CE1	3:A:443:EDO:H12	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:MET:CG	3:D:15:EDO:H11	2.35	0.57
1:A:321:ASN:HD22	7:A:23:JN4:C25	2.18	0.57
1:D:108:ARG:N	4:D:23:DMS:H13	2.20	0.57
1:A:139:VAL:HG11	9:A:454:HOH:O	2.04	0.56
1:D:275:LYS:HD2	3:D:14:EDO:H22	1.86	0.56
1:D:326:LEU:H	5:D:16:PEG:C2	2.17	0.56
1:D:182:GLU:HB2	4:D:8:DMS:C1	2.35	0.56
1:B:182:GLU:HG3	3:B:16:EDO:H22	1.86	0.56
1:C:330:ARG:HD3	1:C:405:TRP:CH2	2.40	0.56
1:B:132:LEU:HD22	1:B:139:VAL:HG22	1.88	0.56
1:A:292:VAL:CG1	1:A:293:THR:N	2.69	0.56
1:D:331:GLN:NE2	4:D:23:DMS:H21	2.17	0.55
1:C:302:ASN:O	1:C:306:ARG:HG3	2.07	0.55
1:C:270:ALA:HB1	1:C:279:LEU:HD11	1.88	0.55
1:D:346:ARG:HH21	1:D:350:ARG:NH2	2.05	0.55
3:B:18:EDO:H12	9:B:527:HOH:O	2.07	0.55
1:D:108:ARG:H	4:D:23:DMS:H12	1.69	0.54
1:B:177:SER:C	3:B:16:EDO:H21	2.27	0.54
1:A:239:LYS:NZ	1:D:239:LYS:HZ3	2.05	0.54
1:C:234:LEU:HB3	3:D:20:EDO:H21	1.89	0.54
1:B:284:LYS:O	1:B:288:GLU:HG3	2.07	0.54
1:C:178:THR:CB	3:C:440:EDO:H21	2.37	0.53
1:D:326:LEU:HG	1:D:330:ARG:HD3	1.90	0.53
1:A:349:GLU:HB3	1:C:147[B]:MET:SD	2.49	0.53
1:D:346:ARG:HH11	5:D:19:PEG:C4	2.21	0.53
1:D:328:LEU:CD2	4:D:23:DMS:H22	2.38	0.53
1:A:292:VAL:HG12	1:A:293:THR:N	2.22	0.53
1:B:327:GLN:HE21	1:B:327:GLN:HA	1.73	0.53
1:A:86:THR:OG1	1:A:89:GLU:HG3	2.08	0.53
1:C:160:HIS:NE2	6:C:17:PO4:O2	2.42	0.53
7:B:21:JN4:H18A	9:B:526:HOH:O	2.08	0.53
1:A:356:PRO:C	1:A:357:MET:HG2	2.29	0.52
1:A:147:MET:SD	1:C:349:GLU:HB3	2.49	0.52
7:D:442:JN4:H18A	9:D:559:HOH:O	2.09	0.52
3:A:21:EDO:H12	1:D:242:GLN:HE22	1.75	0.51
1:C:321[A]:ASN:HB2	1:C:322:PRO:HD3	1.90	0.51
1:D:155:ALA:HA	3:D:17:EDO:C1	2.39	0.51
1:C:116:ARG:CG	1:C:147[A]:MET:HE3	2.40	0.51
3:D:21:EDO:H21	3:D:22:EDO:H12	1.92	0.51
1:C:282:ASP:HB3	1:C:308:GLN:NE2	2.25	0.51
1:C:225:ASP:OD2	5:D:441:PEG:H42	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ILE:O	1:C:147[B]:MET:HG3	2.11	0.50
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.94	0.50
1:B:350:ARG:HB3	9:B:477:HOH:O	2.10	0.50
1:D:308:GLN:HG3	9:D:470:HOH:O	2.10	0.50
1:D:325:PRO:HA	5:D:16:PEG:H21	1.93	0.50
1:A:155:ALA:HA	3:A:17:EDO:C2	2.42	0.50
1:D:262:LYS:CB	5:D:441:PEG:H32	2.41	0.50
1:C:181:LEU:HD21	1:C:298:LEU:HD12	1.92	0.50
1:A:239:LYS:HZ1	1:D:239:LYS:HZ3	1.59	0.49
1:C:321[B]:ASN:HB2	1:C:322:PRO:HD3	1.95	0.49
1:A:350:ARG:HE	3:A:7:EDO:C1	2.25	0.49
1:C:196:ALA:O	1:C:200:HIS:HB3	2.12	0.49
1:B:389:HIS:O	3:B:18:EDO:O2	2.29	0.49
5:D:19:PEG:H21	9:D:476:HOH:O	2.12	0.49
1:C:409:THR:HG22	1:C:409:THR:O	2.13	0.49
1:C:147[A]:MET:HE2	1:C:147[A]:MET:HA	1.94	0.49
1:C:304:SER:O	1:C:308:GLN:HB2	2.13	0.49
1:B:244:GLU:OE2	1:C:254:LYS:HE2	2.13	0.48
1:A:362:ASN:ND2	1:A:362:ASN:N	2.61	0.48
1:A:349:GLU:HB3	1:C:147[B]:MET:CE	2.43	0.48
1:A:356:PRO:O	1:A:357:MET:HG2	2.13	0.48
1:C:221:LEU:O	1:C:221:LEU:HD13	2.13	0.48
1:A:123:HIS:HE1	1:A:127:GLN:HE21	1.60	0.48
9:B:494:HOH:O	1:D:147:MET:HE1	2.13	0.48
1:D:88:GLN:NE2	1:D:89:GLU:HG2	2.29	0.47
1:C:104:LEU:HD11	1:C:109:ILE:HD11	1.95	0.47
1:A:278:ASN:N	1:A:278:ASN:ND2	2.60	0.47
7:D:442:JN4:C10	7:D:442:JN4:C1	2.86	0.47
3:A:443:EDO:H21	9:C:73:HOH:O	2.15	0.47
1:A:242:GLN:OE1	1:D:242:GLN:OE1	2.31	0.47
