



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:27 AM UTC

PDB ID : 4M26 / pdb_00004m26
Title : Crystal structure of non-heme iron oxygenase OrfP in complex with Fe, succinate, and (3S)-hydroxy-L-Arg
Authors : Chang, C.Y.; Liu, Y.C.; Lyu, S.Y.; Wu, C.C.; Li, T.L.
Deposited on : 2013-08-05
Resolution : 2.02 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

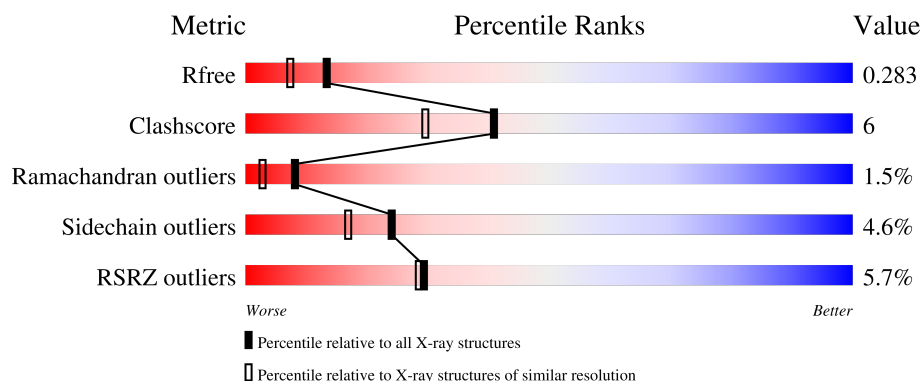
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	364	3% 78% 14% • 8%
1	B	364	5% 74% 9% • 14%
1	C	364	6% 78% 11% • 9%
1	D	364	6% 75% 16% • 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11335 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 L-arginine beta-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	1	0
			2701	1699	491	504	7			
1	B	314	Total	C	N	O	S	0	1	0
			2521	1590	454	470	7			
1	C	332	Total	C	N	O	S	0	0	0
			2660	1676	483	494	7			
1	D	336	Total	C	N	O	S	0	0	0
			2690	1693	487	503	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP G9MBV2
A	-18	GLY	-	expression tag	UNP G9MBV2
A	-17	SER	-	expression tag	UNP G9MBV2
A	-16	SER	-	expression tag	UNP G9MBV2
A	-15	HIS	-	expression tag	UNP G9MBV2
A	-14	HIS	-	expression tag	UNP G9MBV2
A	-13	HIS	-	expression tag	UNP G9MBV2
A	-12	HIS	-	expression tag	UNP G9MBV2
A	-11	HIS	-	expression tag	UNP G9MBV2
A	-10	HIS	-	expression tag	UNP G9MBV2
A	-9	SER	-	expression tag	UNP G9MBV2
A	-8	SER	-	expression tag	UNP G9MBV2
A	-7	GLY	-	expression tag	UNP G9MBV2
A	-6	LEU	-	expression tag	UNP G9MBV2
A	-5	VAL	-	expression tag	UNP G9MBV2
A	-4	PRO	-	expression tag	UNP G9MBV2
A	-3	ARG	-	expression tag	UNP G9MBV2
A	-2	GLY	-	expression tag	UNP G9MBV2
A	-1	SER	-	expression tag	UNP G9MBV2
A	0	HIS	-	expression tag	UNP G9MBV2
B	-19	MET	-	expression tag	UNP G9MBV2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP G9MBV2
B	-17	SER	-	expression tag	UNP G9MBV2
B	-16	SER	-	expression tag	UNP G9MBV2
B	-15	HIS	-	expression tag	UNP G9MBV2
B	-14	HIS	-	expression tag	UNP G9MBV2
B	-13	HIS	-	expression tag	UNP G9MBV2
B	-12	HIS	-	expression tag	UNP G9MBV2
B	-11	HIS	-	expression tag	UNP G9MBV2
B	-10	HIS	-	expression tag	UNP G9MBV2
B	-9	SER	-	expression tag	UNP G9MBV2
B	-8	SER	-	expression tag	UNP G9MBV2
B	-7	GLY	-	expression tag	UNP G9MBV2
B	-6	LEU	-	expression tag	UNP G9MBV2
B	-5	VAL	-	expression tag	UNP G9MBV2
B	-4	PRO	-	expression tag	UNP G9MBV2
B	-3	ARG	-	expression tag	UNP G9MBV2
B	-2	GLY	-	expression tag	UNP G9MBV2
B	-1	SER	-	expression tag	UNP G9MBV2
B	0	HIS	-	expression tag	UNP G9MBV2
C	-19	MET	-	expression tag	UNP G9MBV2
C	-18	GLY	-	expression tag	UNP G9MBV2
C	-17	SER	-	expression tag	UNP G9MBV2
C	-16	SER	-	expression tag	UNP G9MBV2
C	-15	HIS	-	expression tag	UNP G9MBV2
C	-14	HIS	-	expression tag	UNP G9MBV2
C	-13	HIS	-	expression tag	UNP G9MBV2
C	-12	HIS	-	expression tag	UNP G9MBV2
C	-11	HIS	-	expression tag	UNP G9MBV2
C	-10	HIS	-	expression tag	UNP G9MBV2
C	-9	SER	-	expression tag	UNP G9MBV2
C	-8	SER	-	expression tag	UNP G9MBV2
C	-7	GLY	-	expression tag	UNP G9MBV2
C	-6	LEU	-	expression tag	UNP G9MBV2
C	-5	VAL	-	expression tag	UNP G9MBV2
C	-4	PRO	-	expression tag	UNP G9MBV2
C	-3	ARG	-	expression tag	UNP G9MBV2
C	-2	GLY	-	expression tag	UNP G9MBV2
C	-1	SER	-	expression tag	UNP G9MBV2
C	0	HIS	-	expression tag	UNP G9MBV2
D	-19	MET	-	expression tag	UNP G9MBV2
D	-18	GLY	-	expression tag	UNP G9MBV2
D	-17	SER	-	expression tag	UNP G9MBV2

