



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:01 PM UTC

PDB ID : 4DBH / pdb_00004dbh
Title : Crystal structure of Cg1458 with inhibitor
Authors : Ran, T.T.; Wang, W.W.; Xu, D.Q.; Gao, Y.Y.
Deposited on : 2012-01-15
Resolution : 1.94 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

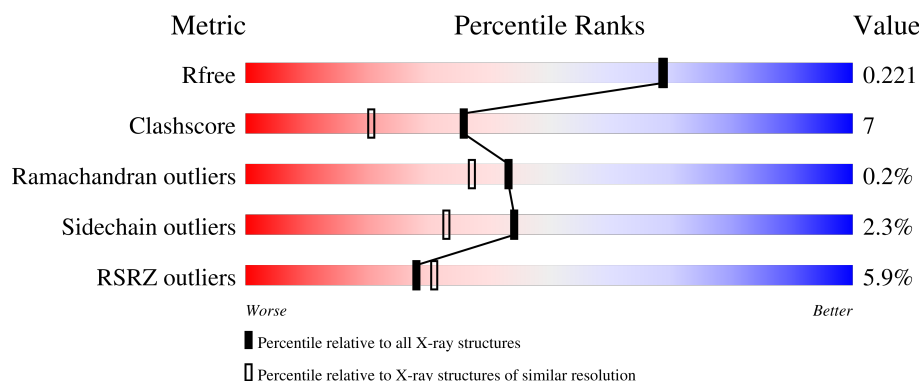
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	288	
1	B	288	

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	OXL	A	402	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4477 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 2-HYDROXYHEPTA-2,4-DIENE-1,7-DIOATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	1	0
			2055	1306	342	396	11			
1	B	269	Total	C	N	O	S	0	1	0
			2040	1298	341	390	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q8NQY2
A	-18	GLY	-	expression tag	UNP Q8NQY2
A	-17	SER	-	expression tag	UNP Q8NQY2
A	-16	SER	-	expression tag	UNP Q8NQY2
A	-15	HIS	-	expression tag	UNP Q8NQY2
A	-14	HIS	-	expression tag	UNP Q8NQY2
A	-13	HIS	-	expression tag	UNP Q8NQY2
A	-12	HIS	-	expression tag	UNP Q8NQY2
A	-11	HIS	-	expression tag	UNP Q8NQY2
A	-10	HIS	-	expression tag	UNP Q8NQY2
A	-9	SER	-	expression tag	UNP Q8NQY2
A	-8	SER	-	expression tag	UNP Q8NQY2
A	-7	GLY	-	expression tag	UNP Q8NQY2
A	-6	LEU	-	expression tag	UNP Q8NQY2
A	-5	VAL	-	expression tag	UNP Q8NQY2
A	-4	PRO	-	expression tag	UNP Q8NQY2
A	-3	ARG	-	expression tag	UNP Q8NQY2
A	-2	GLY	-	expression tag	UNP Q8NQY2
A	-1	SER	-	expression tag	UNP Q8NQY2
A	0	HIS	-	expression tag	UNP Q8NQY2
B	-19	MET	-	expression tag	UNP Q8NQY2
B	-18	GLY	-	expression tag	UNP Q8NQY2
B	-17	SER	-	expression tag	UNP Q8NQY2
B	-16	SER	-	expression tag	UNP Q8NQY2
B	-15	HIS	-	expression tag	UNP Q8NQY2

