Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:59 PM GMT

PDB ID	:	4NE0
Title	:	Crystal structure of non-heme iron oxygenase OrfP D157A mutant in complex with (3S)-hydroxy-L-Arg
Authors	:	Chang, C.Y.; Liu, Y.C.; Lyu, S.Y.; Wu, C.C.; Li, T.L.
Deposited on	:	2013-10-28
Resolution	:	2.17 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

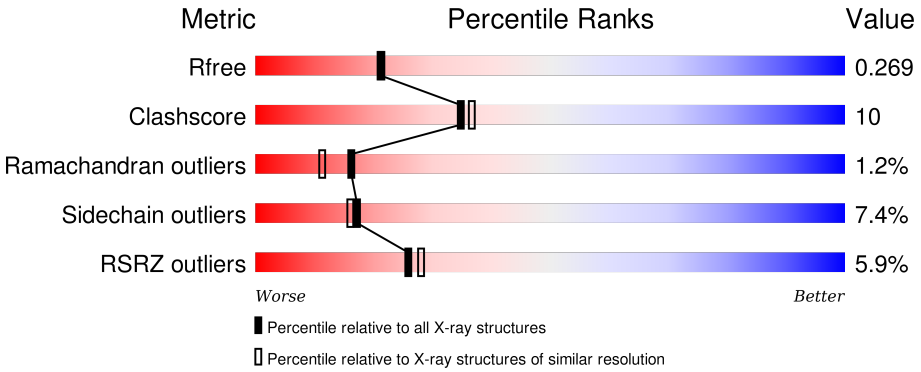
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.17 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}	91344	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	5% 73% 17% • 7%
1	B	364	9% 62% 19% • 16%
1	C	364	4% 69% 15% • • 12%
1	D	364	4% 68% 16% • 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ZZU	D	403	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10692 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	337	Total	C	N	O	S	0	0	0
			2693	1695	488	503	7			
1	B	304	Total	C	N	O	S	0	0	0
			2438	1542	439	451	6			
1	C	322	Total	C	N	O	S	0	0	0
			2576	1625	467	477	7			
1	D	316	Total	C	N	O	S	0	0	0
			2532	1596	460	469	7			

There are 84 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
A	157	ALA	ASP	ENGINEERED MUTATION	UNP G9MBV2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	EXPRESSION TAG	UNP G9MBV2
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
B	157	ALA	ASP	ENGINEERED MUTATION	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
C	157	ALA	ASP	ENGINEERED MUTATION	UNP G9MBV2

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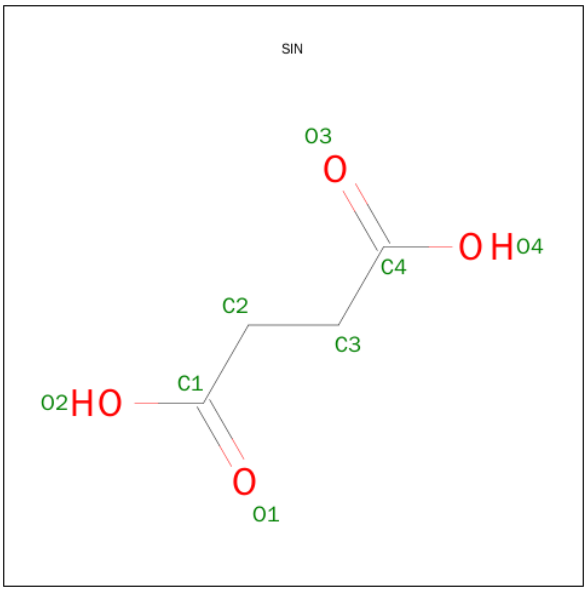
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	EXPRESSION TAG	UNP G9MBV2
D	-18	GLY	-	EXPRESSION TAG	UNP G9MBV2
D	-17	SER	-	EXPRESSION TAG	UNP G9MBV2
D	-16	SER	-	EXPRESSION TAG	UNP G9MBV2
D	-15	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-14	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-13	HIS	-	EXPRESSION TAG	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
D	157	ALA	ASP	ENGINEERED MUTATION	UNP G9MBV2