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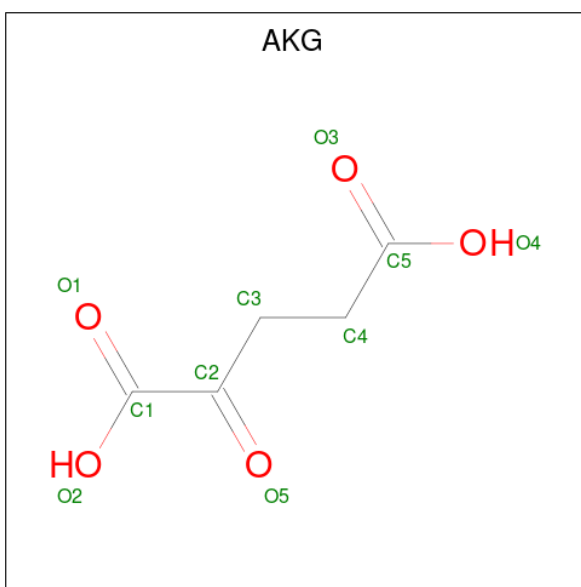
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP G9MBV2
D	-15	HIS	-	expression tag	UNP G9MBV2
D	-14	HIS	-	expression tag	UNP G9MBV2
D	-13	HIS	-	expression tag	UNP G9MBV2
D	-12	HIS	-	expression tag	UNP G9MBV2
D	-11	HIS	-	expression tag	UNP G9MBV2
D	-10	HIS	-	expression tag	UNP G9MBV2
D	-9	SER	-	expression tag	UNP G9MBV2
D	-8	SER	-	expression tag	UNP G9MBV2
D	-7	GLY	-	expression tag	UNP G9MBV2
D	-6	LEU	-	expression tag	UNP G9MBV2
D	-5	VAL	-	expression tag	UNP G9MBV2
D	-4	PRO	-	expression tag	UNP G9MBV2
D	-3	ARG	-	expression tag	UNP G9MBV2
D	-2	GLY	-	expression tag	UNP G9MBV2
D	-1	SER	-	expression tag	UNP G9MBV2
D	0	HIS	-	expression tag	UNP G9MBV2

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

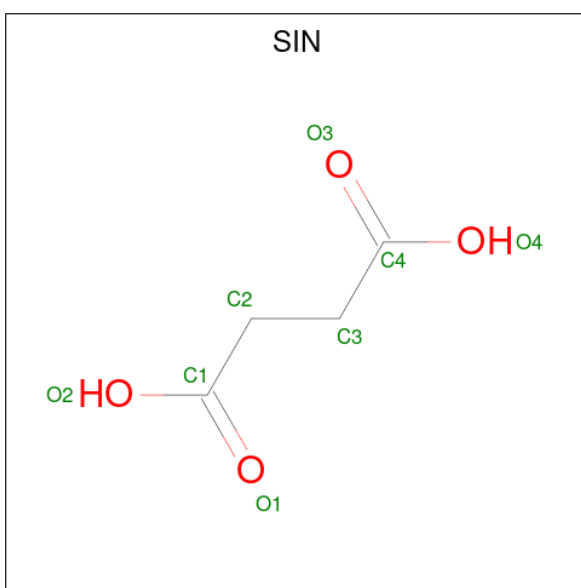
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Fe 2 2	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0

- Molecule 3 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).



