



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:10 AM UTC

PDB ID : 4HDK / pdb_00004hdk
Title : Crystal Structure of ArsAB in Complex with Phloroglucinol
Authors : Newmister, S.A.; Chan, C.H.; Escalante-Semerena, J.C.; Rayment, I.
Deposited on : 2012-10-02
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

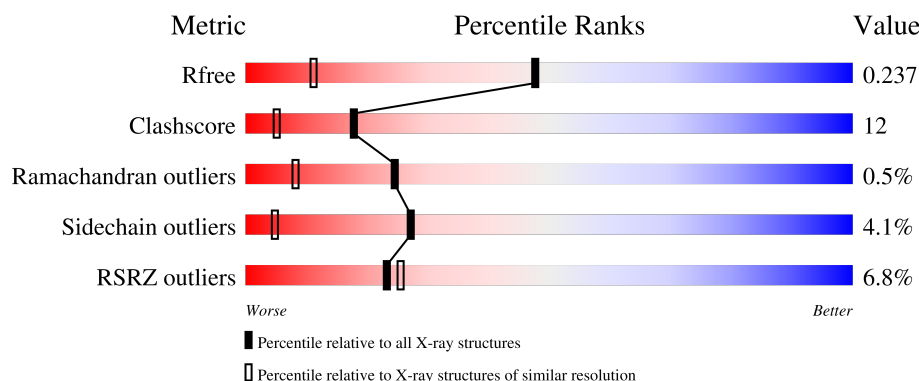
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	348	
2	B	350	

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
5	EDO	A	703	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5435 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 ArsA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	9	0
			2476	1558	431	467	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP F6MZ55
A	0	GLY	-	expression tag	UNP F6MZ55

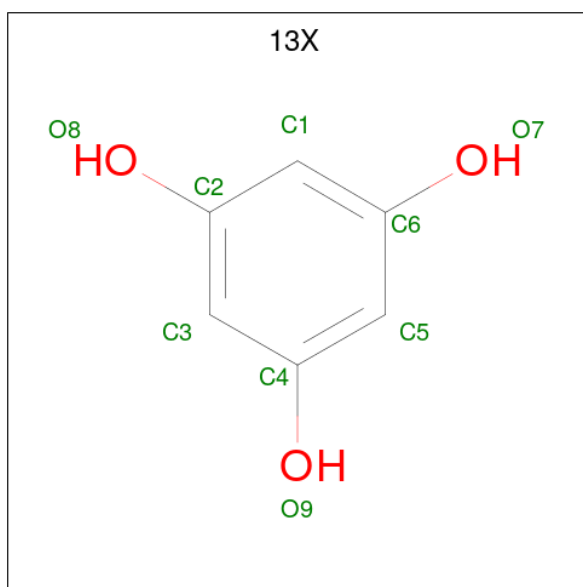
- Molecule 2 is a protein called ArsB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	327	Total	C	N	O	S	0	15	0
			2427	1536	425	443	23			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

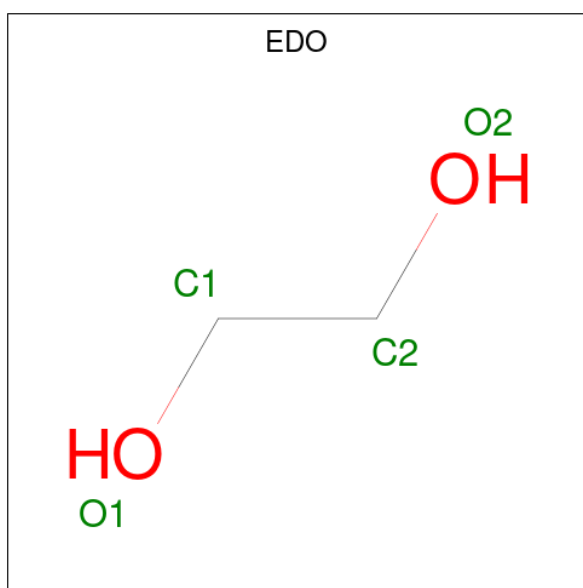
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is benzene-1,3,5-triol (CCD ID: 13X) (formula: C₆H₆O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	6	3		
4	B	1	Total	C	O	0	0
			9	6	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

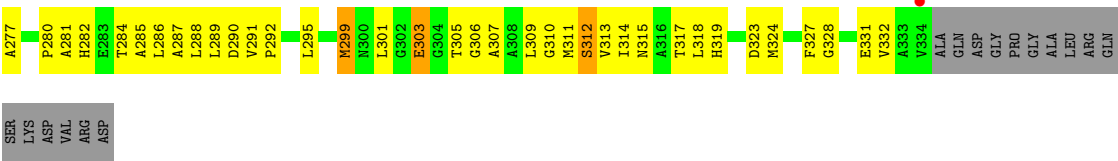
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	203	Total	O	0	0
			203	203		
6	B	298	Total	O	0	0
			298	298		



SER
LYS
ASP
VAL
ARG
ASP

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.78Å 77.36Å 152.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.50 50.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-1.50) 99.5 (50.00-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.189 , 0.223 (Not available) , 0.237	Depositor DCC
R_{free} test set	5021 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5435	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 13X, CL

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	2.18	137/2531 (5.4%)	1.19	15/3424 (0.4%)
2	B	2.36	189/2499 (7.6%)	1.15	11/3392 (0.3%)
All	All	2.27	326/5030 (6.5%)	1.17	26/6816 (0.4%)