1:B:411:PRO:O	1:B:412:GLN:CB	2.63	0.47
1:A:239:LYS:HE3	3:A:21:EDO:O1	2.14	0.47
1:D:123:HIS:CD2	3:D:10:EDO:H22	2.45	0.47
1:B:178:THR:CG2	1:B:181:LEU:HB2	2.44	0.47
1:C:348:ARG:HH22	1:C:360:LYS:HE2	1.79	0.47
1:A:243:GLU:OE1	3:A:443:EDO:H21	2.14	0.47
1:D:123:HIS:HD2	3:D:10:EDO:C2	2.28	0.47
1:A:342:ARG:HD2	9:A:506:HOH:O	2.14	0.47
1:D:224:ASN:OD1	3:D:20:EDO:H11	2.15	0.47
3:A:21:EDO:C1	1:D:242:GLN:HE22	2.28	0.47
1:C:136:LYS:HE2	3:C:5:EDO:O1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:THR:HG23	1:D:350:ARG:HB2	1.96	0.46
1:D:140[B]:ASP:OD1	9:D:479:HOH:O	2.20	0.46
1:C:289:THR:O	1:C:289:THR:HG22	2.16	0.46
3:A:19:EDO:H22	9:A:463:HOH:O	2.14	0.46
1:B:92:LEU:HD23	1:B:112:LEU:HB2	1.97	0.46
1:D:179:PRO:HA	4:D:8:DMS:C1	2.45	0.46
1:D:104:LEU:HD11	1:D:109:ILE:HD11	1.98	0.46
1:A:147:MET:HE3	1:C:350:ARG:HG2	1.98	0.46
1:A:327:GLN:O	1:A:331:GLN:HG3	2.15	0.46
1:A:160:HIS:NE2	6:A:20:PO4:P	2.89	0.46
7:A:23:JN4:H18A	9:A:444:HOH:O	2.15	0.45
1:B:159:TYR:CE1	7:B:21:JN4:H24	2.51	0.45
1:C:94:LYS:HA	1:C:94:LYS:HD2	1.82	0.45
1:B:411:PRO:O	1:B:412:GLN:HB2	2.16	0.45
6:A:20:PO4:P	9:A:486:HOH:O	2.74	0.45
1:B:160:HIS:NE2	6:B:20:PO4:P	2.90	0.45
1:B:108:ARG:NH1	1:B:112:LEU:HD21	2.32	0.45
1:B:147:MET:HE3	1:D:350:ARG:HB3	1.99	0.45
1:D:152:HIS:HE1	3:D:5:EDO:C2	2.23	0.45
3:B:16:EDO:H12	9:B:459:HOH:O	2.16	0.45
1:B:352:MET:HE1	3:B:15:EDO:H11	1.98	0.44
1:D:104:LEU:HD11	1:D:109:ILE:CD1	2.47	0.44
1:D:128:GLU:CG	3:D:18:EDO:H21	2.47	0.44
1:D:321:ASN:HB2	1:D:322:PRO:HD3	1.99	0.44
1:C:275:LYS:CD	3:C:12:EDO:H21	2.47	0.44
1:D:401:ASP:CB	5:D:16:PEG:C4	2.95	0.44
1:A:178:THR:HG22	1:A:181:LEU:HD12	1.99	0.44
1:D:179:PRO:HA	4:D:8:DMS:H13	1.99	0.44
1:C:275:LYS:HD3	3:C:12:EDO:H21	2.00	0.44
1:D:290:LYS:HA	3:D:15:EDO:H21	2.00	0.44
8:C:7:EPE:H101	8:C:7:EPE:H22	1.60	0.44
1:A:151:ASP:O	5:A:440:PEG:H12	2.16	0.44
1:D:323:THR:HB	1:D:395:ILE:HG23	1.98	0.44
1:A:107:PHE:HB2	4:A:442:DMS:H21	1.99	0.44
3:A:7:EDO:H22	1:C:148:THR:HA	1.99	0.43
1:B:108:ARG:CZ	1:B:112:LEU:HD21	2.48	0.43
1:D:223:TYR:CD1	3:D:21:EDO:H11	2.46	0.43
3:A:9:EDO:H11	9:A:482:HOH:O	2.17	0.43
1:D:101:LYS:CA	5:D:12:PEG:H42	2.46	0.43
3:A:21:EDO:H22	1:D:242:GLN:HE22	1.84	0.43
1:C:116:ARG:N	1:C:117:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:TRP:HB2	5:D:12:PEG:H41	2.00	0.43
1:C:152:HIS:HE1	3:C:8:EDO:O1	2.02	0.43
1:C:175:LEU:HD23	3:C:440:EDO:H22	2.00	0.42
1:A:175:LEU:HD23	3:A:10:EDO:H12	2.00	0.42
1:A:292:VAL:CG1	1:A:293:THR:H	2.30	0.42
1:D:270:ALA:HB1	1:D:279:LEU:HD11	2.02	0.42
1:A:293:THR:O	1:A:293:THR:HG23	2.19	0.42
1:B:349:GLU:HG3	1:D:147:MET:SD	2.60	0.42
1:C:104:LEU:HD12	9:C:472:HOH:O	2.20	0.42
1:A:160:HIS:NE2	6:A:20:PO4:O4	2.52	0.42
1:A:136:LYS:N	1:A:136:LYS:HD2	2.35	0.42
1:C:291:LYS:O	1:C:299:LEU:HB3	2.20	0.42
1:C:373:ILE:HA	1:C:377:VAL:HB	2.01	0.42
1:A:321:ASN:HB2	1:A:322:PRO:HD3	2.02	0.42
1:B:324:LYS:HB3	1:B:325:PRO:HD2	2.01	0.42
1:C:116:ARG:CG	1:C:147[A]:MET:CE	2.98	0.42
1:B:178:THR:HG23	1:B:181:LEU:HB2	2.01	0.42
1:B:340:PHE:CE1	3:B:4:EDO:H12	2.55	0.42
1:D:346:ARG:O	1:D:350:ARG:HG2	2.20	0.41
1:A:410:ILE:HA	1:A:411:PRO:HD3	1.93	0.41