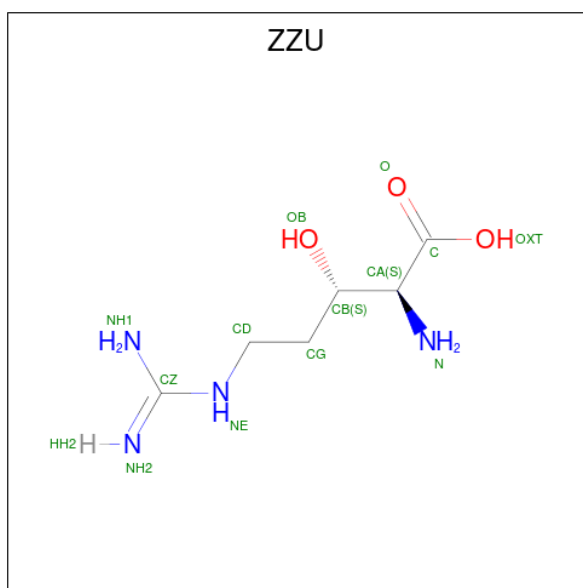
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is SUCCINIC ACID (CCD ID: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			8	4	4		
4	D	1	Total	C	O	0	0
			8	4	4		

- Molecule 5 is (2S,3S)-3-HYDROXYARGININE (CCD ID: ZZU) (formula: $C_6H_{14}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			13	6	4	3		
5	D	1	Total	C	N	O	0	0
			13	6	4	3		

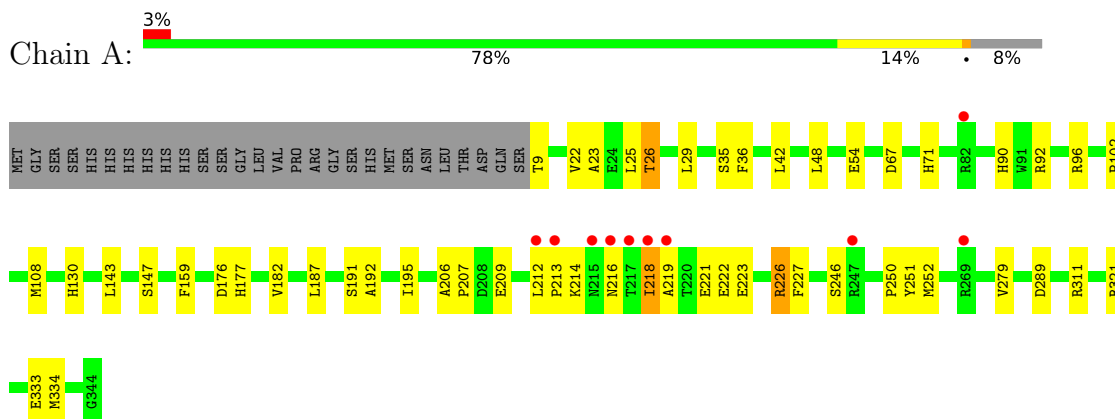
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	213	Total	O	0	0
			213	213		
6	B	144	Total	O	0	0
			144	144		
6	C	204	Total	O	0	0
			204	204		
6	D	135	Total	O	0	0
			135	135		

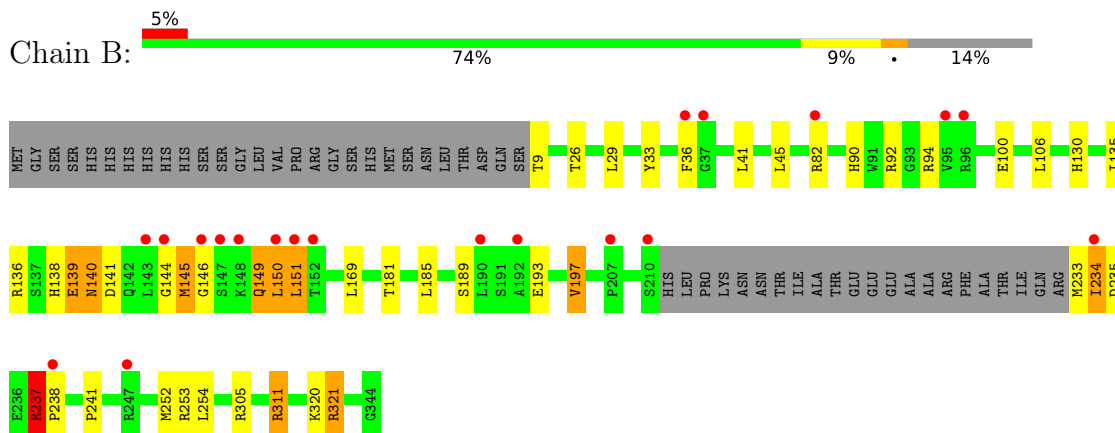
3 Residue-property plots [i](#)

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.

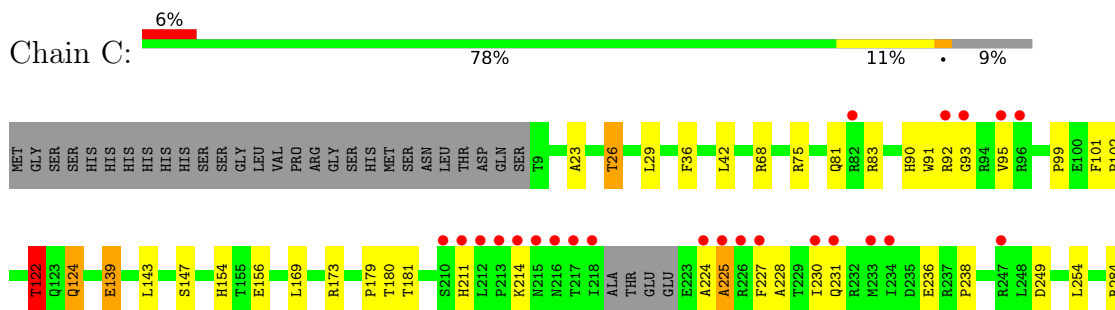
- Molecule 1: L-arginine beta-hydroxylase