All (326) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	211	ARG	C-O	-15.17	1.16	1.23
2	B	268	LYS	C-O	-10.01	1.15	1.24
2	B	68	GLY	C-O	-9.94	1.15	1.24
2	B	166	VAL	C-O	-9.84	1.14	1.24
1	A	330	LEU	C-N	-9.61	1.21	1.33
1	A	83	THR	C-O	-9.15	1.12	1.24
2	B	66	ASP	C-O	-8.98	1.13	1.23
2	B	110	ILE	C-O	-8.96	1.15	1.24
1	A	270[A]	THR	N-CA	-8.80	1.35	1.46
1	A	270[B]	THR	N-CA	-8.80	1.35	1.46
1	A	172	PHE	C-O	-8.60	1.13	1.24
1	A	326	VAL	C-O	-8.50	1.14	1.24
2	B	317	THR	C-O	-8.47	1.14	1.24
1	A	298	HIS	CG-ND1	-8.32	1.29	1.38
1	A	130[A]	ARG	N-CA	-8.27	1.36	1.46
1	A	130[B]	ARG	N-CA	-8.27	1.36	1.46
1	A	89	ALA	C-O	-8.15	1.14	1.24
2	B	272	ILE	C-O	-8.04	1.15	1.24
2	B	246	VAL	C-O	-7.99	1.15	1.24
2	B	250	GLY	C-O	-7.87	1.16	1.24
2	B	299[A]	MET	N-CA	-7.82	1.35	1.46
2	B	299[B]	MET	N-CA	-7.82	1.35	1.46
1	A	241	GLY	C-O	-7.80	1.16	1.23
2	B	11	PRO	C-O	-7.75	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	257	ALA	C-O	-7.70	1.15	1.24
2	B	319	HIS	CG-ND1	-7.60	1.29	1.38
2	B	64	ALA	C-O	-7.54	1.15	1.24
2	B	291	VAL	C-O	-7.53	1.15	1.23
1	A	60	PRO	C-O	-7.50	1.14	1.23
2	B	188	HIS	CG-ND1	-7.47	1.30	1.38
2	B	174	LEU	C-O	-7.44	1.15	1.23
2	B	277	ALA	C-O	-7.43	1.14	1.23
1	A	83	THR	N-CA	-7.32	1.37	1.46
1	A	247	ALA	C-O	-7.25	1.15	1.24
2	B	318	LEU	C-O	-7.24	1.15	1.24
2	B	285	ALA	C-O	-7.23	1.15	1.24
1	A	317	LEU	C-O	-7.21	1.15	1.23
2	B	270	TYR	C-O	-7.20	1.14	1.24
1	A	38	ARG	CA-C	-7.20	1.43	1.52
1	A	318	GLY	C-O	-7.19	1.14	1.23
1	A	171	CYS	C-O	-7.19	1.16	1.23
1	A	263	VAL	C-O	-7.19	1.16	1.24
1	A	227	LYS	C-O	-7.17	1.20	1.23
2	B	313	VAL	C-O	-7.17	1.15	1.24
1	A	324[A]	SER	C-O	-7.16	1.15	1.24
1	A	324[B]	SER	C-O	-7.16	1.15	1.24
2	B	155[A]	ILE	C-O	-7.15	1.16	1.24
2	B	155[B]	ILE	C-O	-7.15	1.16	1.24
2	B	182	ALA	C-O	-7.14	1.15	1.24
2	B	33	SER	C-O	-7.11	1.14	1.24
1	A	103	ALA	C-O	-7.09	1.15	1.24
1	A	63	VAL	C-O	-7.09	1.16	1.24
2	B	63	MET	C-O	-7.09	1.15	1.24
2	B	42[A]	CYS	C-O	-7.04	1.16	1.24
2	B	42[B]	CYS	C-O	-7.04	1.16	1.24
1	A	273	ALA	C-O	-7.02	1.16	1.24
2	B	47	ILE	C-O	-7.00	1.16	1.24
2	B	169	LEU	C-O	-6.97	1.15	1.24
2	B	260	ALA	C-O	-6.96	1.16	1.24
1	A	64	VAL	C-O	-6.92	1.16	1.24
1	A	65	ALA	C-O	-6.89	1.15	1.24
2	B	29	LYS	C-O	-6.89	1.15	1.24
2	B	50	ASN	C-O	-6.87	1.15	1.24
1	A	11	ILE	C-O	-6.84	1.16	1.24
2	B	17	MET	C-O	-6.84	1.16	1.24
2	B	21	GLN	C-O	-6.83	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	LEU	C-O	-6.81	1.16	1.24
2	B	306	GLY	C-O	-6.81	1.15	1.23
2	B	109	ASP	C-O	-6.78	1.15	1.23
2	B	307	ALA	C-O	-6.78	1.16	1.24
2	B	242	GLY	C-O	-6.77	1.16	1.24
1	A	4	LEU	C-O	-6.76	1.16	1.24
2	B	156	ALA	C-O	-6.75	1.16	1.24
2	B	256	ALA	C-O	-6.75	1.16	1.24
2	B	61	ILE	C-O	-6.72	1.16	1.24
2	B	288	LEU	C-O	-6.71	1.16	1.24
1	A	124	VAL	C-O	-6.71	1.16	1.24
2	B	10	LYS	C-O	-6.70	1.17	1.24
2	B	247	VAL	C-O	-6.67	1.17	1.24
1	A	110[A]	MET	C-O	-6.64	1.15	1.23
1	A	110[B]	MET	C-O	-6.64	1.15	1.23
1	A	222	ALA	C-O	-6.63	1.16	1.24
2	B	108	VAL	C-O	-6.63	1.17	1.24
2	B	103	ALA	C-O	-6.63	1.15	1.24
2	B	100	HIS	CG-ND1	-6.62	1.30	1.38
2	B	181[A]	MET	C-O	-6.62	1.16	1.24
2	B	181[B]	MET	C-O	-6.62	1.16	1.24
1	A	300	ILE	C-O	-6.62	1.16	1.24
