



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:36 PM UTC

PDB ID : 5IKY / pdb_00005iky
Title : Apo structure of Obc1, a bifunctional enzyme for quorum sensing-dependent oxalogenesis
Authors : Oh, J.; Rhee, S.
Deposited on : 2016-03-04
Resolution : 2.50 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

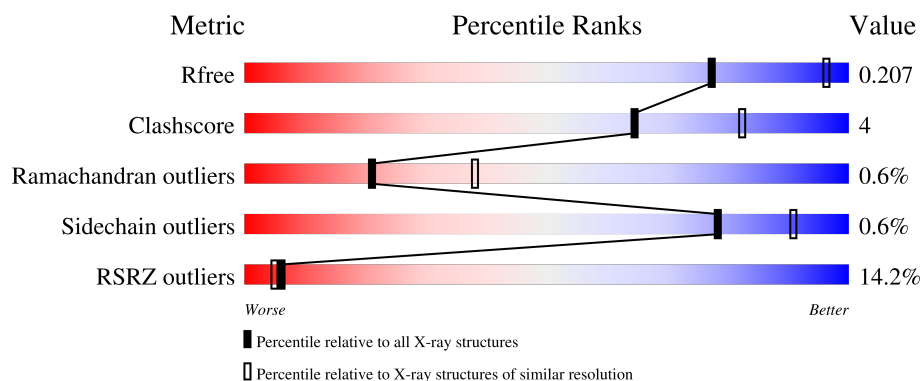
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	1125	13% 83% 9% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8036 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 Oxalate biosynthetic component 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1048	Total	C	N	O	S	0	0	0
			7835	4962	1403	1453	17			

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

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

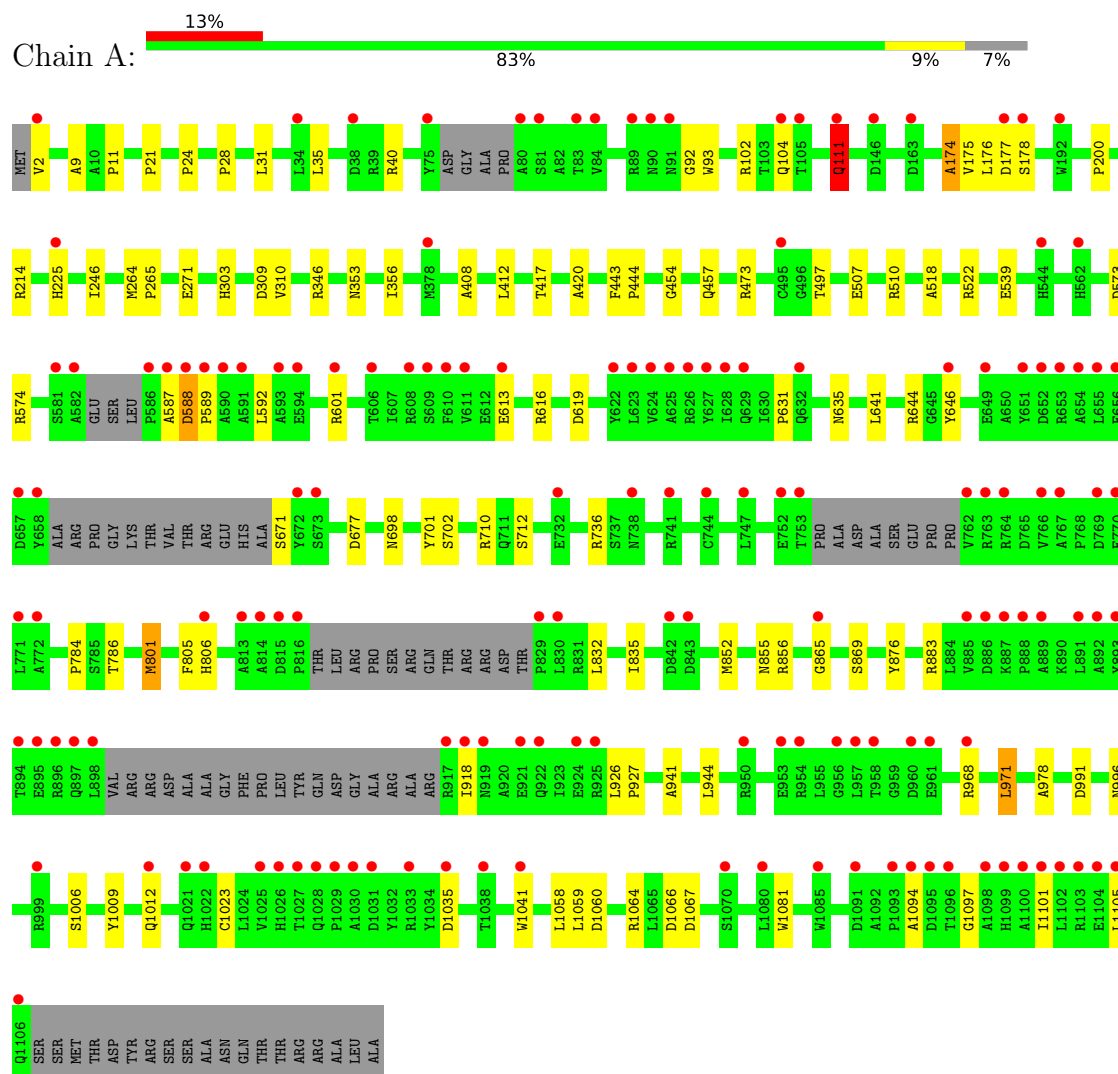
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	200	Total	O	0	0
			200	200		