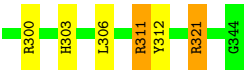


- Molecule 1: L-arginine beta-hydroxylase

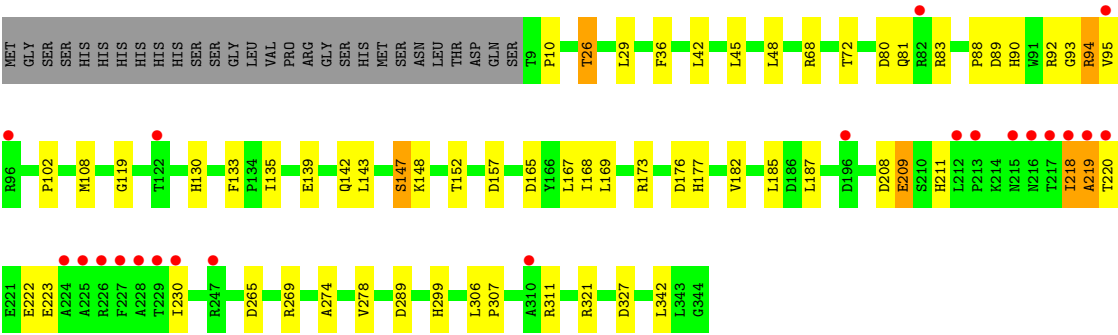


- Molecule 1: L-arginine beta-hydroxylase





● Molecule 1: L-arginine beta-hydroxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.11Å 116.70Å 96.15Å 90.00° 91.47° 90.00°	Depositor
Resolution (Å)	30.00 – 2.02 30.00 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.02) 99.6 (30.00-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.208 , 0.265 (Not available) , 0.283	Depositor DCC
R_{free} test set	4888 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11335	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AKG, SIN, FE, ZZU

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	0.82	0/2771	0.90	2/3768 (0.1%)
1	B	0.79	0/2587	0.85	0/3518
1	C	0.82	0/2729	0.90	1/3710 (0.0%)
1	D	0.77	0/2760	0.86	0/3754
All	All	0.80	0/10847	0.88	3/14750 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	ALA	CA-C-N	5.32	125.58	119.83
1	A	206	ALA	C-N-CA	5.32	125.58	119.83
1	C	180	THR	N-CA-C	-5.01	101.54	109.96

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	2701	0	2618	32	0
1	B	2521	0	2439	31	0
1	C	2660	0	2581	33	0
1	D	2690	0	2606	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0
4	C	8	0	4	0	0
4	D	8	0	4	0	0
5	C	13	0	11	2	0
5	D	13	0	11	0	0
6	A	213	0	0	6	0
6	B	144	0	0	1	0
6	C	204	0	0	2	0
6	D	135	0	0	2	0
All	All	11335	0	10282	135	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 6.