1:C:144:THR:HA	1:C:147[B]:MET:HE2	2.02	0.41
3:D:21:EDO:H12	9:D:468:HOH:O	2.20	0.41
1:D:160:HIS:NE2	6:D:24:PO4:O1	2.54	0.41
1:A:178:THR:HB	3:A:10:EDO:H21	2.02	0.41
1:D:299:LEU:C	1:D:299:LEU:HD13	2.40	0.41
1:A:338:GLU:O	1:A:342:ARG:HG3	2.19	0.41
1:D:349:GLU:C	1:D:351:GLY:H	2.24	0.41
1:C:184:VAL:HG11	1:C:300:LEU:HD12	2.03	0.41
1:A:359:ASP:CG	1:A:362:ASN:HD21	2.24	0.41
1:C:321[B]:ASN:HD22	7:C:18:JN4:C23	2.33	0.41
1:A:293:THR:HG22	1:A:297:VAL:O	2.20	0.41
1:C:278:ASN:H	1:C:278:ASN:ND2	2.19	0.41
1:D:328:LEU:HD23	4:D:23:DMS:C2	2.49	0.41
1:B:151:ASP:OD1	1:D:350:ARG:NH2	2.54	0.41
1:D:346:ARG:NH2	1:D:350:ARG:HH22	2.13	0.41
1:D:128:GLU:HG3	3:D:18:EDO:H21	2.03	0.41
1:B:378:HIS:HB3	1:B:379:PRO:HD3	2.03	0.41
1:D:389:HIS:HA	1:D:390:PRO:HA	1.94	0.41
1:A:186:THR:OG1	3:A:18:EDO:H21	2.21	0.41
1:B:356:PRO:C	1:B:357:MET:HG2	2.41	0.41
1:D:338:GLU:O	1:D:342:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:THR:O	1:A:295:SER:N	2.47	0.41
1:A:323:THR:HB	1:A:395:ILE:HG23	2.03	0.40
1:B:297:VAL:HA	9:B:56:HOH:O	2.20	0.40
1:B:221:LEU:HD12	9:B:78:HOH:O	2.21	0.40
1:A:350:ARG:HG2	1:C:144:THR:HG23	2.03	0.40
1:A:186:THR:HG21	3:A:18:EDO:H21	2.02	0.40
1:A:148:THR:HG23	3:A:443:EDO:H21	2.00	0.40
1:A:302:ASN:ND2	1:A:305:ASP:H	2.19	0.40
1:A:307:ILE:HA	1:A:307:ILE:HD12	1.90	0.40
1:C:342:ARG:HD3	3:C:13:EDO:H12	2.03	0.40
1:D:286:MET:HB2	1:D:286:MET:HE2	1.95	0.40
7:C:18:JN4:O29	7:C:18:JN4:S12	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	327/361 (91%)	319 (98%)	8 (2%)	0	100	100
1	B	323/361 (90%)	316 (98%)	7 (2%)	0	100	100
1	C	325/361 (90%)	317 (98%)	7 (2%)	1 (0%)	46	35
1	D	324/361 (90%)	315 (97%)	8 (2%)	1 (0%)	46	35
All	All	1299/1444 (90%)	1267 (98%)	30 (2%)	2 (0%)	52	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	87	GLU
1	D	349	GLU

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	300/329 (91%)	291 (97%)	9 (3%)	48	38
1	B	297/329 (90%)	285 (96%)	12 (4%)	38	26
1	C	299/329 (91%)	286 (96%)	13 (4%)	35	23
1	D	298/329 (91%)	291 (98%)	7 (2%)	58	51
All	All	1194/1316 (91%)	1153 (97%)	41 (3%)	44	33

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
1	A	116	ARG
1	A	182	GLU
1	A	219	LEU
1	A	222	MET
1	A	278	ASN
1	A	353	GLU
1	A	362	ASN
1	A	409	THR
1	B	90	ASP
1	B	92	LEU
1	B	128	GLU
1	B	219	LEU
1	B	298	LEU
1	B	299	LEU
1	B	308	GLN
1	B	321	ASN
1	B	327	GLN
1	B	386	ASP
1	B	403	ARG
1	B	412	GLN
1	C	86	THR
1	C	90	ASP
1	C	92	LEU

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Mol	Chain	Res	Type
1	C	116	ARG
1	C	219	LEU
1	C	221	LEU
1	C	275	LYS
1	C	280	LEU
1	C	297	VAL
1	C	346	ARG
1	C	362	ASN
1	C	364	SER
1	C	396	LEU
1	D	88	GLN
1	D	89	GLU
1	D	92	LEU
1	D	94	LYS
1	D	245	ASN
1	D	286	MET
1	D	367	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	152	HIS
1	A	216	ASN
1	A	245	ASN
1	A	278	ASN
1	A	302	ASN
1	A	308	GLN
1	A	321	ASN
1	A	331	GLN
1	A	362	ASN
1	A	407	GLN
1	B	88	GLN
1	B	123	HIS
1	B	210	GLN
1	B	214	ASN
1	B	245	ASN
1	B	327	GLN
1	B	362	ASN
1	C	105	HIS
1	C	152	HIS
1	C	245	ASN

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Mol	Chain	Res	Type
1	C	278	ASN
1	C	302	ASN
1	C	308	GLN
1	D	88	GLN
1	D	105	HIS
1	D	123	HIS