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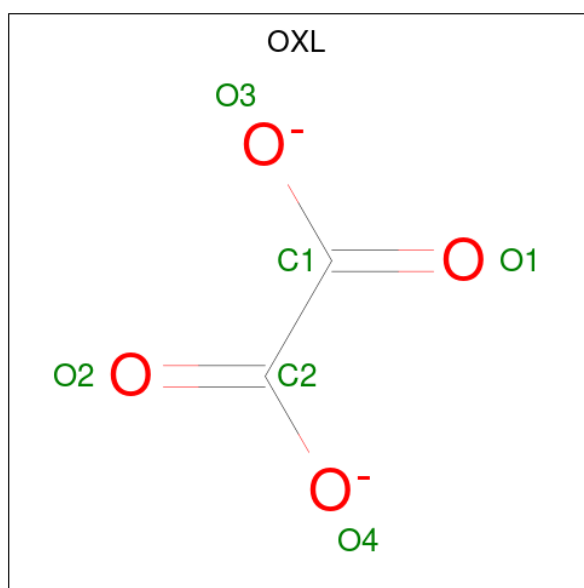
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q8NQY2
B	-13	HIS	-	expression tag	UNP Q8NQY2
B	-12	HIS	-	expression tag	UNP Q8NQY2
B	-11	HIS	-	expression tag	UNP Q8NQY2
B	-10	HIS	-	expression tag	UNP Q8NQY2
B	-9	SER	-	expression tag	UNP Q8NQY2
B	-8	SER	-	expression tag	UNP Q8NQY2
B	-7	GLY	-	expression tag	UNP Q8NQY2
B	-6	LEU	-	expression tag	UNP Q8NQY2
B	-5	VAL	-	expression tag	UNP Q8NQY2
B	-4	PRO	-	expression tag	UNP Q8NQY2
B	-3	ARG	-	expression tag	UNP Q8NQY2
B	-2	GLY	-	expression tag	UNP Q8NQY2
B	-1	SER	-	expression tag	UNP Q8NQY2
B	0	HIS	-	expression tag	UNP Q8NQY2

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 2	O 4	0	0
3	B	1	Total 6	C 2	O 4	0	0

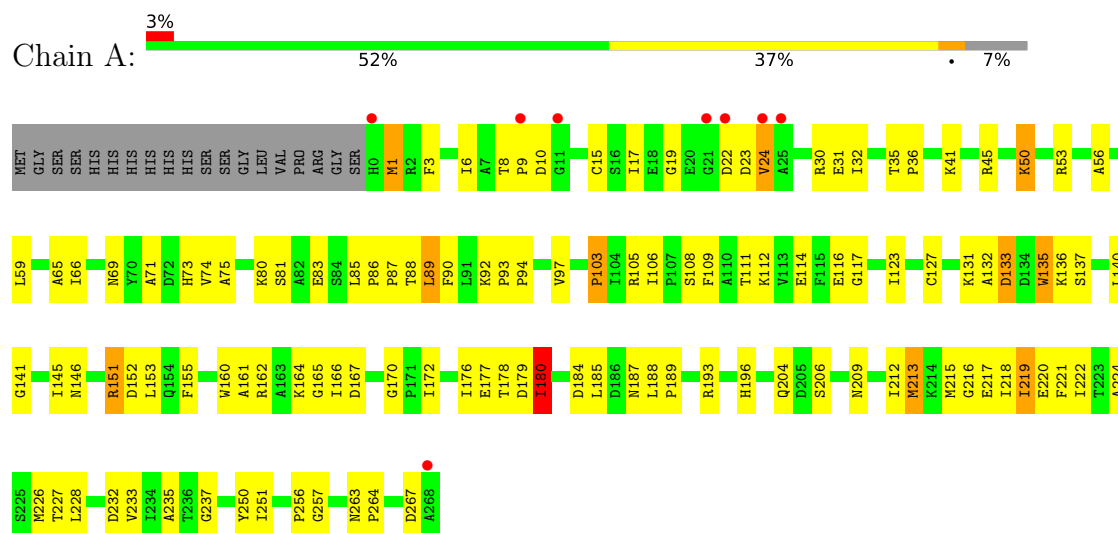
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	215	Total 215	O 215	0	0
4	B	152	Total 152	O 152	0	0