All (135) 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:C:26:THR:HG23	1:C:102:PRO:HB3	1.44	1.00
1:D:26:THR:HG23	1:D:102:PRO:HB3	1.49	0.94
1:C:90:HIS:CD2	1:C:92:ARG:HB2	2.06	0.90
1:A:26:THR:HG23	1:A:102:PRO:HB3	1.58	0.84
1:B:321:ARG:HH11	1:B:321:ARG:HG2	1.42	0.84
1:A:26:THR:HG21	6:A:574:HOH:O	1.77	0.83
1:C:26:THR:HG21	6:C:510:HOH:O	1.83	0.79
1:C:211:HIS:HB3	1:C:230:ILE:HD13	1.64	0.77
1:D:142:GLN:HE22	1:D:152:THR:H	1.33	0.76
1:B:237:ARG:N	1:B:238:PRO:HD3	2.02	0.74
1:D:211:HIS:HB3	1:D:230:ILE:HD13	1.69	0.73
1:A:209:GLU:HA	1:A:212:LEU:HD13	1.71	0.73
1:D:169:LEU:CD2	1:D:321:ARG:HG3	2.18	0.73
1:C:36:PHE:CD1	1:C:36:PHE:O	2.44	0.70
1:B:233:MET:HG3	1:B:234:ILE:H	1.57	0.70
1:D:169:LEU:HD23	1:D:321:ARG:HG3	1.73	0.70
1:D:157:ASP:OD1	1:D:211:HIS:HE1	1.76	0.69
1:C:236:GLU:HG3	1:C:238:PRO:HD3	1.76	0.67
1:D:177:HIS:HD2	1:D:289:ASP:OD1	1.78	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:TRP:CE3	1:C:92:ARG:HA	2.30	0.66
1:D:26:THR:HG23	1:D:102:PRO:CB	2.23	0.66
1:C:95:VAL:HB	6:C:668:HOH:O	1.96	0.65
1:B:149:GLN:HG2	1:B:305:ARG:O	1.96	0.64
1:A:176:ASP:OD2	1:A:311:ARG:NH2	2.31	0.64
1:A:90:HIS:HD2	1:A:92[B]:ARG:H	1.44	0.62
1:B:321:ARG:HG2	1:B:321:ARG:NH1	2.08	0.62
1:B:144:GLY:O	1:B:145:MET:HB2	1.98	0.61
1:C:90:HIS:HD2	1:C:92:ARG:HB2	1.63	0.61
1:C:169:LEU:CD2	1:C:321:ARG:HG3	2.30	0.61
1:B:135:ILE:HG22	1:B:138:HIS:H	1.65	0.61
1:A:90:HIS:HD2	1:A:92[A]:ARG:H	1.46	0.60
1:A:90:HIS:CD2	1:A:92[A]:ARG:HG3	2.36	0.60
1:D:327:ASP:OD1	6:D:536:HOH:O	2.17	0.60
1:C:90:HIS:HD2	1:C:92:ARG:H	1.50	0.60
1:A:90:HIS:CD2	1:A:92[B]:ARG:H	2.20	0.59
1:A:36:PHE:CE1	1:A:108:MET:HG3	2.36	0.59
1:C:169:LEU:HD23	1:C:321:ARG:HG3	1.84	0.59
1:C:122:THR:HG22	1:C:227:PHE:CE2	2.37	0.59
1:A:90:HIS:CD2	1:A:92[A]:ARG:H	2.21	0.58
1:C:139:GLU:HG2	1:C:312:TYR:OH	2.04	0.58
1:B:237:ARG:N	1:B:237:ARG:HD2	2.20	0.56
1:D:209:GLU:C	1:D:211:HIS:H	2.13	0.56
1:A:177:HIS:HD2	1:A:289:ASP:OD1	1.89	0.56
1:A:252:MET:HE1	1:A:279:VAL:HG21	1.87	0.56
1:B:146:GLY:O	1:B:305:ARG:NH2	2.39	0.55
1:B:241:PRO:O	1:B:253:ARG:NH1	2.38	0.54
1:A:187:LEU:HD22	1:A:250:PRO:HD3	1.90	0.53
1:D:169:LEU:HD21	1:D:321:ARG:HG3	1.90	0.53
1:B:26:THR:HG21	1:B:106:LEU:HB2	1.91	0.53
1:D:222:GLU:CD	1:D:223:GLU:H	2.17	0.53
1:B:149:GLN:O	1:B:150:LEU:HB2	2.08	0.53
1:C:225:ALA:HB1	1:C:228:ALA:HB2	1.91	0.53
1:B:151:LEU:HD12	1:B:181:THR:HG21	1.91	0.53
1:B:321:ARG:HH11	1:B:321:ARG:CG	2.19	0.53
1:A:214:LYS:HE3	1:A:218:ILE:HD11	1.89	0.52
1:C:179:PRO:HG2	1:C:306:LEU:HD12	1.91	0.52
1:A:96:ARG:HD3	6:A:629:HOH:O	2.09	0.52
1:D:130:HIS:HD2	1:D:321:ARG:HH12	1.58	0.51
1:D:81:GLN:NE2	1:D:173:ARG:HH11	2.08	0.51
1:D:139:GLU:HG2	1:D:148:LYS:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ALA:HA	1:A:195:ILE:HD12	1.92	0.50
1:C:90:HIS:CD2	1:C:92:ARG:H	2.30	0.50
1:A:223:GLU:HG2	1:A:226:ARG:NH2	2.25	0.50
1:B:139:GLU:C	1:B:141:ASP:H	2.20	0.50
1:A:219:ALA:O	1:A:223:GLU:HB2	2.12	0.50
1:D:10:PRO:O	1:D:72:THR:HG22	2.12	0.50
1:D:90:HIS:HD2	1:D:92:ARG:H	1.60	0.49
1:D:265:ASP:O	1:D:269:ARG:HG3	2.13	0.49
1:B:9:THR:N	6:B:546:HOH:O	2.46	0.48