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

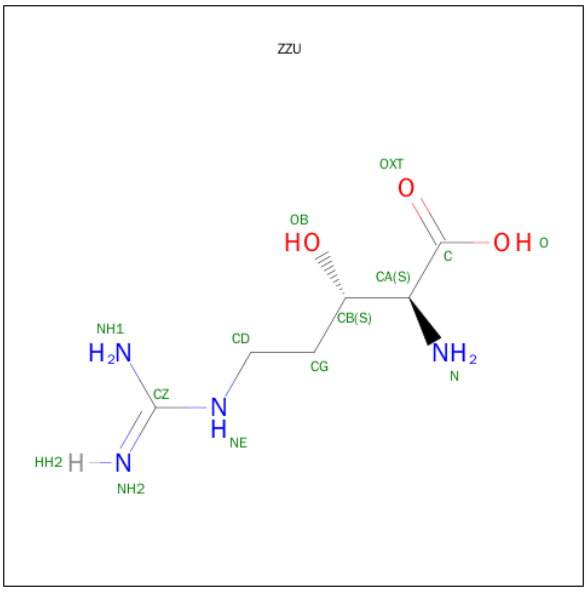
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0

- Molecule 3 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



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

- Molecule 4 is (2S,3S)-3-HYDROXYARGININE (three-letter code: ZZU) (formula: $C_6H_{14}N_4O_3$).



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

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

- Molecule 5 is water.

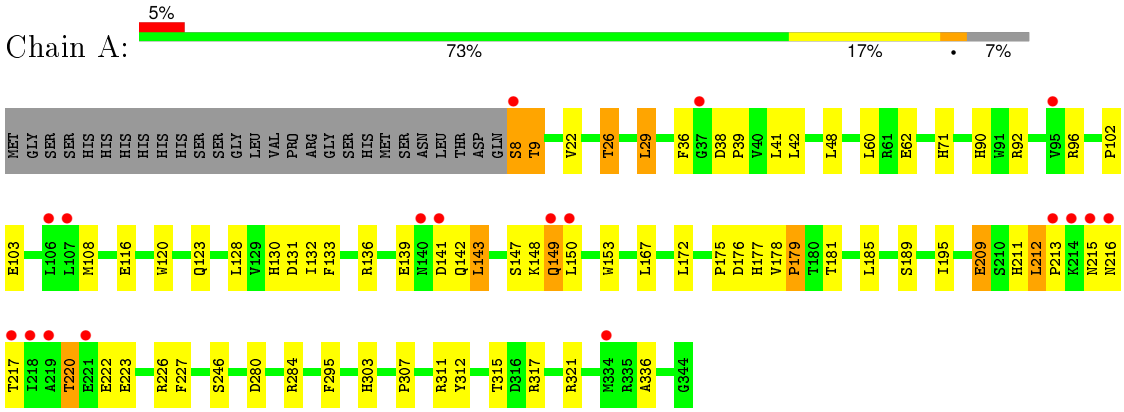
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	138	Total	O	0	0
			138	138		
5	B	73	Total	O	0	0
			73	73		
5	C	100	Total	O	0	0
			100	100		
5	D	96	Total	O	0	0
			96	96		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