1	D	245	ASN
1	D	250	GLN
1	D	278	ASN
1	D	331	GLN
1	D	389	HIS

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 82 ligands modelled in this entry, 8 are monoatomic - leaving 74 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	10	-	3,3,3	0.45	0	2,2,2	0.50	0
3	EDO	A	11	-	3,3,3	0.49	0	2,2,2	0.52	0
3	EDO	A	13	-	3,3,3	0.41	0	2,2,2	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	14	-	3,3,3	0.43	0	2,2,2	0.58	0
3	EDO	A	15	-	3,3,3	0.53	0	2,2,2	0.40	0
3	EDO	A	16	-	3,3,3	0.43	0	2,2,2	0.66	0
3	EDO	A	17	-	3,3,3	0.45	0	2,2,2	0.66	0
3	EDO	A	18	-	3,3,3	0.52	0	2,2,2	0.40	0
3	EDO	A	19	-	3,3,3	0.51	0	2,2,2	0.28	0
6	PO4	A	20	2	4,4,4	0.42	0	6,6,6	0.27	0
3	EDO	A	21	-	3,3,3	0.47	0	2,2,2	0.49	0
7	JN4	A	23	-	29,31,31	4.06	13 (44%)	23,42,42	1.55	3 (13%)
3	EDO	A	4	-	3,3,3	0.44	0	2,2,2	0.54	0
5	PEG	A	440	-	6,6,6	0.45	0	5,5,5	0.49	0
3	EDO	A	441	-	3,3,3	0.54	0	2,2,2	0.41	0
4	DMS	A	442	-	3,3,3	2.41	1 (33%)	3,3,3	0.37	0
3	EDO	A	443	-	3,3,3	0.47	0	2,2,2	0.21	0
3	EDO	A	5	-	3,3,3	0.50	0	2,2,2	0.42	0
4	DMS	A	6	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
3	EDO	A	7	-	3,3,3	0.47	0	2,2,2	0.55	0
3	EDO	A	9	-	3,3,3	0.57	0	2,2,2	0.32	0
3	EDO	B	10	-	3,3,3	0.47	0	2,2,2	0.81	0
3	EDO	B	11	-	3,3,3	0.48	0	2,2,2	0.74	0
3	EDO	B	13	-	3,3,3	0.53	0	2,2,2	0.47	0
3	EDO	B	15	-	3,3,3	0.55	0	2,2,2	0.10	0
3	EDO	B	16	-	3,3,3	0.40	0	2,2,2	0.53	0
3	EDO	B	17	-	3,3,3	0.47	0	2,2,2	0.50	0
3	EDO	B	18	-	3,3,3	0.53	0	2,2,2	0.12	0
3	EDO	B	19	-	3,3,3	0.43	0	2,2,2	0.53	0
6	PO4	B	20	2	4,4,4	0.40	0	6,6,6	0.28	0
7	JN4	B	21	-	29,31,31	4.06	12 (41%)	23,42,42	1.58	4 (17%)
3	EDO	B	4	-	3,3,3	0.49	0	2,2,2	0.53	0
8	EPE	B	6	-	14,15,15	0.45	0	18,20,20	1.96	5 (27%)
4	DMS	B	7	-	3,3,3	2.62	1 (33%)	3,3,3	0.47	0
3	EDO	B	8	-	3,3,3	0.43	0	2,2,2	0.59	0
3	EDO	B	9	-	3,3,3	0.51	0	2,2,2	0.33	0
4	DMS	C	10	-	3,3,3	2.62	1 (33%)	3,3,3	0.48	0
3	EDO	C	11	-	3,3,3	0.50	0	2,2,2	0.41	0
3	EDO	C	12	-	3,3,3	0.52	0	2,2,2	0.36	0
3	EDO	C	13	-	3,3,3	0.54	0	2,2,2	0.30	0
3	EDO	C	14	-	3,3,3	0.50	0	2,2,2	0.29	0
3	EDO	C	15	-	3,3,3	0.47	0	2,2,2	0.44	0
6	PO4	C	17	2	4,4,4	0.34	0	6,6,6	0.30	0
7	JN4	C	18	-	29,31,31	4.14	13 (44%)	23,42,42	1.58	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	C	4	-	3,3,3	0.50	0	2,2,2	0.35	0
3	EDO	C	440	-	3,3,3	0.45	0	2,2,2	0.45	0
3	EDO	C	5	-	3,3,3	0.41	0	2,2,2	0.53	0
3	EDO	C	6	-	3,3,3	0.50	0	2,2,2	0.53	0
8	EPE	C	7	-	14,15,15	0.43	0	18,20,20	1.96	5 (27%)
3	EDO	C	8	-	3,3,3	0.53	0	2,2,2	0.62	0
3	EDO	D	10	-	3,3,3	0.53	0	2,2,2	0.42	0
3	EDO	D	11	-	3,3,3	0.55	0	2,2,2	0.26	0
5	PEG	D	12	-	6,6,6	0.49	0	5,5,5	0.49	0
4	DMS	D	13	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
3	EDO	D	14	-	3,3,3	0.53	0	2,2,2	0.34	0
3	EDO	D	15	-	3,3,3	0.51	0	2,2,2	0.42	0
5	PEG	D	16	-	6,6,6	0.47	0	5,5,5	0.52	0
3	EDO	D	17	-	3,3,3	0.51	0	2,2,2	0.51	0
3	EDO	D	18	-	3,3,3	0.50	0	2,2,2	0.36	0
5	PEG	D	19	-	6,6,6	0.46	0	5,5,5	0.29	0
3	EDO	D	20	-	3,3,3	0.63	0	2,2,2	0.21	0
3	EDO	D	21	-	3,3,3	0.53	0	2,2,2	0.16	0
3	EDO	D	22	-	3,3,3	0.53	0	2,2,2	0.25	0
4	DMS	D	23	-	3,3,3	2.54	1 (33%)	3,3,3	0.43	0
6	PO4	D	24	2	4,4,4	0.32	0	6,6,6	0.28	0
3	EDO	D	4	-	3,3,3	0.53	0	2,2,2	0.27	0