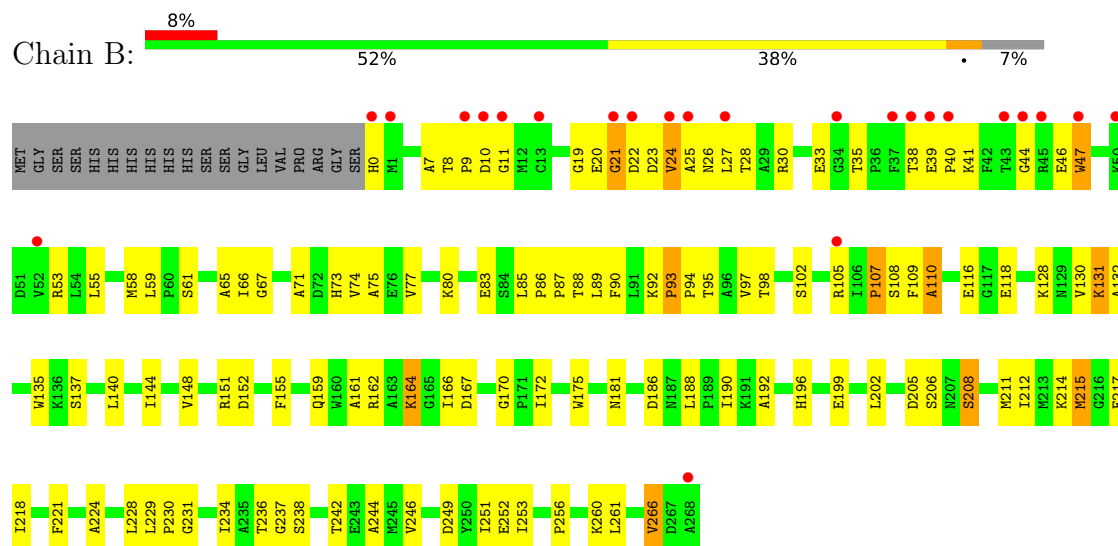
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 2-HYDROXYHEPTA-2,4-DIENE-1,7-DIOATE ISOMERASE



• Molecule 1: 2-HYDROXYHEPTA-2,4-DIENE-1,7-DIOATE ISOMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.04Å 67.24Å 168.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.94 50.00 – 1.94	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-1.94) 96.3 (50.00-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.171 , 0.220 0.181 , 0.221	Depositor DCC
R_{free} test set	1913 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4477	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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: OXL, 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	2.22	99/2103 (4.7%)	1.20	8/2856 (0.3%)
1	B	2.10	87/2088 (4.2%)	1.20	7/2838 (0.2%)
All	All	2.16	186/4191 (4.4%)	1.20	15/5694 (0.3%)