2	B	205	THR	C-O	-6.61	1.16	1.24
2	B	37	PHE	C-O	-6.59	1.16	1.24
2	B	106[A]	ILE	C-O	-6.55	1.17	1.24
2	B	106[B]	ILE	C-O	-6.55	1.17	1.24
1	A	242	GLY	C-O	-6.51	1.15	1.23
2	B	49	GLY	C-O	-6.50	1.15	1.24
2	B	43	LYS	C-O	-6.50	1.16	1.24
2	B	112	VAL	C-O	-6.49	1.16	1.24
1	A	87[A]	MET	C-O	-6.48	1.15	1.24
1	A	87[B]	MET	C-O	-6.48	1.15	1.24
2	B	244	ALA	C-O	-6.45	1.16	1.24
1	A	113	VAL	C-O	-6.44	1.17	1.24
1	A	325	MET	C-O	-6.43	1.16	1.24
2	B	36	SER	C-O	-6.42	1.16	1.24
2	B	251	LEU	C-O	-6.41	1.16	1.24
1	A	69	HIS	C-O	-6.41	1.16	1.24
2	B	299[A]	MET	C-O	-6.40	1.16	1.24
2	B	299[B]	MET	C-O	-6.40	1.16	1.24
2	B	233	VAL	C-O	-6.39	1.16	1.24
2	B	258	LEU	C-O	-6.38	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	284	THR	C-O	-6.37	1.16	1.24
2	B	305	THR	C-O	-6.36	1.16	1.24
1	A	186	ALA	C-O	-6.33	1.16	1.24
1	A	152	GLN	C-O	-6.32	1.16	1.24
2	B	99	ALA	C-O	-6.32	1.16	1.24
2	B	120	PRO	C-O	-6.29	1.15	1.24
2	B	210	ASN	C-O	-6.28	1.15	1.24
2	B	44	LEU	C-O	-6.27	1.16	1.24
2	B	153	VAL	C-O	-6.26	1.17	1.24
1	A	183	THR	C-O	-6.25	1.16	1.24
1	A	327	VAL	C-O	-6.23	1.16	1.24
2	B	14	SER	C-O	-6.23	1.16	1.24
1	A	238	ALA	C-O	-6.23	1.17	1.24
2	B	253	THR	C-O	-6.22	1.16	1.24
2	B	220	ILE	C-O	-6.21	1.17	1.24
2	B	236	ILE	C-O	-6.20	1.17	1.24
1	A	226	ASN	C-O	-6.20	1.16	1.24
1	A	85	ILE	C-O	-6.19	1.17	1.24
2	B	147	GLN	C-O	-6.19	1.16	1.24
2	B	243	ARG	C-O	-6.18	1.15	1.23
2	B	314	ILE	C-O	-6.18	1.17	1.24
2	B	179	ALA	C-O	-6.18	1.16	1.24
1	A	258	ASN	C-O	-6.17	1.15	1.24
2	B	229	ILE	C-O	-6.17	1.17	1.24
1	A	185	SER	C-O	-6.16	1.17	1.24
1	A	99	ALA	C-O	-6.16	1.17	1.24
2	B	45	ALA	C-O	-6.12	1.17	1.24
1	A	250	GLY	C-O	-6.12	1.16	1.23
2	B	287	ALA	C-O	-6.11	1.16	1.24
2	B	145	ALA	C-O	-6.11	1.17	1.24
2	B	223	LYS	C-O	-6.10	1.17	1.24
1	A	61	CYS	C-O	-6.09	1.17	1.24
2	B	245	ALA	C-O	-6.08	1.16	1.23
2	B	249	ASP	C-O	-6.08	1.16	1.24
1	A	98	SER	C-O	-6.07	1.17	1.24
1	A	265	ASP	C-O	-6.06	1.16	1.24
2	B	98	ALA	C-O	-6.06	1.17	1.24
1	A	94	SER	C-O	-6.04	1.17	1.24
2	B	311	MET	C-O	-6.04	1.16	1.24
2	B	20	CYS	C-O	-6.02	1.17	1.24
2	B	177	LEU	C-O	-6.01	1.17	1.24
1	A	244	GLU	C-O	-6.00	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	56	LEU	C-O	-5.99	1.17	1.23
2	B	35	HIS	CG-ND1	-5.99	1.31	1.38
2	B	286	LEU	C-O	-5.98	1.17	1.24
1	A	154	VAL	C-O	-5.97	1.17	1.24
2	B	232	LEU	C-O	-5.96	1.16	1.24
1	A	134	TYR	C-O	-5.96	1.17	1.23
2	B	35	HIS	C-O	-5.95	1.16	1.24
2	B	16	ALA	C-O	-5.94	1.17	1.24
2	B	23	ARG	C-O	-5.93	1.17	1.24
2	B	35	HIS	CD2-NE2	-5.92	1.31	1.37
2	B	190	GLN	CA-C	-5.92	1.45	1.52
2	B	28	THR	C-O	-5.91	1.17	1.23
2	B	65	ALA	C-O	-5.91	1.16	1.23
2	B	227	LEU	C-O	-5.91	1.16	1.24
2	B	230	ALA	C-O	-5.90	1.17	1.24
1	A	118	ALA	C-O	-5.90	1.17	1.23
2	B	7	ALA	C-O	-5.89	1.16	1.24
1	A	47	ALA	C-O	-5.88	1.17	1.24
2	B	259[A]	ILE	C-O	-5.88	1.17	1.24
2	B	259[B]	ILE	C-O	-5.88	1.17	1.24
1	A	147	ARG	C-O	-5.88	1.17	1.24
1	A	126	GLY	C-O	-5.87	1.16	1.24
1	A	321	ILE	C-O	-5.87	1.17	1.24
1	A	303	ARG	C-O	-5.86	1.17	1.24
2	B	144	GLN	C-O	-5.84	1.17	1.24
2	B	148	ALA	C-O	-5.83	1.17	1.24
1	A	38	ARG	N-CA	-5.83	1.39	1.46
2	B	5	LEU	C-O	-5.83	1.17	1.24