3	EDO	D	440	-	3,3,3	0.57	0	2,2,2	0.36	0
5	PEG	D	441	-	6,6,6	0.58	0	5,5,5	0.45	0
7	JN4	D	442	-	29,31,31	4.01	13 (44%)	23,42,42	1.86	5 (21%)
3	EDO	D	5	-	3,3,3	0.43	0	2,2,2	0.59	0
3	EDO	D	6	-	3,3,3	0.54	0	2,2,2	0.40	0
3	EDO	D	7	-	3,3,3	0.43	0	2,2,2	0.47	0
4	DMS	D	8	-	3,3,3	2.63	1 (33%)	3,3,3	0.38	0
4	DMS	D	9	-	3,3,3	2.58	1 (33%)	3,3,3	0.43	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	10	-	-	0/1/1/1	0/0/0/0
3	EDO	A	11	-	-	0/1/1/1	0/0/0/0
3	EDO	A	13	-	-	0/1/1/1	0/0/0/0
3	EDO	A	14	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	15	-	-	0/1/1/1	0/0/0/0
3	EDO	A	16	-	-	0/1/1/1	0/0/0/0
3	EDO	A	17	-	-	0/1/1/1	0/0/0/0
3	EDO	A	18	-	-	0/1/1/1	0/0/0/0
3	EDO	A	19	-	-	0/1/1/1	0/0/0/0
6	PO4	A	20	2	-	0/0/0/0	0/0/0/0
3	EDO	A	21	-	-	0/1/1/1	0/0/0/0
7	JN4	A	23	-	-	0/18/31/31	0/3/3/3
3	EDO	A	4	-	-	0/1/1/1	0/0/0/0
5	PEG	A	440	-	-	0/4/4/4	0/0/0/0
3	EDO	A	441	-	-	0/1/1/1	0/0/0/0
4	DMS	A	442	-	-	0/0/0/0	0/0/0/0
3	EDO	A	443	-	-	0/1/1/1	0/0/0/0
3	EDO	A	5	-	-	0/1/1/1	0/0/0/0
4	DMS	A	6	-	-	0/0/0/0	0/0/0/0
3	EDO	A	7	-	-	0/1/1/1	0/0/0/0
3	EDO	A	9	-	-	0/1/1/1	0/0/0/0
3	EDO	B	10	-	-	0/1/1/1	0/0/0/0
3	EDO	B	11	-	-	0/1/1/1	0/0/0/0
3	EDO	B	13	-	-	0/1/1/1	0/0/0/0
3	EDO	B	15	-	-	0/1/1/1	0/0/0/0
3	EDO	B	16	-	-	0/1/1/1	0/0/0/0
3	EDO	B	17	-	-	0/1/1/1	0/0/0/0
3	EDO	B	18	-	-	0/1/1/1	0/0/0/0
3	EDO	B	19	-	-	0/1/1/1	0/0/0/0
6	PO4	B	20	2	-	0/0/0/0	0/0/0/0
7	JN4	B	21	-	-	0/18/31/31	0/3/3/3
3	EDO	B	4	-	-	0/1/1/1	0/0/0/0
8	EPE	B	6	-	-	0/9/19/19	0/1/1/1
4	DMS	B	7	-	-	0/0/0/0	0/0/0/0
3	EDO	B	8	-	-	0/1/1/1	0/0/0/0
3	EDO	B	9	-	-	0/1/1/1	0/0/0/0
4	DMS	C	10	-	-	0/0/0/0	0/0/0/0
3	EDO	C	11	-	-	0/1/1/1	0/0/0/0
3	EDO	C	12	-	-	0/1/1/1	0/0/0/0
3	EDO	C	13	-	-	0/1/1/1	0/0/0/0
3	EDO	C	14	-	-	0/1/1/1	0/0/0/0
3	EDO	C	15	-	-	0/1/1/1	0/0/0/0
6	PO4	C	17	2	-	0/0/0/0	0/0/0/0
7	JN4	C	18	-	-	0/18/31/31	0/3/3/3
3	EDO	C	4	-	-	0/1/1/1	0/0/0/0
3	EDO	C	440	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	5	-	-	0/1/1/1	0/0/0/0
3	EDO	C	6	-	-	0/1/1/1	0/0/0/0
8	EPE	C	7	-	-	0/9/19/19	0/1/1/1
3	EDO	C	8	-	-	0/1/1/1	0/0/0/0
3	EDO	D	10	-	-	0/1/1/1	0/0/0/0
3	EDO	D	11	-	-	0/1/1/1	0/0/0/0
5	PEG	D	12	-	-	0/4/4/4	0/0/0/0
4	DMS	D	13	-	-	0/0/0/0	0/0/0/0
3	EDO	D	14	-	-	0/1/1/1	0/0/0/0
3	EDO	D	15	-	-	0/1/1/1	0/0/0/0
5	PEG	D	16	-	-	0/4/4/4	0/0/0/0
3	EDO	D	17	-	-	0/1/1/1	0/0/0/0
3	EDO	D	18	-	-	0/1/1/1	0/0/0/0
5	PEG	D	19	-	-	0/4/4/4	0/0/0/0
3	EDO	D	20	-	-	0/1/1/1	0/0/0/0
3	EDO	D	21	-	-	0/1/1/1	0/0/0/0
3	EDO	D	22	-	-	0/1/1/1	0/0/0/0
4	DMS	D	23	-	-	0/0/0/0	0/0/0/0
6	PO4	D	24	2	-	0/0/0/0	0/0/0/0
3	EDO	D	4	-	-	0/1/1/1	0/0/0/0
3	EDO	D	440	-	-	0/1/1/1	0/0/0/0
5	PEG	D	441	-	-	0/4/4/4	0/0/0/0
7	JN4	D	442	-	-	1/18/31/31	0/3/3/3
3	EDO	D	5	-	-	0/1/1/1	0/0/0/0
3	EDO	D	6	-	-	0/1/1/1	0/0/0/0
3	EDO	D	7	-	-	0/1/1/1	0/0/0/0
4	DMS	D	8	-	-	0/0/0/0	0/0/0/0
4	DMS	D	9	-	-	0/0/0/0	0/0/0/0

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	18	JN4	C13-S12	-9.62	1.57	1.72
7	B	21	JN4	C13-S12	-9.34	1.57	1.72
7	D	442	JN4	C13-S12	-8.95	1.58	1.72
7	A	23	JN4	C13-S12	-8.61	1.59	1.72
7	B	21	JN4	O16-C15	-5.29	1.27	1.37
7	A	23	JN4	O16-C15	-5.15	1.27	1.37
7	C	18	JN4	O16-C15	-5.07	1.27	1.37