All (186) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	93	PRO	C-O	-12.23	1.14	1.24
1	A	188	LEU	C-O	-9.93	1.16	1.25
1	A	93	PRO	C-O	-8.95	1.17	1.24
1	A	145	ILE	C-O	-8.80	1.15	1.24
1	A	218	ILE	C-O	-8.72	1.14	1.24
1	A	217	GLU	C-O	-8.72	1.14	1.24
1	A	161	ALA	C-O	-8.62	1.14	1.24
1	A	83	GLU	C-N	-8.36	1.20	1.33
1	A	123	ILE	C-O	-8.10	1.15	1.24
1	B	217	GLU	C-O	-7.69	1.15	1.24
1	A	97	VAL	C-O	-7.67	1.16	1.24
1	A	65	ALA	C-O	-7.66	1.14	1.24
1	A	151	ARG	C-O	-7.64	1.15	1.24
1	A	133	ASP	C-O	-7.59	1.13	1.24
1	A	71	ALA	C-O	-7.43	1.15	1.24
1	B	155	PHE	C-O	-7.38	1.15	1.24
1	A	219	ILE	C-O	-7.34	1.15	1.24
1	A	162	ARG	C-O	-7.21	1.15	1.24
1	B	206	SER	C-O	-7.21	1.17	1.24
1	A	94	PRO	C-O	-7.20	1.15	1.24
1	A	233	VAL	C-O	-7.13	1.16	1.24
1	A	206	SER	C-O	-7.12	1.17	1.24
1	A	137	SER	C-O	-7.12	1.15	1.24
1	A	85	LEU	C-O	-6.98	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	VAL	C-O	-6.95	1.16	1.24
1	A	153	LEU	C-O	-6.94	1.16	1.24
1	B	89	LEU	C-O	-6.90	1.15	1.24
1	B	132	ALA	C-O	-6.88	1.15	1.24
1	A	32	ILE	C-O	-6.86	1.15	1.24
1	A	212	ILE	C-O	-6.84	1.16	1.24
1	B	85	LEU	C-O	-6.83	1.16	1.24
1	B	116	GLU	C-O	-6.81	1.17	1.23
1	A	213	MET	C-O	-6.80	1.15	1.24
1	A	59	LEU	C-O	-6.79	1.15	1.24
1	A	177	GLU	C-O	-6.78	1.15	1.24
1	B	170	GLY	C-O	-6.77	1.14	1.24
1	A	167	ASP	C-O	-6.76	1.15	1.23
1	A	251	ILE	C-O	-6.75	1.16	1.24
1	B	221	PHE	C-O	-6.73	1.16	1.24
1	B	228	LEU	C-O	-6.73	1.15	1.24
1	A	196	HIS	CG-ND1	-6.72	1.30	1.38
1	B	152	ASP	C-O	-6.72	1.16	1.24
1	B	135	TRP	NE1-CE2	-6.70	1.30	1.37
1	B	164	LYS	C-O	-6.67	1.15	1.24
1	A	227	THR	C-O	-6.67	1.16	1.23
1	A	263	ASN	C-O	-6.66	1.15	1.24
1	A	221	PHE	C-O	-6.64	1.16	1.24
1	B	212	ILE	C-O	-6.64	1.16	1.24
1	B	159	GLN	C-O	-6.63	1.16	1.24
1	A	75	ALA	C-O	-6.62	1.16	1.24
1	A	220	GLU	C-O	-6.60	1.16	1.24
1	A	164	LYS	C-O	-6.57	1.14	1.23
1	A	73	HIS	CG-ND1	-6.57	1.31	1.38
1	A	74	VAL	C-O	-6.53	1.16	1.24
1	A	224	ALA	C-O	-6.50	1.15	1.24
1	B	71	ALA	C-O	-6.49	1.16	1.24
1	A	237	GLY	C-O	-6.49	1.16	1.24
1	B	59	LEU	C-O	-6.49	1.16	1.24
1	B	188	LEU	C-O	-6.48	1.16	1.24
1	B	214	LYS	C-O	-6.48	1.15	1.23
1	A	109	PHE	C-O	-6.43	1.15	1.24
1	A	209	ASN	C-O	-6.42	1.15	1.24
1	A	267	ASP	C-O	-6.36	1.16	1.23
1	B	92	LYS	C-O	-6.35	1.16	1.24
1	A	116	GLU	C-O	-6.31	1.17	1.23
1	B	144	ILE	C-O	-6.31	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	181	ASN	C-O	-6.31	1.15	1.24