1	A	43	VAL	C-O	-5.83	1.16	1.24
2	B	309	LEU	C-O	-5.83	1.16	1.24
1	A	20	ASP	C-O	-5.82	1.17	1.24
1	A	40	GLU	C-O	-5.80	1.17	1.24
2	B	171	GLU	C-O	-5.79	1.16	1.23
2	B	324	MET	C-O	-5.79	1.16	1.23
2	B	188	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	67	ALA	C-O	-5.78	1.16	1.23
2	B	271	LEU	C-O	-5.77	1.17	1.24
1	A	121	LEU	C-O	-5.77	1.16	1.24
1	A	57	LEU	C-O	-5.76	1.16	1.24
1	A	295	GLU	C-O	-5.75	1.16	1.23
1	A	100	ASN	C-O	-5.75	1.17	1.24
2	B	292	PRO	C-O	-5.75	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	116	LEU	C-O	-5.73	1.16	1.24
2	B	264	VAL	C-O	-5.73	1.17	1.24
2	B	267	VAL	C-O	-5.71	1.17	1.24
2	B	69	VAL	C-O	-5.69	1.18	1.24
2	B	218	LEU	C-O	-5.69	1.17	1.24
1	A	196	ALA	C-O	-5.69	1.16	1.23
2	B	159	GLU	C-O	-5.68	1.17	1.24
1	A	179	ILE	C-O	-5.67	1.18	1.24
2	B	57[A]	GLU	C-O	-5.67	1.17	1.24
2	B	57[B]	GLU	C-O	-5.67	1.17	1.24
2	B	55	ALA	C-O	-5.66	1.17	1.23
1	A	268	ASN	C-O	-5.65	1.17	1.24
2	B	118	HIS	CG-ND1	-5.64	1.32	1.38
1	A	248	LEU	C-O	-5.64	1.17	1.24
1	A	262	VAL	C-O	-5.64	1.18	1.24
1	A	310	CYS	C-O	-5.64	1.16	1.24
1	A	288	PHE	C-O	-5.64	1.17	1.24
1	A	182	THR	C-O	-5.61	1.16	1.24
2	B	87	PHE	C-O	-5.60	1.17	1.24
1	A	236	VAL	C-O	-5.60	1.17	1.24
2	B	34	LEU	C-O	-5.60	1.16	1.24
1	A	145	MET	C-O	-5.59	1.17	1.23
1	A	88	THR	C-O	-5.58	1.17	1.24
1	A	249	ALA	C-O	-5.58	1.17	1.24
1	A	112	VAL	C-O	-5.58	1.18	1.24
2	B	150	GLU	C-O	-5.58	1.17	1.24
1	A	287	MET	C-O	-5.58	1.17	1.23
1	A	313	LEU	C-O	-5.56	1.16	1.24
2	B	183	ILE	C-O	-5.56	1.17	1.24
2	B	96	VAL	C-O	-5.56	1.17	1.24
2	B	139	ALA	C-O	-5.56	1.17	1.24
1	A	286	TYR	C-O	-5.55	1.16	1.24
2	B	263	LEU	C-O	-5.54	1.17	1.24
2	B	265	PRO	C-O	-5.54	1.17	1.24
2	B	212	PRO	C-O	-5.53	1.17	1.23
1	A	93	ILE	C-O	-5.53	1.17	1.24
1	A	235	ASP	C-O	-5.51	1.17	1.24
1	A	232	ASP	C-O	-5.50	1.17	1.24
1	A	329	MET	C-O	-5.49	1.17	1.24
1	A	97	ALA	C-O	-5.49	1.16	1.23
1	A	122	SER	C-O	-5.49	1.17	1.24
2	B	219	ASP	C-O	-5.48	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	225	GLY	C-O	-5.47	1.18	1.23
2	B	115	ASP	C-O	-5.46	1.17	1.23
2	B	240	ALA	C-O	-5.46	1.17	1.24
2	B	146	ILE	C-O	-5.46	1.17	1.24
2	B	238	GLY	C-O	-5.46	1.17	1.23
2	B	315	ASN	C-O	-5.45	1.17	1.24
2	B	119	SER	C-O	-5.45	1.18	1.24
2	B	13	ASP	C-O	-5.44	1.16	1.23
2	B	176	GLY	C-O	-5.44	1.17	1.23
1	A	84	THR	C-O	-5.44	1.17	1.24
1	A	8	VAL	C-O	-5.43	1.17	1.24
1	A	160	ILE	C-O	-5.42	1.17	1.24
2	B	39	HIS	CG-ND1	-5.41	1.32	1.38
2	B	331	GLU	C-O	-5.39	1.17	1.24
2	B	142	ARG	C-O	-5.39	1.17	1.24
1	A	245	LEU	C-O	-5.38	1.17	1.24
2	B	48	SER	C-O	-5.38	1.17	1.24
2	B	170	GLY	C-O	-5.37	1.17	1.23
1	A	311	LEU	C-O	-5.37	1.17	1.24
2	B	137	GLY	C-O	-5.34	1.16	1.24
1	A	5	GLN	C-O	-5.34	1.17	1.24
1	A	167	HIS	CG-ND1	-5.34	1.32	1.38
1	A	173	CYS	C-O	-5.34	1.17	1.24
1	A	101	ALA	C-O	-5.33	1.17	1.24
2	B	239	ALA	C-O	-5.33	1.18	1.24
2	B	275	HIS	CD2-NE2	-5.33	1.31	1.37
2	B	221	LEU	C-O	-5.32	1.18	1.24
2	B	213	ASN	C-O	-5.32	1.17	1.24
2	B	282	HIS	CG-ND1	-5.32	1.32	1.38
1	A	312	GLU	C-O	-5.31	1.17	1.23
2	B	327	PHE	C-O	-5.31	1.18	1.24
1	A	66	SER	C-O	-5.30	1.17	1.24
2	B	160	ILE	C-O	-5.30	1.18	1.24
1	A	75	VAL	C-O	-5.30	1.17	1.24