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: Oxalate biosynthetic component 1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	230.81Å 230.81Å 253.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.77 – 2.50 38.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.77-2.50) 99.6 (38.77-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.198 , 0.227 0.207 , 0.207	Depositor DCC
R_{free} test set	4574 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8036	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: 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	0.31	0/8011	0.74	3/10954 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	454	GLY	CA-C-N	5.46	125.29	119.28
1	A	454	GLY	C-N-CA	5.46	125.29	119.28
1	A	111	GLN	CB-CA-C	5.11	118.64	110.62

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	7835	0	7516	60	0
2	A	1	0	0	0	0
3	A	200	0	0	3	0
All	All	8036	0	7516	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 4.

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:A:111:GLN:HE21	1:A:111:GLN:HA	1.40	0.85
1:A:174:ALA:O	1:A:177:ASP:N	2.18	0.73
1:A:111:GLN:HA	1:A:111:GLN:NE2	2.04	0.71
1:A:698:ASN:HD21	1:A:702:SER:HB2	1.56	0.71
1:A:174:ALA:O	1:A:176:LEU:N	2.25	0.70
1:A:177:ASP:OD1	1:A:178:SER:N	2.26	0.69
1:A:35:LEU:O	1:A:40:ARG:NH2	2.25	0.68
1:A:613:GLU:OE2	1:A:616:ARG:NH1	2.27	0.67
1:A:111:GLN:HE21	1:A:111:GLN:CA	2.08	0.66
1:A:1064:ARG:NH1	3:A:1304:HOH:O	2.29	0.65
1:A:601:ARG:NH1	1:A:701:TYR:OH	2.29	0.65
1:A:677:ASP:O	1:A:736:ARG:NH2	2.31	0.64
1:A:303:HIS:O	1:A:574:ARG:NH2	2.34	0.61
1:A:539:GLU:OE1	1:A:712:SER:OG	2.21	0.59
1:A:309:ASP:OD1	1:A:522:ARG:NH2	2.36	0.57
1:A:1060:ASP:OD1	1:A:1064:ARG:N	2.31	0.57
1:A:876:TYR:HB2	1:A:944:LEU:HD22	1.88	0.56
1:A:588:ASP:H	1:A:589:PRO:HD2	1.72	0.54
1:A:1097:GLY:O	1:A:1101:ILE:HG13	2.08	0.54
1:A:996:ASN:ND2	1:A:1058:LEU:O	2.41	0.54
1:A:457:GLN:N	3:A:1310:HOH:O	2.42	0.53
1:A:786:THR:HG23	1:A:852:MET:HB2	1.91	0.53
1:A:225:HIS:HD2	1:A:473:ARG:NH1	2.07	0.53
1:A:507:GLU:OE2	1:A:510:ARG:NH1	2.43	0.52
1:A:806:HIS:HB2	1:A:832:LEU:HD22	1.91	0.52
1:A:28:PRO:HD2	1:A:31:LEU:HD12	1.93	0.51