1	A	160	TRP	NE1-CE2	-6.28	1.30	1.37
1	B	238	SER	C-O	-6.28	1.15	1.24
1	A	136	LYS	C-O	-6.27	1.16	1.24
1	A	30	ARG	C-O	-6.26	1.16	1.24
1	B	128	LYS	C-O	-6.26	1.16	1.23
1	A	140	LEU	C-O	-6.26	1.16	1.24
1	B	256	PRO	C-O	-6.22	1.16	1.23
1	A	66	ILE	C-O	-6.21	1.16	1.23
1	A	53	ARG	C-O	-6.20	1.16	1.24
1	B	65	ALA	C-O	-6.19	1.16	1.23
1	A	88	THR	C-O	-6.19	1.16	1.23
1	B	109	PHE	C-O	-6.15	1.16	1.24
1	B	231	GLY	C-O	-6.14	1.15	1.24
1	A	132	ALA	C-O	-6.11	1.17	1.24
1	A	187	ASN	C-O	-6.09	1.16	1.24
1	A	204	GLN	C-O	-6.07	1.16	1.23
1	B	95	THR	C-O	-6.07	1.16	1.24
1	B	86	PRO	C-O	-6.06	1.17	1.24
1	A	256	PRO	C-O	-6.06	1.15	1.23
1	B	196	HIS	CD2-NE2	-6.05	1.31	1.37
1	B	74	VAL	C-O	-6.02	1.17	1.24
1	A	127	CYS	C-O	-6.01	1.16	1.23
1	A	146	ASN	C-O	-6.00	1.17	1.23
1	B	108	SER	C-O	-5.98	1.16	1.24
1	A	69	ASN	C-O	-5.97	1.15	1.23
1	B	61	SER	C-O	-5.96	1.16	1.24
1	B	77	VAL	C-O	-5.95	1.17	1.24
1	A	6	ILE	C-O	-5.94	1.18	1.24
1	A	117	GLY	C-O	-5.93	1.18	1.24
1	A	170	GLY	C-O	-5.92	1.16	1.24
1	A	92	LYS	C-O	-5.92	1.16	1.24
1	A	235	ALA	C-O	-5.91	1.16	1.24
1	B	53	ARG	C-O	-5.89	1.17	1.24
1	A	232	ASP	C-O	-5.89	1.16	1.23
1	B	28	THR	C-O	-5.87	1.16	1.24
1	A	228	LEU	C-O	-5.87	1.16	1.24
1	B	137	SER	C-O	-5.87	1.16	1.24
1	B	167	ASP	C-O	-5.84	1.16	1.23
1	A	152	ASP	C-O	-5.84	1.17	1.24
1	A	185	LEU	C-O	-5.82	1.16	1.24
1	A	184	ASP	C-O	-5.81	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	ALA	C-O	-5.81	1.17	1.24
1	B	66	ILE	C-O	-5.75	1.17	1.24
1	B	130	VAL	C-O	-5.74	1.16	1.24
1	A	172	ILE	C-O	-5.74	1.18	1.24
1	A	80	LYS	C-O	-5.73	1.16	1.23
1	B	83	GLU	C-O	-5.72	1.17	1.24
1	B	161	ALA	C-O	-5.72	1.17	1.24
1	B	218	ILE	C-O	-5.72	1.17	1.24
1	A	189	PRO	C-O	-5.71	1.17	1.23
1	A	166	ILE	C-O	-5.71	1.17	1.24
1	A	81	SER	C-O	-5.70	1.16	1.23
1	A	108	SER	C-O	-5.68	1.16	1.24
1	B	58	MET	C-O	-5.67	1.17	1.23
1	B	151	ARG	C-O	-5.66	1.17	1.24
1	B	172	ILE	C-O	-5.65	1.18	1.24
1	B	140	LEU	C-O	-5.65	1.17	1.24
1	A	264	PRO	C-O	-5.65	1.17	1.23
1	B	88	THR	C-O	-5.63	1.17	1.23
1	A	257	GLY	C-O	-5.62	1.15	1.24
1	B	73	HIS	CG-ND1	-5.60	1.32	1.38
1	A	165	GLY	C-O	-5.58	1.16	1.23
1	B	253	ILE	C-O	-5.58	1.17	1.24
1	B	148	VAL	C-O	-5.58	1.18	1.24
1	B	261	LEU	C-O	-5.57	1.17	1.24
1	B	35	THR	C-O	-5.56	1.17	1.24
1	A	193	ARG	C-O	-5.56	1.17	1.24
1	B	162	ARG	C-O	-5.55	1.17	1.24
1	B	196	HIS	CG-ND1	-5.54	1.32	1.38
1	A	86	PRO	C-O	-5.54	1.18	1.24
