



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:26 PM UTC

PDB ID : 1I8J / pdb_00001i8j
Title : CRYSTAL STRUCTURE OF PORPHOBILINOGEN SYNTHASE COM-
PLEXED WITH THE INHIBITOR 4,7-DIOXOSEBACIC ACID
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Deposited on : 2001-03-14
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

<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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

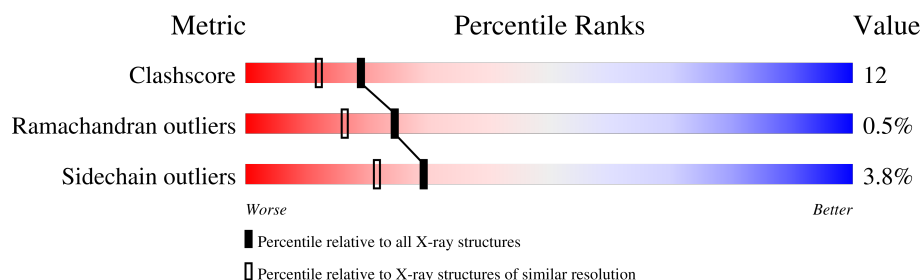
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	323	
1	B	323	

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
4	DSB	A	350	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5254 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 PORPHOBILINOGEN SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2453	1533	427	475	18			
1	B	323	Total	C	N	O	S	0	0	0
			2453	1533	427	475	18			

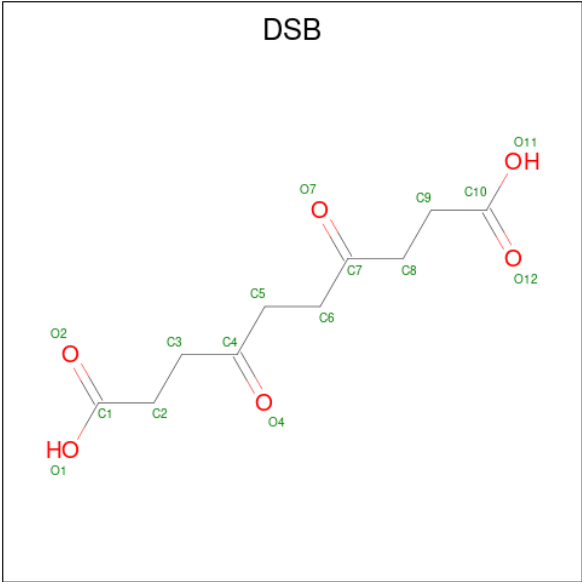
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 4,7-DIOXOSEBACIC ACID (CCD ID: DSB) (formula: C₁₀H₁₄O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	10	4		
4	B	1	Total	C	O	0	0
			14	10	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	164	Total	O	0	0
			164	164		
5	B	152	Total	O	0	0
			152	152		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: PORPHOBILINOGEN SYNTHASE

Chain A: 



• Molecule 1: PORPHOBILINOGEN SYNTHASE

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.74Å 128.74Å 142.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (35.00-1.90)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5254	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.08	2/2491 (0.1%)	1.27	19/3362 (0.6%)
1	B	1.07	6/2491 (0.2%)	1.26	22/3362 (0.7%)
All	All	1.08	8/4982 (0.2%)	1.26	41/6724 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	53	MET	SD-CE	9.48	2.03	1.79
1	B	271	VAL	CA-CB	7.50	1.61	1.54
1	A	131	VAL	CA-CB	7.19	1.62	1.54
1	B	39	GLU	CA-C	6.81	1.61	1.52
1	B	39	GLU	CB-CG	5.78	1.69	1.52
1	B	72	ILE	CA-CB	5.33	1.60	1.54
1	A	277	MET	SD-CE	-5.32	1.66	1.79
1	B	114	VAL	CA-CB	5.15	1.60	1.54