1:A:856:ARG:HG2	1:A:978:ALA:HB2	1.92	0.51
1:A:1023:CYS:HB3	1:A:1059:LEU:HD11	1.93	0.51
1:A:801:MET:HE3	1:A:805:PHE:HE2	1.76	0.50
1:A:855:ASN:ND2	1:A:869:SER:HB3	2.26	0.50
1:A:214:ARG:NH2	3:A:1313:HOH:O	2.46	0.49
1:A:619:ASP:OD2	1:A:671:SER:N	2.46	0.48
1:A:1066:ASP:OD1	1:A:1067:ASP:N	2.47	0.48
1:A:587:ALA:HB3	1:A:592:LEU:HD22	1.96	0.48
1:A:1035:ASP:HA	1:A:1081:TRP:HE1	1.79	0.47
1:A:518:ALA:O	1:A:522:ARG:HG3	2.14	0.47
1:A:710:ARG:NH2	1:A:1006:SER:O	2.32	0.47
1:A:1041:TRP:CE3	1:A:1105:LEU:HD11	2.50	0.47
1:A:92:GLY:HA3	1:A:104:GLN:OE1	2.15	0.46
1:A:991:ASP:OD2	1:A:1009:TYR:OH	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:926:LEU:O	1:A:968:ARG:NE	2.47	0.46
1:A:11:PRO:HD2	1:A:225:HIS:O	2.16	0.45
1:A:883:ARG:NH2	1:A:927:PRO:O	2.42	0.45
1:A:641:LEU:HB3	1:A:646:TYR:HB2	1.98	0.44
1:A:93:TRP:CE2	1:A:102:ARG:HG3	2.53	0.44
1:A:784:PRO:HD3	1:A:835:ILE:HB	1.99	0.43
1:A:417:THR:HG23	1:A:420:ALA:H	1.83	0.43
1:A:1041:TRP:CZ3	1:A:1105:LEU:HD11	2.52	0.43
1:A:443:PHE:HA	1:A:444:PRO:HD2	1.88	0.43
1:A:214:ARG:HD2	1:A:271:GLU:OE2	2.18	0.43
1:A:353:ASN:OD1	1:A:356:ILE:HG12	2.20	0.42
1:A:9:ALA:HB1	1:A:497:THR:HG21	2.02	0.41
1:A:264:MET:HB2	1:A:265:PRO:HD3	2.03	0.41
1:A:408:ALA:O	1:A:412:LEU:HD12	2.21	0.41
1:A:310:VAL:HA	1:A:346:ARG:O	2.21	0.41
1:A:21:PRO:HG3	1:A:200:PRO:CB	2.51	0.41
1:A:941:ALA:HB1	1:A:971:LEU:HD11	2.02	0.41
1:A:573:ASP:OD1	1:A:644:ARG:NH2	2.55	0.40
1:A:24:PRO:HG2	1:A:246:ILE:HD11	2.03	0.40
1:A:631:PRO:O	1:A:635:ASN:ND2	2.52	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	1034/1125 (92%)	993 (96%)	35 (3%)	6 (1%)	21 38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	ALA

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Mol	Chain	Res	Type
1	A	175	VAL
1	A	1094	ALA
1	A	588	ASP
1	A	918	ILE
1	A	865	GLY

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	775/922 (84%)	770 (99%)	5 (1%)	78 91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	111	GLN
1	A	801	MET
1	A	971	LEU
1	A	1012	GLN

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	111	GLN
1	A	225	HIS
1	A	305	GLN
1	A	354	HIS
1	A	481	ASN
1	A	578	HIS