1	B	175	TRP	NE1-CE2	-5.54	1.31	1.37
1	B	249	ASP	C-O	-5.48	1.16	1.23
1	A	135	TRP	NE1-CE2	-5.45	1.31	1.37
1	B	110	ALA	C-O	-5.45	1.17	1.23
1	A	114	GLU	C-O	-5.41	1.17	1.23
1	A	135	TRP	C-O	-5.41	1.17	1.24
1	B	107	PRO	C-O	-5.40	1.17	1.23
1	B	205	ASP	C-O	-5.39	1.17	1.24
1	B	98	THR	C-O	-5.37	1.17	1.23
1	A	216	GLY	C-O	-5.35	1.17	1.23
1	B	246	VAL	C-O	-5.33	1.18	1.23
1	B	202	LEU	C-O	-5.32	1.17	1.24
1	A	89	LEU	C-O	-5.32	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	ASP	C-O	-5.31	1.18	1.23
1	A	103	PRO	C-O	-5.30	1.18	1.23
1	A	17	ILE	C-O	-5.30	1.18	1.24
1	B	102	SER	C-O	-5.30	1.16	1.24
1	A	141	GLY	C-O	-5.30	1.17	1.23
1	A	222	ILE	C-O	-5.29	1.18	1.24
1	B	118	GLU	C-O	-5.28	1.17	1.23
1	B	252	GLU	C-O	-5.27	1.17	1.24
1	B	199	GLU	C-O	-5.26	1.18	1.24
1	A	215	MET	C-O	-5.26	1.18	1.24
1	A	263	ASN	CA-C	5.25	1.58	1.52
1	A	41	LYS	C-O	-5.25	1.17	1.24
1	B	260	LYS	C-O	-5.23	1.17	1.24
1	B	215	MET	C-O	-5.22	1.18	1.24
1	A	111	THR	C-O	-5.21	1.17	1.23
1	B	224	ALA	C-O	-5.21	1.17	1.24
1	A	31	GLU	C-O	-5.19	1.17	1.23
1	A	83	GLU	C-O	-5.17	1.18	1.24
1	B	190	ILE	C-O	-5.15	1.18	1.24
1	B	242	THR	C-O	-5.14	1.17	1.23
1	B	192	ALA	C-O	-5.13	1.18	1.23
1	A	155	PHE	C-O	-5.13	1.18	1.24
1	B	55	LEU	C-O	-5.12	1.16	1.23
1	B	244	ALA	C-O	-5.10	1.17	1.23
1	B	7	ALA	C-O	-5.10	1.17	1.24
1	B	94	PRO	C-O	-5.09	1.17	1.24
1	B	251	ILE	C-O	-5.09	1.18	1.24
1	B	208	SER	C-O	-5.08	1.17	1.24
1	A	176	ILE	C-O	-5.08	1.18	1.24
1	B	266	VAL	C-O	-5.07	1.18	1.23
1	A	50	LYS	C-O	-5.07	1.17	1.24
1	B	186	ASP	C-O	-5.06	1.17	1.24
1	B	166	ILE	C-O	-5.04	1.18	1.24
1	A	250	TYR	C-O	-5.04	1.18	1.23
1	B	234	ILE	C-O	-5.02	1.18	1.24
1	A	180	ILE	C-O	-5.00	1.18	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ASP	N-CA-C	-9.35	99.59	112.30
1	A	15	CYS	CA-C-N	8.74	135.02	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	CYS	C-N-CA	8.74	135.02	122.09
1	A	135	TRP	N-CA-C	7.65	119.61	111.28
1	B	44	GLY	N-CA-C	-6.98	106.17	114.48
1	A	106	ILE	N-CA-C	6.83	114.66	107.76
1	B	135	TRP	N-CA-C	6.29	118.94	111.33
1	A	56	ALA	N-CA-C	-6.12	102.57	109.60
1	B	24	VAL	CB-CA-C	-5.86	101.68	111.29
1	A	15	CYS	O-C-N	-5.56	116.92	123.25
1	A	19	GLY	N-CA-C	5.56	118.02	111.63
1	B	21	GLY	N-CA-C	-5.48	102.25	111.73
1	B	22	ASP	N-CA-C	5.07	118.89	109.56
1	B	237	GLY	N-CA-C	5.05	116.75	111.95
1	B	181	ASN	CB-CA-C	5.01	119.34	109.72