7	D	442	JN4	O16-C15	-5.03	1.27	1.37
7	D	442	JN4	C3-C4	2.06	1.54	1.51
7	C	18	JN4	C7-N9	2.16	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	21	JN4	C7-N9	2.19	1.44	1.39
7	A	23	JN4	C7-N9	2.26	1.44	1.39
7	C	18	JN4	C3-C4	2.54	1.54	1.51
7	D	442	JN4	C7-N9	2.63	1.45	1.39
7	A	23	JN4	C3-C4	2.75	1.55	1.51
7	D	442	JN4	C28-C24	3.02	1.45	1.38
7	C	18	JN4	C28-C24	3.03	1.45	1.38
7	B	21	JN4	C28-C24	3.07	1.45	1.38
7	A	23	JN4	C28-C24	3.18	1.45	1.38
7	D	442	JN4	C21-N20	3.26	1.43	1.35
7	B	21	JN4	C21-N20	3.40	1.43	1.35
7	B	21	JN4	C25-C23	3.45	1.46	1.38
7	C	18	JN4	C21-N20	3.48	1.44	1.35
7	D	442	JN4	C25-C23	3.57	1.46	1.38
7	C	18	JN4	C11-C10	3.60	1.49	1.29
7	A	23	JN4	C11-C10	3.63	1.49	1.29
7	B	21	JN4	C11-C10	3.64	1.49	1.29
7	A	23	JN4	C21-N20	3.64	1.44	1.35
7	D	442	JN4	C11-C10	3.66	1.49	1.29
7	A	23	JN4	C25-C23	3.72	1.46	1.38
7	C	18	JN4	C25-C23	3.81	1.46	1.38
7	A	23	JN4	C7-N2	3.91	1.44	1.36
7	C	18	JN4	C7-N2	3.99	1.44	1.36
7	D	442	JN4	C7-N2	4.00	1.44	1.36
4	A	442	DMS	O-S	4.03	1.77	1.50
7	B	21	JN4	C7-N2	4.14	1.44	1.36
4	D	23	DMS	O-S	4.33	1.80	1.50
4	D	9	DMS	O-S	4.33	1.80	1.50
4	B	7	DMS	O-S	4.38	1.80	1.50
4	C	10	DMS	O-S	4.42	1.80	1.50
4	D	8	DMS	O-S	4.43	1.80	1.50
4	A	6	DMS	O-S	4.46	1.80	1.50
7	B	21	JN4	C10-N9	4.51	1.43	1.32
4	D	13	DMS	O-S	4.53	1.81	1.50
7	A	23	JN4	C10-N9	4.64	1.44	1.32
7	C	18	JN4	C10-N9	4.72	1.44	1.32
7	D	442	JN4	C10-N9	4.81	1.44	1.32
7	D	442	JN4	C18-C17	4.92	1.49	1.31
7	B	21	JN4	C18-C17	4.95	1.49	1.31
7	C	18	JN4	C18-C17	4.95	1.49	1.31
7	A	23	JN4	C18-C17	4.96	1.49	1.31
7	B	21	JN4	C14-C13	5.24	1.53	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	442	JN4	C14-C13	5.30	1.53	1.41
7	C	18	JN4	C14-C13	5.37	1.53	1.41
7	A	23	JN4	C14-C13	5.54	1.54	1.41
7	D	442	JN4	C14-C5	14.20	1.69	1.39
7	B	21	JN4	C14-C5	14.31	1.69	1.39
7	A	23	JN4	C14-C5	14.45	1.69	1.39
7	C	18	JN4	C14-C5	14.64	1.70	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	21	JN4	C14-C5-C4	-5.06	108.35	113.61
7	D	442	JN4	C14-C5-C4	-4.76	108.66	113.61
7	A	23	JN4	C14-C5-C4	-4.61	108.81	113.61
7	C	18	JN4	C14-C5-C4	-4.61	108.81	113.61
7	C	18	JN4	O29-C21-N20	-3.07	118.23	123.72
7	D	442	JN4	O8-C7-N2	-3.06	117.09	121.77
7	B	21	JN4	O29-C21-N20	-2.56	119.16	123.72
7	A	23	JN4	O29-C21-N20	-2.53	119.19	123.72
7	D	442	JN4	O29-C21-N20	-2.24	119.72	123.72
8	C	7	EPE	O2S-S-C10	-2.17	105.06	106.91
8	B	6	EPE	C6-N1-C2	2.10	113.44	108.90
7	B	21	JN4	N9-C7-N2	2.12	118.99	115.97
7	C	18	JN4	N9-C7-N2	2.49	119.51	115.97
8	B	6	EPE	C7-N4-C5	2.93	118.78	111.27
8	C	7	EPE	O1S-S-C10	3.08	109.53	106.91
8	B	6	EPE	C5-N4-C3	3.24	115.92	108.90
7	B	21	JN4	O16-C15-C14	3.36	118.19	111.10
7	C	18	JN4	O16-C15-C14	3.40	118.27	111.10
8	C	7	EPE	C7-N4-C5	3.44	120.08	111.27
8	C	7	EPE	C7-N4-C3	3.47	120.16	111.27
8	B	6	EPE	C7-N4-C3	3.54	120.34	111.27
7	D	442	JN4	O16-C15-C14	3.61	118.71	111.10
7	A	23	JN4	O16-C15-C14	3.72	118.94	111.10
8	C	7	EPE	C5-N4-C3	4.19	117.98	108.90
7	D	442	JN4	N9-C7-N2	4.36	122.17	115.97
8	B	6	EPE	O1S-S-C10	4.91	111.09	106.91

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	442	JN4	N2-C7-N9-C10

There are no ring outliers.