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	HIS	N-CA-C	9.23	121.34	111.28
1	B	191	TYR	N-CA-C	-8.74	95.49	109.39
1	A	191	TYR	N-CA-C	-7.61	98.20	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ALA	N-CA-C	7.33	119.91	111.11
1	A	220	MET	N-CA-C	7.19	120.26	110.55
1	B	313	ALA	N-CA-C	7.05	119.86	111.33
1	A	192	SER	N-CA-C	6.82	118.36	111.07
1	A	136	GLY	N-CA-C	-6.79	101.59	110.29
1	A	109	VAL	CA-C-N	6.78	127.33	119.47
1	A	109	VAL	C-N-CA	6.78	127.33	119.47
1	B	219	GLN	N-CA-C	-6.71	101.04	110.50
1	B	86	GLU	N-CA-C	6.65	118.60	111.36
1	B	271	VAL	N-CA-C	6.57	119.95	110.09
1	A	271	VAL	N-CA-C	6.50	117.56	110.21
1	B	136	GLY	N-CA-C	-6.37	98.08	113.18
1	A	86	GLU	N-CA-C	6.16	118.80	111.71
1	B	134	GLU	N-CA-C	-6.10	104.70	111.71
1	B	146	LEU	N-CA-C	-6.08	104.73	111.36
1	B	30	LEU	N-CA-C	6.07	119.72	109.76
1	A	12	LYS	N-CA-C	6.07	117.97	111.36
1	A	81	SER	N-CA-C	6.03	120.09	109.96
1	B	224	ASN	N-CA-C	5.99	119.07	108.24
1	B	141	ALA	N-CA-C	-5.92	104.91	111.36
1	B	81	SER	N-CA-C	5.72	119.24	110.20
1	B	220	MET	N-CA-C	5.67	117.85	110.53
1	A	4	ILE	N-CA-C	-5.61	105.63	111.58
1	B	236	GLU	N-CA-C	-5.58	105.28	111.36
1	B	89	SER	N-CA-C	5.52	119.11	112.38
1	A	236	GLU	N-CA-C	-5.47	105.31	111.28
1	A	253	ASP	N-CA-C	-5.39	105.49	111.36
1	B	249	GLY	N-CA-C	5.38	119.39	112.83
1	A	41	ASP	N-CA-C	5.34	120.28	113.55
1	B	41	ASP	N-CA-C	5.33	120.43	113.88
1	B	216	LYS	N-CA-C	5.29	119.22	112.87
1	B	54	ARG	N-CA-C	-5.26	102.06	109.96
1	A	30	LEU	N-CA-C	5.23	118.33	109.76
1	A	20	PHE	N-CA-C	5.20	119.31	112.92
1	B	115	MET	N-CA-C	-5.18	100.79	109.24
1	B	197	SER	N-CA-C	5.08	117.41	110.55
1	B	4	ILE	N-CA-C	-5.06	105.22	112.35
1	A	224	ASN	N-CA-C	5.03	117.35	108.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	TYR	Sidechain

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	2453	0	2403	59	1
1	B	2453	0	2404	71	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	14	0	12	8	0
4	B	14	0	12	5	0
5	A	164	0	0	3	0
5	B	152	0	0	3	0
All	All	5254	0	4831	115	2