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	2055	0	2059	22	0
1	B	2040	0	2038	39	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
4	A	215	0	0	0	0
4	B	152	0	0	0	0
All	All	4477	0	4097	60	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 7.

All (60) 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:8:THR:HB	1:B:9:PRO:CD	1.70	1.22
1:B:8:THR:HB	1:B:9:PRO:HD2	1.38	1.03
1:B:8:THR:HB	1:B:9:PRO:HD3	1.43	0.98
1:B:208:SER:HB2	1:B:211:MET:HE3	1.67	0.77
1:B:8:THR:CB	1:B:9:PRO:HD2	2.14	0.76
1:B:24:VAL:CG2	1:B:25:ALA:N	2.48	0.76
1:A:1:MET:HE2	1:A:3:PHE:CZ	2.24	0.73
1:B:24:VAL:HG23	1:B:25:ALA:N	2.02	0.73
1:B:8:THR:C	1:B:10:ASP:N	2.43	0.71
1:B:8:THR:C	1:B:10:ASP:H	1.96	0.71
1:A:112:LYS:HD3	1:A:151:ARG:HB2	1.76	0.67
1:B:105[A]:ARG:HG2	1:B:266:VAL:CG2	2.25	0.66
1:A:131:LYS:NZ	1:A:133:ASP:OD1	2.30	0.65
1:B:10:ASP:OD1	1:B:10:ASP:C	2.38	0.65
1:B:20:GLU:OE2	1:B:21:GLY:N	2.29	0.65
1:B:10:ASP:OD1	1:B:11:GLY:N	2.30	0.65
1:A:23:ASP:OD1	1:A:24:VAL:N	2.30	0.64
1:B:23:ASP:OD1	1:B:23:ASP:C	2.37	0.64
1:B:20:GLU:O	1:B:21:GLY:C	2.41	0.64
1:A:1:MET:CE	1:A:3:PHE:CE1	2.82	0.63
1:B:19:GLY:HA3	1:B:27:LEU:HD23	1.81	0.62
1:A:178:THR:O	1:A:180:ILE:HD12	2.00	0.62
1:A:8:THR:C	1:A:10:ASP:N	2.59	0.59
1:B:23:ASP:HB3	1:B:26:ASN:HD22	1.68	0.58
1:A:8:THR:C	1:A:10:ASP:H	2.11	0.58
1:A:1:MET:CE	1:A:3:PHE:CZ	2.87	0.57
1:B:8:THR:CB	1:B:9:PRO:HD3	2.20	0.55
1:B:47:TRP:N	1:B:47:TRP:CE3	2.74	0.55
1:B:8:THR:O	1:B:10:ASP:N	2.41	0.54
1:A:23:ASP:OD1	1:A:23:ASP:C	2.51	0.53
1:B:47:TRP:HE3	1:B:47:TRP:H	1.56	0.52
1:A:89:LEU:C	1:A:89:LEU:HD23	2.35	0.51
1:B:8:THR:CB	1:B:9:PRO:CD	2.46	0.51
1:B:9:PRO:HD2	1:B:10:ASP:H	1.75	0.50
1:B:9:PRO:CD	1:B:10:ASP:H	2.24	0.49
1:B:8:THR:OG1	1:B:10:ASP:HB3	2.14	0.47
1:A:1:MET:HE1	1:A:3:PHE:CE1	2.50	0.47
1:B:90:PHE:CE2	1:B:164:LYS:HD3	2.50	0.47
1:A:135:TRP:HB2	1:A:219:ILE:HD13	1.97	0.47
1:A:10:ASP:CG	1:A:45:ARG:HH12	2.24	0.45
1:A:89:LEU:HD23	1:A:90:PHE:N	2.32	0.44
1:B:33:GLU:N	1:B:41:LYS:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:THR:HB	1:A:36:PRO:CD	2.47	0.44
1:B:215:MET:HE1	1:B:236:THR:HG21	1.99	0.44
1:A:103:PRO:HG2	1:A:105[A]:ARG:NH1	2.33	0.43
1:B:24:VAL:HG22	1:B:25:ALA:H	1.83	0.43
1:B:229:LEU:HB3	1:B:230:PRO:HD2	1.99	0.43
1:B:9:PRO:CD	1:B:10:ASP:N	2.82	0.43
1:B:39:GLU:HA	1:B:40:PRO:HD2	1.80	0.43
1:A:87:PRO:HG2	1:A:213:MET:HG3	2.01	0.43
1:B:24:VAL:HA	1:B:27:LEU:HB2	2.01	0.42
1:A:8:THR:O	1:A:10:ASP:N	2.52	0.42
1:A:10:ASP:CB	1:A:45:ARG:HH12	2.33	0.42
1:B:38:THR:O	1:B:39:GLU:C	2.62	0.42
1:A:226:MET:HE2	1:B:93:PRO:HG3	2.02	0.41
1:B:8:THR:O	1:B:9:PRO:C	2.63	0.41
1:B:67:GLY:O	1:B:87:PRO:HA	2.21	0.41
1:B:131:LYS:HA	1:B:131:LYS:HD2	1.93	0.40
1:A:1:MET:HE2	1:A:1:MET:HB2	1.69	0.40
1:B:107:PRO:HD2	1:B:110:ALA:HB3	2.03	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	268/288 (93%)	256 (96%)	11 (4%)	1 (0%)	30	22
1	B	268/288 (93%)	251 (94%)	17 (6%)	0	100	100
All	All	536/576 (93%)	507 (95%)	28 (5%)	1 (0%)	43	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	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	225/240 (94%)	221 (98%)	4 (2%)	51	43
1	B	221/240 (92%)	215 (97%)	6 (3%)	39	26
All	All	446/480 (93%)	436 (98%)	10 (2%)	44	35