46 monomers are involved in 134 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	10	EDO	2	0
3	A	17	EDO	1	0
3	A	18	EDO	2	0
3	A	19	EDO	1	0
6	A	20	PO4	3	0
3	A	21	EDO	4	0
7	A	23	JN4	2	0
5	A	440	PEG	1	0
4	A	442	DMS	1	0
3	A	443	EDO	8	0
3	A	7	EDO	3	0
3	A	9	EDO	1	0
3	B	15	EDO	7	0
3	B	16	EDO	6	0
3	B	18	EDO	5	0
6	B	20	PO4	1	0
7	B	21	JN4	2	0
3	B	4	EDO	1	0
3	C	11	EDO	1	0
3	C	12	EDO	2	0
3	C	13	EDO	3	0
3	C	14	EDO	2	0
6	C	17	PO4	1	0
7	C	18	JN4	4	0
3	C	440	EDO	3	0
3	C	5	EDO	1	0
8	C	7	EPE	2	0
3	C	8	EDO	1	0
3	D	10	EDO	3	0
5	D	12	PEG	7	0
4	D	13	DMS	1	0
3	D	14	EDO	1	0
3	D	15	EDO	3	0
5	D	16	PEG	6	0
3	D	17	EDO	2	0
3	D	18	EDO	2	0
5	D	19	PEG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	20	EDO	2	0
3	D	21	EDO	5	0
3	D	22	EDO	1	0
4	D	23	DMS	11	0
6	D	24	PO4	1	0
5	D	441	PEG	4	0
7	D	442	JN4	3	0
3	D	5	EDO	5	0
4	D	8	DMS	4	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	329/361 (91%)	0.53	35 (10%) 8 8	14, 28, 58, 86	0
1	B	325/361 (90%)	0.49	29 (8%) 12 13	17, 34, 50, 79	0
1	C	325/361 (90%)	0.63	39 (12%) 6 6	17, 32, 62, 81	0
1	D	324/361 (89%)	0.34	23 (7%) 19 21	14, 24, 50, 69	0
All	All	1303/1444 (90%)	0.50	126 (9%) 10 11	14, 29, 56, 86	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	356	PRO	7.4
1	C	294	SER	7.3
1	C	351	GLY	5.6
1	D	362	ASN	5.5
1	A	293	THR	5.4
1	A	296	GLY	5.3
1	D	354	ILE	5.3
1	C	353	GLU	5.2
1	A	295	SER	5.1
1	C	295	SER	5.1
1	A	361	HIS	5.1
1	C	362	ASN	5.0
1	A	356	PRO	4.9
1	A	294	SER	4.9
1	C	363	ALA	4.9
1	C	354	ILE	4.9
1	A	362	ASN	4.8
1	A	363	ALA	4.6
1	A	411	PRO	4.6
1	A	354	ILE	4.6
1	C	87	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	353	GLU	4.5
1	C	293	THR	4.4
1	C	361	HIS	4.3
1	C	297	VAL	4.3
1	B	88	GLN	4.3
1	A	375	TYR	4.3
1	D	363	ALA	4.2
1	A	410	ILE	4.2
1	B	90	ASP	3.9
1	D	357	MET	3.9
1	D	361	HIS	3.9
1	A	357	MET	3.9
1	D	356	PRO	3.9
1	D	355	SER	3.8
1	A	299	LEU	3.8
1	C	357	MET	3.7
1	A	84	VAL	3.7
1	C	296	GLY	3.7
1	B	94	LYS	3.6
1	B	108	ARG	3.6
1	C	375	TYR	3.6
1	B	412	GLN	3.6
1	C	410	ILE	3.5
1	D	375	TYR	3.5
1	A	297	VAL	3.4
1	D	353	GLU	3.4
1	C	292	VAL	3.4
1	B	91	VAL	3.3
1	C	86	THR	3.3
1	C	289	THR	3.3
1	D	90	ASP	3.3
1	C	168	VAL	3.3
1	A	352	MET	3.3
1	A	317	ALA	3.2
1	B	139	VAL	3.2
1	C	409	THR	3.2
1	A	359	ASP	3.2
1	C	291	LYS	3.2
1	B	133	LYS	3.2
1	C	319	LEU	3.1
1	A	83	GLY	3.0
1	A	355	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	196	ALA	2.9
1	C	301	ASP	2.8
1	D	88	GLN	2.8
1	A	316	CYS	2.8
1	B	168	VAL	2.8
1	C	316	CYS	2.8
1	C	299	LEU	2.7
1	C	355	SER	2.7
1	C	317	ALA	2.7
1	B	301	ASP	2.7
1	D	314	VAL	2.6
1	D	198	ALA	2.6
1	D	89	GLU	2.6
1	B	130	ASP	2.6
1	B	362	ASN	2.6
1	D	193	ALA	2.6
1	A	168	VAL	2.6
1	A	351	GLY	2.6
1	C	348	ARG	2.6
1	B	356	PRO	2.5
1	A	291	LYS	2.5
1	B	257	ARG	2.5
1	A	348	ARG	2.5
1	C	302	ASN	2.4
1	B	136	LYS	2.4
1	C	320	SER	2.4
1	D	317	ALA	2.4
1	C	359	ASP	2.4
1	B	196	ALA	2.4
1	C	364	SER	2.4
1	C	314	VAL	2.3
1	B	89	GLU	2.3
1	A	350	ARG	2.3
1	D	168	VAL	2.3
1	B	118	LEU	2.3
1	B	286	MET	2.3
1	A	360	LYS	2.3
1	C	367	LYS	2.3
1	C	175	LEU	2.2
1	B	193	ALA	2.2
1	D	410	ILE	2.2
1	B	353	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	172	THR	2.2
1	B	165	ALA	2.2
1	B	375	TYR	2.2
1	A	409	THR	2.2
1	A	292	VAL	2.2
1	B	295	SER	2.2
1	C	303	TYR	2.1
1	B	294	SER	2.1
1	A	319	LEU	2.1
1	D	316	CYS	2.1
1	D	404	GLU	2.1
1	B	112	LEU	2.1
1	B	97	GLU	2.1
1	A	301	ASP	2.1
1	D	358	CYS	2.1
1	A	288	GLU	2.0
1	C	360	LYS	2.0
1	A	314	VAL	2.0
1	B	363	ALA	2.0
1	C	88	GLN	2.0
1	B	199	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	D	22	4/4	0.89	0.34	23.38	28,37,38,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	EDO	B	11	4/4	0.91	0.27	17.87	39,40,42,43	0
3	EDO	D	21	4/4	0.90	0.33	14.51	29,30,31,37	0