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 (115) 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:53:MET:SD	1:B:53:MET:CE	2.03	1.47
1:B:194:LYS:NZ	1:B:246:LYS:HE2	1.55	1.17
1:A:194:LYS:NZ	1:A:246:LYS:HE2	1.65	1.11
1:A:277:MET:HE1	1:B:278:ILE:HG12	1.37	1.02
1:B:194:LYS:NZ	1:B:246:LYS:CE	2.32	0.94
1:A:287:ILE:HD13	1:B:277:MET:HE3	1.53	0.90
1:A:277:MET:CE	1:B:278:ILE:HG12	2.03	0.88
1:B:246:LYS:HE2	4:B:350:DSB:C7	2.02	0.88
1:A:278:ILE:HA	1:B:277:MET:HE2	1.56	0.88
1:B:126:HIS:CE1	1:B:132:LEU:HD13	2.12	0.84
1:A:277:MET:HE2	1:B:278:ILE:HA	1.57	0.83
1:A:194:LYS:NZ	1:A:246:LYS:CE	2.41	0.83
1:A:246:LYS:HE2	4:A:350:DSB:C7	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:GLU:OE2	1:B:83:HIS:HE1	1.66	0.78
1:A:292:VAL:HG11	1:B:277:MET:HE1	1.67	0.76
1:B:39:GLU:OE2	1:B:83:HIS:CE1	2.38	0.76
1:B:246:LYS:CE	4:B:350:DSB:C7	2.64	0.75
1:B:39:GLU:CD	1:B:83:HIS:HE1	1.97	0.72
1:A:246:LYS:CE	4:A:350:DSB:C7	2.69	0.69
1:A:278:ILE:HG12	1:B:277:MET:HE1	1.72	0.69
1:A:277:MET:CE	1:B:278:ILE:HA	2.22	0.69
1:A:246:LYS:NZ	4:A:350:DSB:H82	2.08	0.67
1:B:58:LYS:HE3	1:B:59:HIS:NE2	2.09	0.66
1:B:194:LYS:HZ3	1:B:246:LYS:HE2	1.50	0.66
1:A:196:ALA:HA	1:A:219:GLN:HE21	1.61	0.64
1:B:38:GLU:HG2	1:B:82:HIS:HD2	1.63	0.63
1:B:196:ALA:HA	1:B:219:GLN:HE21	1.64	0.62
1:A:278:ILE:HG12	1:B:277:MET:CE	2.29	0.62
1:A:151:VAL:HG21	5:A:670:HOH:O	1.99	0.61
1:A:292:VAL:HG11	1:B:277:MET:CE	2.29	0.61
1:B:315:ASP:N	1:B:315:ASP:OD1	2.35	0.59
1:A:45:ALA:HA	1:A:53:MET:HG2	1.84	0.59
4:A:350:DSB:H92	4:A:350:DSB:H51	1.85	0.59
1:B:263:GLU:HG2	5:B:499:HOH:O	2.02	0.58
1:B:58:LYS:HE3	1:B:59:HIS:CD2	2.38	0.58
1:A:100:ARG:O	1:A:104:ILE:HG13	2.02	0.58
1:A:315:ASP:OD2	1:A:319:LYS:HE3	2.04	0.58
1:B:53:MET:HE3	1:B:53:MET:HB2	1.86	0.58
1:A:1:THR:HG22	1:A:2:ASP:H	1.69	0.57
1:B:275:TYR:CD2	1:B:311:TYR:HB2	2.39	0.57
1:B:38:GLU:O	1:B:40:ILE:HG23	2.05	0.56
4:A:350:DSB:H51	4:A:350:DSB:C9	2.35	0.56
1:B:246:LYS:NZ	4:B:350:DSB:C7	2.68	0.56
1:A:46:VAL:HG11	1:A:206:ALA:HB2	1.88	0.55
1:B:126:HIS:ND1	1:B:128:HIS:HB2	2.22	0.55
1:B:162:ALA:HA	1:B:189:MET:O	2.07	0.55
1:B:73:ARG:NH1	5:B:523:HOH:O	2.40	0.54
1:B:164:SER:HB3	1:B:191:TYR:CE1	2.44	0.53
1:A:287:ILE:CD1	1:B:277:MET:HE3	2.31	0.53
1:A:119:CYS:SG	1:A:129:CYS:HB3	2.50	0.51
1:B:96:GLY:O	1:B:100:ARG:HG3	2.11	0.51
1:B:41:ASP:O	1:B:58:LYS:HE2	2.11	0.51
1:B:53:MET:CE	1:B:53:MET:CG	2.87	0.51
1:A:278:ILE:HA	1:B:277:MET:CE	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:HD21	1:A:168:ASP:O	2.10	0.51
1:A:277:MET:HE2	1:B:278:ILE:CA	2.33	0.50