2	B	323	ASP	C-O	-5.29	1.17	1.24
2	B	165	GLN	C-O	-5.29	1.17	1.24
2	B	97	PHE	C-O	-5.29	1.18	1.24
2	B	273	GLY	C-O	-5.29	1.15	1.23
2	B	217	PRO	C-O	-5.28	1.17	1.24
1	A	165	VAL	C-O	-5.27	1.17	1.24
1	A	323	ALA	C-O	-5.27	1.18	1.24
2	B	152	GLY	C-O	-5.27	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	HIS	CD2-NE2	-5.26	1.32	1.37
1	A	335	TYR	C-O	-5.25	1.18	1.24
1	A	22	VAL	C-O	-5.25	1.18	1.24
2	B	52	ARG	C-O	-5.25	1.18	1.24
2	B	274	SER	C-O	-5.25	1.17	1.24
1	A	114	ASP	C-O	-5.23	1.17	1.24
1	A	25[A]	LYS	C-O	-5.23	1.18	1.24
1	A	25[B]	LYS	C-O	-5.23	1.18	1.24
1	A	341	LEU	C-O	-5.23	1.18	1.24
2	B	83	ARG	C-O	-5.22	1.18	1.24
1	A	158	ILE	C-O	-5.21	1.18	1.24
2	B	228	ALA	C-O	-5.19	1.18	1.24
2	B	185	ALA	C-O	-5.18	1.18	1.24
1	A	162	ASN	C-O	-5.18	1.18	1.24
2	B	102	GLN	C-O	-5.18	1.17	1.23
1	A	328	ASP	C-O	-5.17	1.18	1.24
2	B	312	SER	C-O	-5.17	1.18	1.24
2	B	24	VAL	C-O	-5.15	1.18	1.24
1	A	285	GLU	C-O	-5.15	1.17	1.24
2	B	289	LEU	C-O	-5.14	1.17	1.24
1	A	255	SER	C-O	-5.13	1.18	1.24
2	B	94	ILE	C-O	-5.13	1.17	1.24
2	B	175	GLY	C-O	-5.12	1.17	1.24
2	B	168	GLY	C-O	-5.12	1.15	1.23
1	A	53	LEU	C-O	-5.12	1.18	1.24
1	A	177	MET	C-O	-5.10	1.18	1.23
2	B	207	ILE	C-O	-5.10	1.18	1.24
1	A	129	HIS	CD2-NE2	-5.09	1.32	1.37
1	A	251	VAL	C-O	-5.09	1.18	1.24
1	A	71	VAL	C-O	-5.09	1.17	1.24
2	B	101	VAL	C-O	-5.09	1.18	1.24
2	B	104[A]	ARG	C-O	-5.08	1.17	1.23
2	B	104[B]	ARG	C-O	-5.08	1.17	1.23
1	A	144	ALA	C-O	-5.08	1.18	1.24
1	A	119	GLY	C-O	-5.07	1.17	1.24
2	B	30	PRO	C-O	-5.07	1.17	1.23
2	B	231	GLY	C-O	-5.07	1.17	1.23
1	A	54	ASN	C-O	-5.07	1.18	1.24
1	A	151	ILE	C-O	-5.06	1.18	1.24
1	A	292	LEU	C-O	-5.06	1.18	1.24
1	A	237	LEU	C-O	-5.06	1.18	1.24
2	B	192	LEU	CA-C	-5.06	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	295	LEU	C-O	-5.05	1.18	1.24
1	A	290	SER	C-O	-5.05	1.17	1.24
1	A	149	GLN	C-O	-5.04	1.18	1.24
1	A	46	TYR	C-O	-5.04	1.18	1.24
2	B	15	ILE	C-O	-5.02	1.18	1.24
1	A	156	THR	C-O	-5.01	1.18	1.24
2	B	328	GLY	C-O	-5.01	1.17	1.23
2	B	310	GLY	C-O	-5.01	1.17	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	LEU	O-C-N	9.17	133.92	123.19
1	A	83	THR	N-CA-C	-8.99	101.37	111.71
1	A	124	VAL	N-CA-C	8.56	115.35	107.56
1	A	85	ILE	CB-CA-C	-8.35	101.28	111.97
2	B	163	GLY	N-CA-C	7.99	126.50	115.00
2	B	223	LYS	N-CA-C	7.23	118.95	111.14
2	B	190	GLN	N-CA-C	-6.87	101.96	108.07
1	A	239	LYS	N-CA-C	6.82	118.50	111.14
1	A	29	VAL	N-CA-C	6.38	116.53	110.53
2	B	190	GLN	CA-C-N	6.38	126.33	119.76
2	B	190	GLN	C-N-CA	6.38	126.33	119.76
2	B	48	SER	N-CA-C	6.12	118.03	111.36
1	A	294	GLY	N-CA-C	-6.11	102.20	111.42
2	B	303[A]	GLU	CA-C-O	-5.87	113.75	121.08
2	B	303[B]	GLU	CA-C-O	-5.87	113.75	121.08
1	A	203	ARG	N-CA-C	5.85	118.75	110.50
1	A	29	VAL	CB-CA-C	-5.82	104.40	112.02
1	A	30	LEU	N-CA-C	-5.57	102.94	110.68
1	A	38	ARG	CA-C-O	-5.50	113.88	120.10
2	B	190	GLN	O-C-N	5.35	126.86	121.56
1	A	80	PRO	CA-C-N	5.31	128.86	120.47
1	A	80	PRO	C-N-CA	5.31	128.86	120.47
1	A	130[A]	ARG	CA-C-O	-5.19	115.30	121.32
1	A	130[B]	ARG	CA-C-O	-5.19	115.30	121.32
2	B	91	GLN	N-CA-C	5.14	119.65	113.17
2	B	209	VAL	N-CA-C	5.11	115.88	110.72