5	PEG	D	16	7/7	0.65	0.40	13.96	36,43,47,55	0
3	EDO	B	19	4/4	0.92	0.44	10.82	35,36,39,40	0
3	EDO	C	15	4/4	0.80	0.27	10.76	33,37,39,46	0
3	EDO	A	16	4/4	0.80	0.26	9.12	34,37,44,45	0
3	EDO	D	20	4/4	0.80	0.26	7.54	32,33,40,40	0
3	EDO	A	21	4/4	0.93	0.35	7.15	37,38,40,44	0
3	EDO	C	14	4/4	0.82	0.21	6.90	33,35,40,43	0
3	EDO	C	13	4/4	0.74	0.37	6.41	27,33,40,48	0
4	DMS	B	7	4/4	0.89	0.29	6.27	40,44,50,61	0
3	EDO	D	6	4/4	0.80	0.30	6.27	39,44,47,52	0
3	EDO	D	14	4/4	0.81	0.22	6.08	39,40,50,51	0
3	EDO	D	17	4/4	0.89	0.20	6.06	28,29,37,44	0
3	EDO	A	11	4/4	0.89	0.25	5.99	33,34,42,43	0
3	EDO	A	17	4/4	0.85	0.23	5.92	34,36,38,43	0
6	PO4	B	20	5/5	0.88	0.21	5.84	24,24,26,31	2
5	PEG	A	440	7/7	0.77	0.29	5.48	31,38,41,43	0
3	EDO	B	16	4/4	0.95	0.31	5.44	37,39,40,45	0
3	EDO	A	15	4/4	0.82	0.21	5.40	41,44,45,46	0
3	EDO	B	18	4/4	0.87	0.23	4.44	33,37,39,42	0
4	DMS	D	13	4/4	0.89	0.25	4.26	34,35,42,53	0
8	EPE	B	6	15/15	0.89	0.28	4.21	43,54,60,62	0
3	EDO	A	443	4/4	0.76	0.22	4.11	26,33,41,42	0
5	PEG	D	441	7/7	0.84	0.18	3.92	16,34,35,36	0
3	EDO	D	15	4/4	0.88	0.27	3.91	37,39,39,53	0
3	EDO	B	15	4/4	0.89	0.37	3.65	29,36,39,44	0
4	DMS	D	9	4/4	0.89	0.23	3.57	34,42,43,59	0
5	PEG	D	19	7/7	0.83	0.29	3.45	34,42,48,51	0
3	EDO	B	13	4/4	0.87	0.17	3.19	35,41,44,49	0
5	PEG	D	12	7/7	0.82	0.21	3.16	26,32,46,50	0
3	EDO	D	5	4/4	0.90	0.17	3.16	24,35,37,41	0
8	EPE	C	7	15/15	0.92	0.23	2.84	34,50,68,71	0
3	EDO	A	9	4/4	0.80	0.27	2.72	38,40,45,46	0
3	EDO	C	12	4/4	0.88	0.18	2.62	40,45,47,52	0
6	PO4	C	17	5/5	0.94	0.19	2.48	22,22,30,35	1
3	EDO	A	10	4/4	0.89	0.18	2.23	36,38,40,42	0
3	EDO	C	4	4/4	0.92	0.13	2.02	36,40,43,51	0
3	EDO	B	8	4/4	0.88	0.19	1.98	37,41,46,53	0
3	EDO	D	440	4/4	0.87	0.17	1.80	21,25,29,33	0
6	PO4	A	20	5/5	0.91	0.21	1.79	20,22,29,32	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	EDO	C	8	4/4	0.85	0.20	1.68	35,38,39,40	0
3	EDO	A	4	4/4	0.93	0.11	1.65	25,26,30,31	0
4	DMS	C	10	4/4	0.92	0.15	1.52	36,42,51,60	0
6	PO4	D	24	5/5	0.93	0.18	1.51	22,22,25,25	3
3	EDO	C	11	4/4	0.85	0.15	1.41	38,43,44,46	0
3	EDO	A	19	4/4	0.86	0.26	1.33	47,50,50,55	0
7	JN4	A	23	29/29	0.82	0.23	1.32	32,43,77,82	0
4	DMS	A	442	4/4	0.95	0.19	1.30	34,41,44,50	0
3	EDO	C	5	4/4	0.90	0.18	1.21	38,40,41,44	0
4	DMS	D	23	4/4	0.88	0.21	1.04	20,39,43,45	0
3	EDO	B	9	4/4	0.83	0.14	0.75	31,38,38,39	0
3	EDO	B	4	4/4	0.86	0.17	0.57	34,44,44,47	0
7	JN4	B	21	29/29	0.92	0.14	0.56	29,35,56,64	0
7	JN4	D	442	29/29	0.87	0.17	0.51	28,40,63,67	0
3	EDO	D	4	4/4	0.95	0.10	0.38	23,24,27,31	0
7	JN4	C	18	29/29	0.90	0.17	0.33	32,40,57,65	0
3	EDO	C	6	4/4	0.92	0.13	0.18	39,39,41,46	0
3	EDO	C	440	4/4	0.91	0.14	0.15	43,43,44,49	0
3	EDO	A	14	4/4	0.94	0.11	-0.05	24,30,30,37	0
3	EDO	A	7	4/4	0.90	0.11	-0.37	39,42,43,45	0
3	EDO	B	10	4/4	0.90	0.13	-0.51	32,33,41,48	0
3	EDO	D	7	4/4	0.94	0.11	-0.55	28,29,32,37	0
2	ZN	A	2	1/1	0.99	0.08	-1.21	25,25,25,25	1
2	ZN	C	1	1/1	1.00	0.10	-1.35	24,24,24,24	0
2	ZN	D	2	1/1	0.99	0.07	-1.40	24,24,24,24	1
2	ZN	D	1	1/1	1.00	0.09	-1.54	21,21,21,21	0
2	ZN	A	1	1/1	1.00	0.10	-1.55	22,22,22,22	0
2	ZN	B	2	1/1	0.98	0.08	-1.55	27,27,27,27	1
2	ZN	C	2	1/1	0.99	0.08	-1.68	24,24,24,24	1
2	ZN	B	1	1/1	0.99	0.07	-1.93	25,25,25,25	0
3	EDO	A	18	4/4	0.91	0.22	-	21,38,41,44	0
3	EDO	D	11	4/4	0.90	0.18	-	38,40,44,45	0
4	DMS	D	8	4/4	0.85	0.32	-	37,47,52,62	0
3	EDO	D	10	4/4	0.77	0.17	-	38,45,47,49	0
3	EDO	B	17	4/4	0.88	0.25	-	44,47,52,55	0
4	DMS	A	6	4/4	0.91	0.30	-	42,43,44,55	0
3	EDO	A	13	4/4	0.94	0.13	-	25,30,38,42	0
3	EDO	A	441	4/4	0.88	0.28	-	33,39,44,45	0
3	EDO	A	5	4/4	0.88	0.13	-	42,43,46,48	0
3	EDO	D	18	4/4	0.82	0.24	-	41,43,44,47	0

6.5 Other polymers

There are no such residues in this entry.