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	24	VAL
1	A	50	LYS
1	A	180	ILE
1	B	0	HIS
1	B	30	ARG
1	B	46	GLU
1	B	47	TRP
1	B	80	LYS
1	B	131	LYS

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

Mol	Chain	Res	Type
1	A	26	ASN
1	A	181	ASN
1	A	201	GLN
1	A	210	GLN
1	B	26	ASN
1	B	129	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 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	$\# Z > 2$
3	OXL	A	402	2	5,5,5	3.60	3 (60%)	6,6,6	2.87	4 (66%)
3	OXL	B	402	2	5,5,5	3.42	3 (60%)	6,6,6	2.18	2 (33%)

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	OXL	A	402	2	-	4/4/4/4	-
3	OXL	B	402	2	-	0/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	OXL	C2-C1	-6.65	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	OXL	C2-C1	-6.63	1.43	1.54
3	A	402	OXL	O3-C1	-3.23	1.21	1.30
3	B	402	OXL	O3-C1	-2.75	1.23	1.30
3	A	402	OXL	O4-C2	-2.72	1.23	1.30
3	B	402	OXL	O4-C2	-2.40	1.24	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	OXL	O3-C1-C2	3.98	120.55	112.83
3	A	402	OXL	O4-C2-C1	3.94	120.47	112.83
3	B	402	OXL	O3-C1-C2	3.71	120.03	112.83
3	B	402	OXL	O1-C1-C2	-3.24	113.88	120.63
3	A	402	OXL	O2-C2-C1	-3.23	113.90	120.63
3	A	402	OXL	O1-C1-C2	-2.67	115.06	120.63

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	OXL	O3-C1-C2-O4
3	A	402	OXL	O1-C1-C2-O2
3	A	402	OXL	O1-C1-C2-O4
3	A	402	OXL	O3-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	269/288 (93%)	-0.10	8 (2%) 52 58	7, 14, 39, 66	1 (0%)
1	B	269/288 (93%)	0.16	24 (8%) 15 17	8, 17, 54, 74	1 (0%)
All	All	538/576 (93%)	0.03	32 (5%) 28 31	7, 15, 49, 74	2 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	PRO	4.7
1	B	9	PRO	3.9
1	B	22	ASP	3.8
1	B	24	VAL	3.6
1	A	22	ASP	3.3
1	B	40	PRO	3.2
1	B	43	THR	3.2
1	A	268	ALA	3.2
1	B	11	GLY	3.1
1	B	0	HIS	3.1
1	A	21	GLY	3.0
1	B	21	GLY	2.9
1	B	10	ASP	2.9
1	A	0	HIS	2.9
1	B	38	THR	2.8
1	A	24	VAL	2.8
1	A	25	ALA	2.7
1	B	37	PHE	2.7
1	B	44	GLY	2.6
1	B	50	LYS	2.4
1	B	39	GLU	2.4
1	B	268	ALA	2.4
1	B	34	GLY	2.3
1	B	45	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	47	TRP	2.3
1	A	11	GLY	2.2
1	B	27	LEU	2.2
1	B	25	ALA	2.2
1	B	13	CYS	2.2
1	B	105[A]	ARG	2.1
1	B	1	MET	2.1
1	B	52	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(Å ²)	Q<0.9
2	MG	B	403	1/1	0.91	0.05	25,25,25,25	0
2	MG	A	401	1/1	0.93	0.05	12,12,12,12	0
3	OXL	A	402	6/6	0.94	0.09	16,19,21,23	0
3	OXL	B	402	6/6	0.95	0.08	18,22,23,23	0
2	MG	B	401	1/1	0.99	0.02	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.