5.3.3 RNA ⓘ

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	1048/1125 (93%)	0.68	149 (14%) 6 5	39, 75, 123, 171	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	816	PRO	12.5
1	A	582	ALA	9.9
1	A	771	LEU	6.6
1	A	815	ASP	6.6
1	A	1094	ALA	6.6
1	A	658	TYR	6.5
1	A	1027	THR	6.4
1	A	922	GLN	6.3
1	A	627	TYR	5.7
1	A	654	ALA	5.5
1	A	770	GLU	5.3
1	A	80	ALA	5.2
1	A	628	ILE	5.1
1	A	762	VAL	5.1
1	A	1096	THR	4.9
1	A	2	VAL	4.9
1	A	887	LYS	4.9
1	A	1105	LEU	4.9
1	A	672	TYR	4.8
1	A	753	THR	4.6
1	A	953	GLU	4.6
1	A	105	THR	4.6
1	A	1026	HIS	4.5
1	A	888	PRO	4.5
1	A	886	ASP	4.5
1	A	1031	ASP	4.5
1	A	586	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	653	ARG	4.3
1	A	829	PRO	4.3
1	A	622	TYR	4.3
1	A	898	LEU	4.3
1	A	1106	GLN	4.2
1	A	649	GLU	4.2
1	A	917	ARG	4.2
1	A	842	ASP	4.1
1	A	919	ASN	4.1
1	A	610	PHE	4.1
1	A	921	GLU	4.1
1	A	495	CYS	3.9
1	A	1095	ASP	3.9
1	A	958	THR	3.9
1	A	889	ALA	3.8
1	A	581	SER	3.8
1	A	918	ILE	3.8
1	A	885	VAL	3.8
1	A	83	THR	3.8
1	A	589	PRO	3.7
1	A	591	ALA	3.6
1	A	177	ASP	3.6
1	A	646	TYR	3.6
1	A	1041	TRP	3.5
1	A	1029	PRO	3.4
1	A	89	ARG	3.4
1	A	84	VAL	3.4
1	A	738	ASN	3.3
1	A	1098	ALA	3.3
1	A	1028	GLN	3.3
1	A	91	ASN	3.3
1	A	1080	LEU	3.3
1	A	593	ALA	3.2
1	A	606	THR	3.2
1	A	1093	PRO	3.2
1	A	895	GLU	3.2
1	A	892	ALA	3.1
1	A	624	VAL	3.1
1	A	893	TYR	3.1
1	A	772	ALA	3.1
1	A	814	ALA	3.1
1	A	588	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	609	SER	3.1
1	A	111	GLN	3.0
1	A	957	LEU	3.0
1	A	1035	ASP	3.0
1	A	1033	ARG	3.0
1	A	75	TYR	3.0
1	A	950	ARG	3.0
1	A	924	GLU	2.9
1	A	1038	THR	2.9
1	A	590	ALA	2.9
1	A	225	HIS	2.9
1	A	925	ARG	2.9
1	A	843	ASP	2.9
1	A	613	GLU	2.9
1	A	896	ARG	2.8
1	A	378	MET	2.8
1	A	629	GLN	2.8
1	A	655	LEU	2.8
1	A	626	ARG	2.7
1	A	1103	ARG	2.7
1	A	38	ASP	2.7
1	A	651	TYR	2.7
1	A	1100	ALA	2.7
1	A	178	SER	2.7
1	A	1085	TRP	2.7
1	A	813	ALA	2.6
1	A	1030	ALA	2.6
1	A	744	CYS	2.6
1	A	1070	SER	2.6
1	A	960	ASP	2.6
1	A	954	ARG	2.5
1	A	741	ARG	2.5
1	A	897	GLN	2.5
1	A	673	SER	2.5
1	A	999	ARG	2.5
1	A	81	SER	2.5
1	A	894	THR	2.5
1	A	657	ASP	2.5
1	A	891	LEU	2.5
1	A	806	HIS	2.5
1	A	601	ARG	2.5
1	A	656	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	766	VAL	2.4
1	A	830	LEU	2.4
1	A	1099	HIS	2.4
1	A	865	GLY	2.4
1	A	594	GLU	2.4
1	A	34	LEU	2.3
1	A	608	ARG	2.3
1	A	769	ASP	2.3
1	A	1091	ASP	2.3
1	A	611	VAL	2.3
1	A	90	ASN	2.3
1	A	625	ALA	2.3
1	A	623	LEU	2.3
1	A	163	ASP	2.3
1	A	1104	GLU	2.3
1	A	732	GLU	2.2
1	A	961	GLU	2.2
1	A	767	ALA	2.2
1	A	544	HIS	2.2
1	A	1021	GLN	2.2
1	A	587	ALA	2.2
1	A	562	HIS	2.2
1	A	652	ASP	2.2
1	A	752	GLU	2.2
1	A	1025	VAL	2.2
1	A	747	LEU	2.2
1	A	1012	GLN	2.1
1	A	104	GLN	2.1
1	A	1102	LEU	2.1
1	A	1022	HIS	2.1
1	A	968	ARG	2.1
1	A	632	GLN	2.1
1	A	764	ARG	2.1
1	A	956	GLY	2.1
1	A	1101	ILE	2.1
1	A	763	ARG	2.0
1	A	192	TRP	2.0
1	A	146	ASP	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 [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
2	MG	A	1201	1/1	0.95	0.10	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.