1:B:237:ARG:H	1:B:238:PRO:HD3	1.78	0.48
1:A:23:ALA:O	1:A:26:THR:HG22	2.13	0.48
1:D:218:ILE:HG22	1:D:219:ALA:H	1.78	0.48
1:D:176:ASP:OD1	1:D:311:ARG:NH2	2.47	0.48
1:B:92:ARG:C	1:B:94:ARG:H	2.23	0.47
1:B:193:GLU:O	1:B:197:VAL:HG12	2.14	0.47
1:C:311:ARG:HH11	1:C:311:ARG:HB2	1.79	0.47
1:D:142:GLN:NE2	1:D:152:THR:H	2.08	0.47
1:D:165:ASP:OD1	1:D:299:HIS:CE1	2.68	0.47
1:A:130:HIS:ND1	6:A:636:HOH:O	2.35	0.47
1:A:159:PHE:CG	1:A:207:PRO:HA	2.50	0.47
1:D:220:THR:HG22	1:D:220:THR:O	2.16	0.46
1:C:36:PHE:O	1:C:36:PHE:HD1	1.98	0.46
1:D:80:ASP:OD2	1:D:83:ARG:HB2	2.16	0.46
1:D:299:HIS:ND1	6:D:629:HOH:O	2.35	0.45
1:C:154:HIS:CE1	5:C:403:ZZU:HG2C	2.51	0.45
1:D:36:PHE:CE1	1:D:108:MET:HG3	2.52	0.45
1:A:9:THR:HG21	1:A:71:HIS:CE1	2.52	0.45
1:A:222:GLU:OE1	1:A:222:GLU:N	2.49	0.45
1:B:136:ARG:O	1:B:139:GLU:HB2	2.18	0.44
1:C:169:LEU:HD23	1:C:321:ARG:CG	2.48	0.44
1:B:36:PHE:HA	1:B:41:LEU:HD23	1.98	0.44
1:B:100:GLU:HG3	1:B:320:LYS:HE3	1.99	0.44
1:C:91:TRP:CE2	1:C:124:GLN:HG2	2.53	0.44
1:D:119:GLY:O	1:D:342:LEU:HA	2.18	0.43
1:D:157:ASP:OD1	1:D:211:HIS:CE1	2.65	0.43
1:C:26:THR:HG23	1:C:102:PRO:CB	2.30	0.43
1:B:237:ARG:N	1:B:238:PRO:CD	2.75	0.43
1:B:252:MET:HE2	1:B:254:LEU:HD22	1.99	0.43
1:A:333:GLU:HG2	6:A:657:HOH:O	2.18	0.43
1:C:101:PHE:HB3	1:C:102:PRO:HD3	2.00	0.43
1:A:22:VAL:O	1:A:26:THR:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:ASP:OD1	1:D:299:HIS:HE1	2.01	0.43
1:C:156:GLU:OE2	5:C:403:ZZU:N	2.52	0.43
1:B:139:GLU:O	1:B:141:ASP:N	2.49	0.43
1:B:33:TYR:CD2	1:B:41:LEU:HB2	2.54	0.43
1:D:89:ASP:O	1:D:135:ILE:HG12	2.19	0.43
1:A:54:GLU:HG3	6:A:561:HOH:O	2.18	0.43
1:D:88:PRO:HG2	1:D:133:PHE:CE2	2.54	0.43
1:D:274:ALA:O	1:D:278:VAL:HG23	2.19	0.43
1:B:150:LEU:HB3	1:B:151:LEU:H	1.65	0.42
1:C:181:THR:O	1:C:303:HIS:HA	2.19	0.42
1:D:168:ILE:O	1:D:321:ARG:HA	2.18	0.42
1:A:26:THR:HG23	1:A:102:PRO:CB	2.40	0.42
1:B:311:ARG:HH11	1:B:311:ARG:HB2	1.84	0.42
1:D:209:GLU:C	1:D:211:HIS:N	2.77	0.42
1:A:35:SER:HB2	6:A:578:HOH:O	2.18	0.42
1:C:23:ALA:O	1:C:26:THR:HG22	2.19	0.42
1:C:81:GLN:NE2	1:C:173:ARG:HH11	2.16	0.42
1:C:249:ASP:CG	1:C:300:ARG:HH22	2.27	0.42
1:A:226:ARG:HG3	1:A:334:MET:HA	2.01	0.42
1:A:213:PRO:HG3	1:A:227:PHE:HB3	2.00	0.42
1:C:81:GLN:HE22	1:C:173:ARG:HE	1.67	0.41
1:D:208:ASP:C	1:D:209:GLU:O	2.62	0.41
1:D:148:LYS:O	1:D:307:PRO:HB3	2.20	0.41
1:D:130:HIS:HD2	1:D:321:ARG:NH1	2.19	0.41
1:C:90:HIS:HD2	1:C:92:ARG:N	2.14	0.41
1:C:83:ARG:O	1:C:99:PRO:HB2	2.21	0.41
1:A:67:ASP:OD2	1:A:251:TYR:OH	2.38	0.41
1:C:81:GLN:NE2	1:C:173:ARG:HE	2.18	0.41
1:D:93:GLY:O	1:D:94:ARG:O	2.39	0.40
1:B:135:ILE:HD12	1:B:145:MET:HG3	2.03	0.40
1:A:25:LEU:O	1:A:29:LEU:HG	2.21	0.40
1:B:90:HIS:CD2	1:B:92:ARG:HD2	2.56	0.40
1:D:143:LEU:HD21	1:D:209:GLU:HB2	2.03	0.40
1:B:233:MET:CG	1:B:234:ILE:H	2.31	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	335/364 (92%)	325 (97%)	9 (3%)	1 (0%)	36	31
1	B	311/364 (85%)	295 (95%)	9 (3%)	7 (2%)	5	1
1	C	328/364 (90%)	311 (95%)	11 (3%)	6 (2%)	6	2
1	D	334/364 (92%)	314 (94%)	14 (4%)	6 (2%)	6	2
All	All	1308/1456 (90%)	1245 (95%)	43 (3%)	20 (2%)	8	3