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	2476	0	2557	70	0
2	B	2427	0	2561	64	0
3	A	1	0	0	1	0
4	A	9	0	4	3	0
4	B	9	0	4	0	0
5	A	4	0	6	0	0
5	B	8	0	12	0	0
6	A	203	0	0	10	0
6	B	298	0	0	15	0
All	All	5435	0	5144	124	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 (124) 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:259:ARG:HG2	1:A:259:ARG:HH11	1.17	1.09
1:A:33:ALA:HB2	2:B:78:MET:HE1	1.09	1.09
1:A:32:SER:OG	2:B:77:GLN:HA	1.55	1.06
1:A:33:ALA:HB2	2:B:78:MET:CE	1.86	1.05
1:A:87[A]:MET:HE1	1:A:90[A]:ASN:HD22	1.20	1.03
2:B:243:ARG:HD3	6:B:544:HOH:O	1.60	1.01
1:A:75:VAL:HG12	1:A:218:ILE:CD1	1.90	1.00
2:B:181[A]:MET:HE1	2:B:280:PRO:HB2	1.42	0.97
2:B:104[B]:ARG:NH2	6:B:694:HOH:O	1.98	0.96
1:A:2:SER:HB3	1:A:5:GLN:HE21	1.32	0.95
1:A:36:LEU:HD22	2:B:299[A]:MET:HE3	1.47	0.93
1:A:205:THR:HG22	1:A:206:GLY:H	1.33	0.92
1:A:2:SER:CB	1:A:5:GLN:HE21	1.85	0.90
1:A:36:LEU:HD22	2:B:299[A]:MET:CE	2.05	0.87
2:B:108:VAL:HG21	2:B:155[A]:ILE:HD13	1.58	0.85
1:A:83:THR:HG23	1:A:87[B]:MET:SD	2.17	0.85
1:A:83:THR:CG2	1:A:87[B]:MET:SD	2.66	0.83
2:B:42[B]:CYS:SG	6:B:772:HOH:O	2.20	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181[A]:MET:CE	2:B:280:PRO:HB2	2.10	0.81
1:A:205:THR:HG22	1:A:206:GLY:N	1.95	0.81
1:A:87[A]:MET:CE	1:A:90[A]:ASN:HD22	1.94	0.80
2:B:243:ARG:CD	6:B:544:HOH:O	2.23	0.80
1:A:280:HIS:HD2	1:A:282:LEU:H	1.31	0.78
2:B:190:GLN:CB	2:B:191:PRO:HD2	2.15	0.76
1:A:75:VAL:CG1	1:A:218:ILE:CD1	2.63	0.76
1:A:292:LEU:HB2	6:A:909:HOH:O	1.85	0.76
1:A:75:VAL:CG1	1:A:218:ILE:HD13	2.17	0.74
2:B:251:LEU:O	2:B:255[A]:THR:HG23	1.87	0.74
2:B:172:MET:HE2	2:B:303[B]:GLU:CD	2.13	0.74
2:B:211:ARG:HD3	6:B:703:HOH:O	1.87	0.74
2:B:190:GLN:HB2	2:B:191:PRO:HD2	1.70	0.73
2:B:69:VAL:HG23	2:B:69:VAL:O	1.89	0.72
1:A:200:VAL:HG13	1:A:297:ALA:HB2	1.70	0.72
1:A:259:ARG:HG2	1:A:259:ARG:NH1	1.91	0.71
1:A:87[A]:MET:HE1	1:A:90[A]:ASN:ND2	2.03	0.71
2:B:211:ARG:HG3	2:B:211:ARG:HH11	1.54	0.70
1:A:87[A]:MET:SD	4:A:702:13X:C1	2.79	0.70
2:B:2:LEU:HG	2:B:3:GLU:OE2	1.92	0.70
1:A:295:GLU:HB2	1:A:296:PRO:HD2	1.74	0.70
1:A:130[A]:ARG:NH1	6:A:928:HOH:O	2.25	0.69
1:A:83:THR:HG22	1:A:87[B]:MET:SD	2.32	0.69
2:B:184[A]:VAL:HG23	2:B:192:LEU:HD11	1.76	0.66
2:B:47:ILE:O	2:B:243:ARG:HD2	1.96	0.66
1:A:75:VAL:HG12	1:A:218:ILE:HD12	1.78	0.66
1:A:295:GLU:HB2	1:A:296:PRO:CD	2.27	0.65
1:A:69:HIS:HE1	1:A:244:GLU:OE2	1.80	0.63
1:A:200:VAL:HG12	1:A:200:VAL:O	1.97	0.63
1:A:36:LEU:CD2	2:B:299[A]:MET:HE3	2.25	0.63
1:A:130[B]:ARG:NH2	3:A:701:CL:CL	2.69	0.61
1:A:205:THR:CG2	1:A:206:GLY:H	2.11	0.61
1:A:36:LEU:HD22	2:B:299[B]:MET:SD	2.42	0.60
2:B:181[A]:MET:HE1	2:B:280:PRO:CB	2.26	0.60
1:A:36:LEU:CD2	2:B:299[A]:MET:CE	2.78	0.60
2:B:214:ALA:HA	2:B:220:ILE:HD11	1.85	0.59
2:B:181[B]:MET:HE1	2:B:280:PRO:HB2	1.84	0.59
2:B:177:LEU:O	2:B:181[B]:MET:HG3	2.03	0.58
2:B:164:CYS:N	6:B:728:HOH:O	2.37	0.58
1:A:161:VAL:O	1:A:165:VAL:HG13	2.05	0.57
2:B:184[A]:VAL:HG11	2:B:255[A]:THR:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181[A]:MET:HE1	2:B:280:PRO:O	2.04	0.56
1:A:280:HIS:CD2	1:A:282:LEU:H	2.17	0.55
2:B:133:ASN:C	2:B:133:ASN:HD22	2.14	0.55
2:B:69:VAL:O	2:B:69:VAL:CG2	2.56	0.54
2:B:211:ARG:HG3	2:B:211:ARG:NH1	2.23	0.53
1:A:284:LYS:HE2	6:A:999:HOH:O	2.09	0.53
1:A:200:VAL:O	1:A:200:VAL:CG1	2.57	0.53
2:B:184[A]:VAL:CG1	2:B:255[A]:THR:HG22	2.38	0.53
2:B:172:MET:HE2	2:B:303[B]:GLU:OE2	2.09	0.52
1:A:73:ARG:HB2	6:A:981:HOH:O	2.09	0.52
1:A:215:LYS:HD3	6:A:893:HOH:O	2.09	0.52
2:B:108:VAL:CG2	2:B:155[A]:ILE:HD13	2.37	0.52
2:B:133:ASN:HD22	2:B:135:THR:H	1.58	0.52
1:A:148:GLU:H	1:A:148:GLU:CD	2.18	0.51
2:B:181[B]:MET:CE	2:B:280:PRO:HB2	2.39	0.51
1:A:87[A]:MET:SD	4:A:702:13X:H6	2.50	0.51
1:A:110[B]:MET:HG3	6:A:826:HOH:O	2.10	0.51
1:A:145:MET:HG2	1:A:238:ALA:HA	1.93	0.50
1:A:31:GLN:O	1:A:32:SER:HB3	2.11	0.50
2:B:172:MET:CE	2:B:303[B]:GLU:CD	2.84	0.50
1:A:36:LEU:HA	2:B:299[B]:MET:HG2	1.93	0.49
2:B:42[A]:CYS:SG	6:B:700:HOH:O	2.39	0.49
2:B:186[B]:CYS:SG	2:B:220:ILE:HG12	2.52	0.49
2:B:290[B]:ASP:OD2	6:B:596:HOH:O	2.20	0.49
2:B:2:LEU:CB	6:B:715:HOH:O	2.60	0.48
1:A:266:GLY:O	1:A:270[B]:THR:HG23	2.12	0.48
2:B:2:LEU:HB2	6:B:715:HOH:O	2.13	0.48
2:B:190:GLN:HB2	2:B:191:PRO:CD	2.42	0.48
1:A:85:ILE:HG13	6:A:818:HOH:O	2.13	0.48
2:B:181[A]:MET:HE1	2:B:280:PRO:C	2.38	0.48
1:A:32:SER:O	2:B:77:GLN:HB3	2.14	0.48
2:B:108:VAL:HG21	2:B:155[A]:ILE:CD1	2.38	0.47
1:A:87[A]:MET:HE2	4:A:702:13X:O7	2.15	0.47
1:A:2:SER:HB3	1:A:5:GLN:NE2	2.14	0.46
1:A:292:LEU:HD23	1:A:309:ALA:HB3	1.97	0.46
2:B:190:GLN:CB	2:B:191:PRO:CD	2.89	0.46
1:A:292:LEU:N	6:A:909:HOH:O	2.48	0.46
1:A:75:VAL:HG12	1:A:218:ILE:HD11	1.91	0.46
2:B:193:PRO:HA	2:B:194:GLY:HA2	1.59	0.46
1:A:29:VAL:O	1:A:31:GLN:HG2	2.15	0.46
2:B:268:LYS:HD3	2:B:268:LYS:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:GLY:C	6:B:728:HOH:O	2.59	0.45
2:B:136:GLU:HB2	6:B:789:HOH:O	2.17	0.44
1:A:139:PHE:HA	1:A:142:GLY:O	2.18	0.44
2:B:15:ILE:HG12	6:B:717:HOH:O	2.17	0.44
1:A:31:GLN:O	1:A:32:SER:CB	2.66	0.43
1:A:29:VAL:C	1:A:31:GLN:N	2.77	0.43
1:A:200:VAL:CG1	1:A:297:ALA:HB2	2.44	0.43
2:B:243:ARG:HD2	6:B:544:HOH:O	2.06	0.43
2:B:10:LYS:HD2	2:B:10:LYS:HA	1.65	0.43
1:A:15:ASP:OD1	1:A:15:ASP:C	2.62	0.42
1:A:85:ILE:HG23	1:A:121:LEU:HD21	2.00	0.42
1:A:81:ILE:HD13	6:A:929:HOH:O	2.19	0.42
1:A:295:GLU:CB	1:A:296:PRO:CD	2.95	0.42
1:A:148:GLU:CD	1:A:148:GLU:N	2.77	0.42
2:B:280:PRO:O	2:B:281:ALA:HB3	2.20	0.42
1:A:83:THR:HB	1:A:179:ILE:HD11	2.02	0.41
1:A:69:HIS:HD2	6:A:803:HOH:O	2.04	0.41
2:B:154:ARG:HG3	6:B:708:HOH:O	2.20	0.41
1:A:81:ILE:HA	1:A:179:ILE:HG21	2.03	0.41
2:B:133:ASN:ND2	2:B:135:THR:H	2.19	0.41
1:A:38:ARG:HH11	1:A:308[A]:GLU:HB3	1.87	0.40
2:B:63:MET:HE1	2:B:155[A]:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/348 (96%)	327 (98%)	6 (2%)	2 (1%)	21	6
2	B	338/350 (97%)	331 (98%)	6 (2%)	1 (0%)	36	17
All	All	673/698 (96%)	658 (98%)	12 (2%)	3 (0%)	24	12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	GLY
1	A	309	ALA
2	B	193	PRO