1:B:53:MET:CE	1:B:53:MET:HB2	2.42	0.50
1:B:192:SER:HB2	1:B:232:SER:HA	1.94	0.50
1:A:273:GLY:O	1:A:277:MET:HG3	2.12	0.49
1:B:38:GLU:O	1:B:39:GLU:C	2.55	0.49
1:B:202:PRO:HB2	1:B:272:SER:HB2	1.94	0.49
1:B:46:VAL:HG11	1:B:206:ALA:HB2	1.95	0.49
1:B:1:THR:HG22	1:B:2:ASP:N	2.28	0.49
1:B:38:GLU:CG	1:B:82:HIS:HD2	2.26	0.48
1:B:45:ALA:HA	1:B:53:MET:HG2	1.96	0.48
1:A:38:GLU:HG3	1:A:82:HIS:HD2	1.78	0.48
1:A:246:LYS:NZ	4:A:350:DSB:C7	2.76	0.48
1:A:246:LYS:NZ	4:A:350:DSB:C8	2.77	0.48
1:A:277:MET:HE3	1:B:287:ILE:HD13	1.95	0.48
1:B:126:HIS:ND1	1:B:132:LEU:HD13	2.29	0.48
1:A:292:VAL:CG1	1:B:277:MET:HE1	2.41	0.48
1:B:35:PHE:HB3	1:B:80:ILE:HD11	1.95	0.48
1:B:195:PHE:CD1	1:B:222:PRO:HA	2.49	0.47
1:A:1:THR:HG22	1:A:2:ASP:N	2.29	0.47
1:B:41:ASP:HA	1:B:58:LYS:HE2	1.96	0.47
1:A:32:LEU:HD13	1:A:313:ALA:HB3	1.96	0.47
1:A:277:MET:HB3	1:B:277:MET:HB3	1.96	0.47
1:A:164:SER:O	1:A:194:LYS:HE2	2.14	0.47
1:B:143:LEU:HD22	1:B:170:GLN:HA	1.96	0.47
1:A:202:PRO:HB2	1:A:272:SER:HB2	1.96	0.47
1:A:43:TYR:OH	1:A:63:GLU:HG2	2.16	0.46
1:A:33:PRO:HB2	1:A:311:TYR:CE1	2.51	0.46
1:A:88:GLY:HA2	1:A:123:TYR:O	2.15	0.46
1:A:30:LEU:HD11	1:A:322:LEU:HD12	1.98	0.45
1:A:164:SER:HB3	1:A:191:TYR:CE1	2.51	0.45
1:B:33:PRO:HB2	1:B:311:TYR:CE1	2.52	0.44
1:A:119:CYS:SG	1:A:120:PHE:N	2.89	0.43
1:B:273:GLY:O	1:B:277:MET:HG3	2.18	0.43
1:B:40:ILE:HD12	1:B:42:ASP:O	2.19	0.43
5:A:603:HOH:O	1:B:139:ASN:HB2	2.19	0.43
4:B:350:DSB:H51	4:B:350:DSB:H91	1.99	0.43
1:A:67:ILE:HA	1:A:314:LEU:HD13	2.01	0.43
1:A:278:ILE:CA	1:B:277:MET:HE2	2.38	0.43
1:A:64:ILE:HD12	1:A:64:ILE:HA	1.86	0.42
1:B:49:MET:HE2	1:B:49:MET:HB3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:SER:HB2	1:B:194:LYS:HE3	2.00	0.42
1:B:31:VAL:HG11	1:B:309:PHE:CE1	2.54	0.42
1:B:30:LEU:HD11	1:B:322:LEU:HD12	2.01	0.42
1:B:64:ILE:HG23	1:B:109:VAL:HG23	2.01	0.42
1:A:48:ALA:HB2	1:A:205:GLU:OE1	2.19	0.42
1:B:106:LYS:HE2	5:B:674:HOH:O	2.18	0.42
1:A:126:HIS:ND1	1:A:128:HIS:HB2	2.35	0.42
1:A:244:MET:HA	1:A:267:GLY:O	2.19	0.42
1:A:236:GLU:HG2	5:A:636:HOH:O	2.20	0.41
1:A:32:LEU:HD23	1:A:67:ILE:HD13	2.02	0.41
1:B:191:TYR:CE2	4:B:350:DSB:H61	2.54	0.41
1:A:55:ILE:HG12	1:A:63:GLU:HG3	2.03	0.41
1:A:93:ARG:C	1:A:95:ASP:N	2.78	0.41
1:A:220:MET:HB2	1:A:220:MET:HE3	1.85	0.41
1:A:281:ALA:HB2	1:B:277:MET:HA	2.02	0.41
1:A:133:CYS:O	1:A:134:GLU:C	2.62	0.41
1:B:164:SER:HB3	1:B:191:TYR:CD1	2.56	0.40
1:A:246:LYS:HE2	4:A:350:DSB:C6	2.51	0.40
1:A:190:SER:OG	1:A:235:ASP:OD2	2.37	0.40
1:B:164:SER:HB2	1:B:194:LYS:CE	2.52	0.40