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	139	GLU
1	B	145	MET
1	D	94	ARG
1	B	140	ASN
1	B	234	ILE
1	B	235	ASP
1	C	224	ALA
1	D	218	ILE
1	D	219	ALA
1	B	150	LEU
1	C	147	SER
1	D	209	GLU
1	A	147	SER
1	B	237	ARG
1	C	122	THR
1	C	225	ALA
1	D	95	VAL
1	D	147	SER
1	C	93	GLY
1	C	124	GLN

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	287/311 (92%)	275 (96%)	12 (4%)	26	20
1	B	269/311 (86%)	255 (95%)	14 (5%)	21	13
1	C	283/311 (91%)	269 (95%)	14 (5%)	22	15
1	D	286/311 (92%)	274 (96%)	12 (4%)	26	20
All	All	1125/1244 (90%)	1073 (95%)	52 (5%)	24	17

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	A	42	LEU
1	A	48	LEU
1	A	143	LEU
1	A	182	VAL
1	A	191	SER
1	A	216	ASN
1	A	218	ILE
1	A	221	GLU
1	A	226	ARG
1	A	246	SER
1	A	321	ARG
1	B	29	LEU
1	B	45	LEU
1	B	82	ARG
1	B	130	HIS
1	B	140	ASN
1	B	149	GLN
1	B	151	LEU
1	B	169	LEU
1	B	185	LEU
1	B	189	SER
1	B	197	VAL
1	B	237	ARG

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Mol	Chain	Res	Type
1	B	311	ARG
1	B	321	ARG
1	C	26	THR
1	C	29	LEU
1	C	42	LEU
1	C	68	ARG
1	C	75	ARG
1	C	122	THR
1	C	139	GLU
1	C	143	LEU
1	C	214	LYS
1	C	231	GLN
1	C	254	LEU
1	C	284	ARG
1	C	311	ARG
1	C	321	ARG
1	D	26	THR
1	D	29	LEU
1	D	42	LEU
1	D	45	LEU
1	D	48	LEU
1	D	68	ARG
1	D	147	SER
1	D	167	LEU
1	D	182	VAL
1	D	185	LEU
1	D	187	LEU
1	D	306	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	81	GLN
1	A	90	HIS
1	A	138	HIS
1	A	177	HIS
1	A	215	ASN
1	B	57	GLN
1	B	81	GLN
1	B	90	HIS
1	B	142	GLN

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Mol	Chain	Res	Type
1	B	177	HIS
1	C	57	GLN
1	C	81	GLN
1	C	90	HIS
1	C	127	HIS
1	C	130	HIS
1	C	142	GLN
1	C	177	HIS
1	C	290	GLN
1	D	57	GLN
1	D	81	GLN
1	D	90	HIS
1	D	130	HIS
1	D	142	GLN
1	D	177	HIS
1	D	211	HIS
1	D	215	ASN
1	D	216	ASN
1	D	263	GLN
1	D	290	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 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	SIN	C	402	2	7,7,7	1.30	0	8,8,8	1.33	2 (25%)
4	SIN	D	402	2	7,7,7	1.33	0	8,8,8	0.96	0
3	AKG	A	403	2	9,9,9	1.85	1 (11%)	11,11,11	1.85	4 (36%)
5	ZZU	C	403	2	11,12,12	1.04	0	10,15,15	1.13	1 (10%)
5	ZZU	D	403	2	11,12,12	0.93	0	10,15,15	1.25	2 (20%)
3	AKG	B	402	2	9,9,9	1.76	1 (11%)	11,11,11	1.87	3 (27%)

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	SIN	C	402	2	-	2/5/5/5	-
4	SIN	D	402	2	-	2/5/5/5	-
3	AKG	A	403	2	-	1/9/9/9	-
5	ZZU	C	403	2	-	3/14/14/14	-
5	ZZU	D	403	2	-	4/14/14/14	-
3	AKG	B	402	2	-	4/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	AKG	C2-C1	-4.66	1.46	1.53
3	B	402	AKG	C2-C1	-3.85	1.47	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	AKG	C3-C2-C1	4.01	122.67	115.86
3	A	403	AKG	O1-C1-C2	-3.72	117.18	121.81
5	D	403	ZZU	OXT-C-O	-2.96	117.36	124.08
3	A	403	AKG	C3-C2-C1	2.88	120.75	115.86
5	C	403	ZZU	OXT-C-O	-2.61	118.16	124.08
3	B	402	AKG	O2-C1-C2	2.51	120.55	113.59
3	B	402	AKG	O1-C1-C2	-2.28	118.97	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	AKG	O4-C5-C4	2.21	120.99	114.00
3	A	403	AKG	O2-C1-C2	2.16	119.58	113.59
5	D	403	ZZU	OXT-C-CA	2.06	121.25	114.15
4	C	402	SIN	O4-C4-C3	2.06	120.51	114.00
4	C	402	SIN	O3-C4-C3	-2.03	116.64	123.09