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	264/264 (100%)	252 (96%)	12 (4%)	24	4
2	B	253/256 (99%)	244 (96%)	9 (4%)	31	6
All	All	517/520 (99%)	496 (96%)	21 (4%)	27	5

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	23	LYS
1	A	25[A]	LYS
1	A	25[B]	LYS
1	A	53	LEU
1	A	139	PHE
1	A	165	VAL
1	A	197	PRO
1	A	208	SER
1	A	213	LYS
1	A	259	ARG
1	A	306	GLN
2	B	2	LEU
2	B	77	GLN
2	B	78	MET
2	B	133	ASN
2	B	190	GLN
2	B	195	LEU
2	B	198	ARG
2	B	301	LEU

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Mol	Chain	Res	Type
2	B	312	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	69	HIS
1	A	258	ASN
1	A	268	ASN
1	A	277	ASN
1	A	280	HIS
2	B	133	ASN

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, 1 is monoatomic - leaving 5 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	13X	A	702	-	9,9,9	1.74	1 (11%)	12,12,12	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	403	-	3,3,3	1.13	0	2,2,2	0.61	0
5	EDO	A	703	-	3,3,3	1.49	1 (33%)	2,2,2	2.09	1 (50%)
5	EDO	B	401	-	3,3,3	0.94	0	2,2,2	0.36	0
4	13X	B	402	-	9,9,9	1.10	1 (11%)	12,12,12	1.26	1 (8%)