All (2) 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:B:39:GLU:OE2	1:B:39:GLU:OE2[8_665]	1.35	0.85
1:A:39:GLU:OE2	1:A:39:GLU:OE2[8_666]	2.16	0.04

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	321/323 (99%)	309 (96%)	12 (4%)	0	100	100
1	B	321/323 (99%)	312 (97%)	6 (2%)	3 (1%)	14	6
All	All	642/646 (99%)	621 (97%)	18 (3%)	3 (0%)	24	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	GLU
1	B	210	ALA
1	B	129	CYS

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	250/258 (97%)	238 (95%)	12 (5%)	23	15
1	B	250/258 (97%)	243 (97%)	7 (3%)	38	32
All	All	500/516 (97%)	481 (96%)	19 (4%)	29	21

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	7	PRO
1	A	27	LEU
1	A	28	ASN
1	A	62	ARG
1	A	95	ASP
1	A	144	GLU
1	A	152	VAL
1	A	211	LEU
1	A	218	TYR
1	A	236	GLU
1	A	315	ASP
1	B	7	PRO

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Mol	Chain	Res	Type
1	B	27	LEU
1	B	62	ARG
1	B	64	ILE
1	B	111	GLU
1	B	263	GLU
1	B	315	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	82	HIS
1	A	83	HIS
1	A	107	GLN
1	A	149	GLN
1	A	172	GLN
1	A	219	GLN
1	B	82	HIS
1	B	83	HIS
1	B	170	GLN
1	B	219	GLN
1	B	270	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](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
4	DSB	B	350	1	13,13,15	0.98	0	14,14,18	1.45	2 (14%)
4	DSB	A	350	1	13,13,15	0.70	0	14,14,18	1.32	3 (21%)

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
4	DSB	B	350	1	-	4/11/11/15	-
4	DSB	A	350	1	-	5/11/11/15	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	350	DSB	C8-C9-C10	-3.04	106.56	114.51
4	A	350	DSB	O2-C1-C2	-2.42	115.43	123.09
4	A	350	DSB	O12-C10-C9	-2.14	116.31	123.09
4	A	350	DSB	C3-C2-C1	-2.13	108.94	114.51
4	B	350	DSB	O12-C10-C9	-2.11	116.42	123.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	350	DSB	C5-C6-C7-C8
4	A	350	DSB	C7-C8-C9-C10
4	B	350	DSB	C2-C3-C4-C5
4	A	350	DSB	C6-C7-C8-C9
4	B	350	DSB	C1-C2-C3-C4
4	B	350	DSB	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	B	350	DSB	O2-C1-C2-C3
4	A	350	DSB	C2-C3-C4-C5
4	A	350	DSB	O11-C10-C9-C8

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	350	DSB	5	0
4	A	350	DSB	8	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.