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	403	ZZU	NE-CD-CG-CB
5	D	403	ZZU	CA-CB-CG-CD
5	D	403	ZZU	NE-CD-CG-CB
5	C	403	ZZU	OXT-C-CA-N
3	B	402	AKG	O1-C1-C2-O5
3	A	403	AKG	C1-C2-C3-C4
5	D	403	ZZU	OB-CB-CG-CD
3	B	402	AKG	O2-C1-C2-O5
3	B	402	AKG	O2-C1-C2-C3
4	D	402	SIN	C2-C3-C4-O3
4	D	402	SIN	C2-C3-C4-O4
5	D	403	ZZU	CG-CD-NE-CZ
4	C	402	SIN	C2-C3-C4-O4
3	B	402	AKG	O1-C1-C2-C3
4	C	402	SIN	C2-C3-C4-O3
5	C	403	ZZU	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	403	ZZU	2	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	336/364 (92%)	0.07	10 (2%) 52 52	11, 34, 63, 128	5 (1%)
1	B	314/364 (86%)	0.49	20 (6%) 25 24	20, 41, 83, 113	4 (1%)
1	C	332/364 (91%)	0.19	23 (6%) 23 22	21, 34, 93, 134	4 (1%)
1	D	336/364 (92%)	0.46	22 (6%) 25 24	24, 43, 81, 143	3 (0%)
All	All	1318/1456 (90%)	0.30	75 (5%) 29 28	11, 38, 82, 143	16 (1%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	THR	5.9
1	A	218	ILE	5.8
1	D	225	ALA	5.7
1	C	92	ARG	5.6
1	A	82	ARG	5.3
1	B	151	LEU	5.1
1	B	148	LYS	4.9
1	B	150	LEU	4.9
1	D	218	ILE	4.9
1	C	230	ILE	4.8
1	A	269	ARG	4.8
1	C	224	ALA	4.7
1	C	95	VAL	4.6
1	B	143	LEU	4.5
1	B	82	ARG	4.3
1	D	224	ALA	4.2
1	D	230	ILE	4.1
1	C	82	ARG	4.0
1	A	216	ASN	4.0
1	C	234	ILE	4.0
1	D	82	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	220	THR	3.9
1	C	93	GLY	3.8
1	D	216	ASN	3.7
1	C	212	LEU	3.6
1	C	213	PRO	3.5
1	B	146	GLY	3.5
1	B	147	SER	3.5
1	C	217	THR	3.4
1	B	144	GLY	3.4
1	D	217	THR	3.3
1	D	213	PRO	3.3
1	B	234	ILE	3.3
1	C	96	ARG	3.2
1	C	216	ASN	3.2
1	B	36	PHE	3.1
1	C	218	ILE	3.1
1	C	225	ALA	3.0
1	D	212	LEU	3.0
1	B	95	VAL	3.0
1	D	219	ALA	2.9
1	B	96	ARG	2.8
1	D	95	VAL	2.8
1	A	219	ALA	2.7
1	A	212	LEU	2.7
1	A	213	PRO	2.7
1	B	210	SER	2.7
1	C	210	SER	2.7
1	B	192	ALA	2.7
1	C	215	ASN	2.7
1	D	226	ARG	2.7
1	C	231	GLN	2.7
1	D	96	ARG	2.7
1	B	152	THR	2.6
1	C	227	PHE	2.6
1	D	227	PHE	2.6
1	D	228	ALA	2.6
1	D	229	THR	2.6
1	D	122	THR	2.5
1	B	37	GLY	2.5
1	B	247	ARG	2.5
1	A	215	ASN	2.4
1	D	247	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	207	PRO	2.3
1	C	214	LYS	2.3
1	C	233	MET	2.3
1	B	238	PRO	2.3
1	C	211	HIS	2.2
1	B	190	LEU	2.1
1	C	247	ARG	2.1
1	D	310	ALA	2.1
1	D	196	ASP	2.0
1	C	226	ARG	2.0
1	D	215	ASN	2.0
1	A	247	ARG	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
3	AKG	B	402	10/10	0.79	0.13	40,49,53,57	0
5	ZZU	D	403	13/13	0.87	0.10	39,46,49,52	0
4	SIN	C	402	8/8	0.89	0.08	31,32,39,39	0
5	ZZU	C	403	13/13	0.91	0.10	36,47,58,61	0
3	AKG	A	403	10/10	0.94	0.07	29,33,38,38	0
4	SIN	D	402	8/8	0.94	0.07	33,36,37,38	0
2	FE	A	402	1/1	0.98	0.14	55,55,55,55	0
2	FE	B	401	1/1	0.98	0.04	40,40,40,40	0
2	FE	C	401	1/1	0.99	0.02	30,30,30,30	0
2	FE	A	401	1/1	1.00	0.01	31,31,31,31	0
2	FE	D	401	1/1	1.00	0.01	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.