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	13X	A	702	-	-	-	0/1/1/1
5	EDO	B	403	-	-	1/1/1/1	-
5	EDO	A	703	-	-	1/1/1/1	-
5	EDO	B	401	-	-	0/1/1/1	-
4	13X	B	402	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	13X	C3-C2	-3.38	1.34	1.39
5	A	703	EDO	O1-C1	2.31	1.53	1.42
4	B	402	13X	C1-C6	2.12	1.42	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	703	EDO	O1-C1-C2	-2.81	91.02	112.39
4	B	402	13X	O9-C4-C3	-2.03	114.53	119.85

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	703	EDO	O1-C1-C2-O2
5	B	403	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	702	13X	3	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	332/348 (95%)	0.71	30 (9%)	15 16	9, 21, 40, 78	9 (2%)
2	B	327/350 (93%)	0.25	15 (4%)	37 41	8, 16, 39, 70	15 (4%)
All	All	659/698 (94%)	0.48	45 (6%)	23 25	8, 19, 40, 78	24 (3%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308[A]	GLU	6.0
2	B	193	PRO	5.6
1	A	29	VAL	5.1
1	A	80	PRO	4.9
1	A	76	VAL	4.9
2	B	334	VAL	4.8
1	A	292	LEU	4.2
1	A	81	ILE	4.1
2	B	195	LEU	4.0
1	A	32	SER	3.9
2	B	215	ALA	3.3
2	B	70	ALA	3.2
2	B	194	GLY	3.1
1	A	316	ARG	3.0
2	B	191	PRO	3.0
1	A	294	GLY	3.0
1	A	207	ILE	3.0
1	A	204	GLY	3.0
2	B	196	ALA	2.9
2	B	2	LEU	2.9
2	B	189	GLY	2.8
1	A	17	VAL	2.8
2	B	214	ALA	2.6
2	B	200	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	53	LEU	2.6
1	A	205	THR	2.5
1	A	16	THR	2.5
1	A	28	GLY	2.5
2	B	82	ALA	2.4
1	A	213	LYS	2.4
1	A	200	VAL	2.4
1	A	30	LEU	2.4
2	B	69	VAL	2.3
1	A	343	ASN	2.3
1	A	18	ILE	2.3
1	A	123	TYR	2.3
1	A	13	ARG	2.2
1	A	27	ALA	2.1
1	A	56	ALA	2.1
1	A	51	GLY	2.1
1	A	293	SER	2.1
1	A	24	THR	2.0
1	A	31	GLN	2.0
2	B	77	GLN	2.0
1	A	225	VAL	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
5	EDO	A	703	4/4	0.73	0.16	27,30,34,38	0
5	EDO	B	401	4/4	0.87	0.14	25,28,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	13X	B	402	9/9	0.89	0.10	31,34,35,46	0
4	13X	A	702	9/9	0.91	0.09	15,17,19,22	0
5	EDO	B	403	4/4	0.93	0.10	20,25,27,31	0
3	CL	A	701	1/1	0.94	0.10	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.