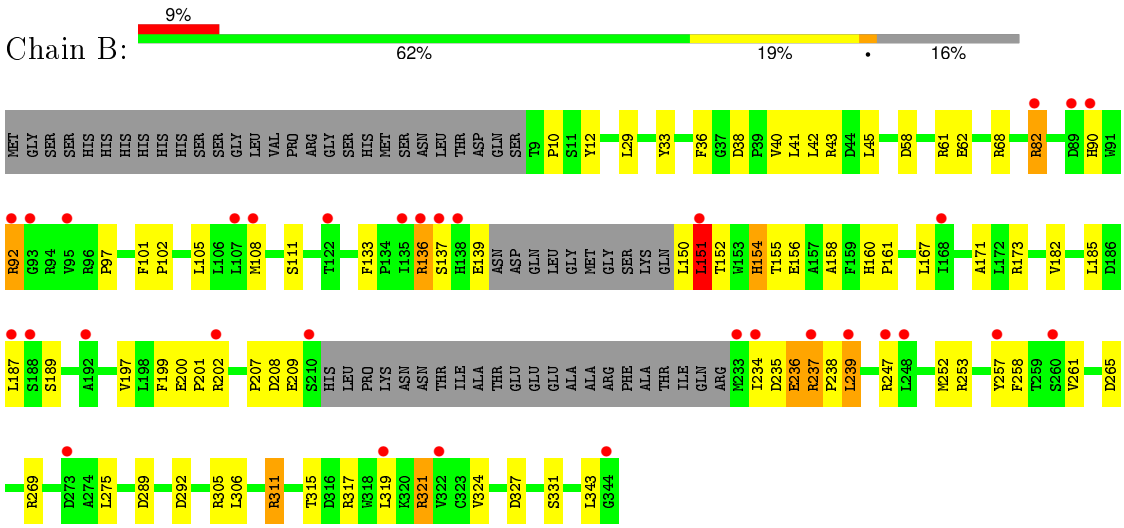
- Molecule 1: L-arginine beta-hydroxylase

Chain A:



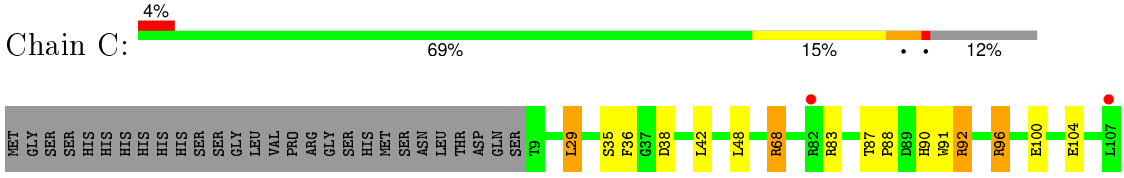
- Molecule 1: L-arginine beta-hydroxylase

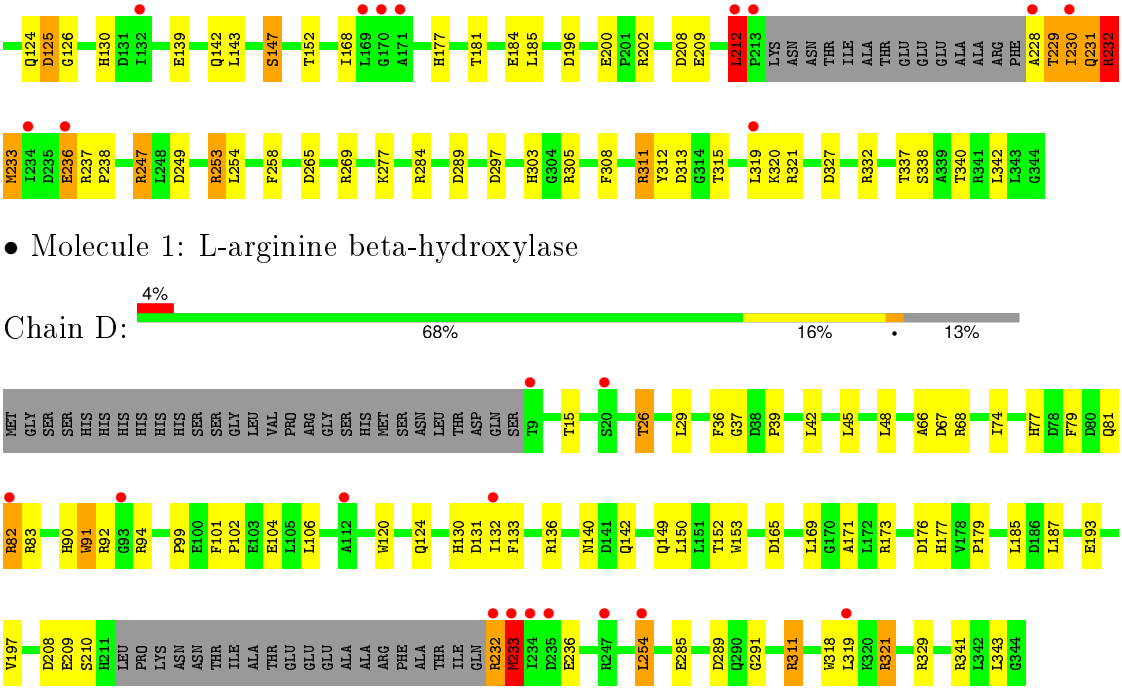
Chain B:



- Molecule 1: L-arginine beta-hydroxylase

Chain C:





- Molecule 1: L-arginine beta-hydroxylase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.86Å 117.33Å 95.81Å 90.00° 91.33° 90.00°	Depositor
Resolution (Å)	30.00 – 2.17 23.95 – 2.17	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.00-2.17) 96.9 (23.95-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 2.17Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.210 , 0.269 0.210 , 0.269	Depositor DCC
R_{free} test set	3823 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	33.1	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.3	EDS
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 76424 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10692	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZZU, FE, SIN

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	0.91	2/2763 (0.1%)	0.97	2/3758 (0.1%)
1	B	0.81	0/2503	0.92	2/3405 (0.1%)
1	C	0.92	0/2644	1.04	11/3596 (0.3%)
1	D	0.85	4/2599 (0.2%)	0.96	5/3533 (0.1%)
All	All	0.88	6/10509 (0.1%)	0.97	20/14292 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	TRP	CD2-CE2	6.60	1.49	1.41
1	D	153	TRP	CD2-CE2	5.74	1.48	1.41
1	D	120	TRP	CD2-CE2	5.50	1.48	1.41
1	D	91	TRP	CD2-CE2	5.45	1.47	1.41
1	A	153	TRP	CD2-CE2	5.20	1.47	1.41
1	D	318	TRP	CD2-CE2	5.19	1.47	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	247	ARG	NE-CZ-NH1	-9.77	115.41	120.30
1	C	305	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	C	305	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	C	253	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	D	341	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	317	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	C	83	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	C	212	LEU	CA-CB-CG	6.10	129.33	115.30
1	C	247	ARG	NE-CZ-NH2	6.07	123.34	120.30
1	C	83	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	D	254	LEU	CA-CB-CG	5.84	128.74	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	321	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	173	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	D	341	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	29	LEU	CB-CG-CD1	5.53	120.40	111.00
1	C	319	LEU	CA-CB-CG	5.42	127.76	115.30
1	B	327	ASP	CB-CG-OD1	5.33	123.10	118.30
1	C	29	LEU	CB-CG-CD1	5.15	119.75	111.00
1	C	332	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	D	165	ASP	CB-CG-OD1	-5.04	113.76	118.30

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	2693	0	2612	48	0
1	B	2438	0	2361	47	0
1	C	2576	0	2501	69	0
1	D	2532	0	2452	40	0
2	A	1	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	C	8	0	4	0	0
3	D	8	0	4	1	0
4	C	13	0	11	1	0
4	D	13	0	12	0	0
5	A	138	0	0	3	2
5	B	73	0	0	1	0
5	C	100	0	0	1	0
5	D	96	0	0	1	2
All	All	10692	0	9957	200	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (200) 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:130:HIS:CE1	1:A:321:ARG:HH11	1.62	1.18
1:B:82:ARG:HH11	1:B:82:ARG:HG2	1.01	1.14
1:C:229:THR:HA	1:C:230:ILE:HB	1.35	1.09
1:D:82:ARG:HG3	1:D:82:ARG:HH21	1.11	1.08
1:B:237:ARG:HB3	1:B:238:PRO:HD3	1.30	1.08
1:D:26:THR:HG23	1:D:102:PRO:HB3	1.36	1.07
1:D:169:LEU:HD23	1:D:321:ARG:HG3	1.35	1.04
1:B:237:ARG:CB	1:B:238:PRO:HD3	1.89	1.03
1:C:236:GLU:HG3	1:C:238:PRO:HD3	1.42	0.99
1:D:82:ARG:HG3	1:D:82:ARG:NH2	1.71	0.97
1:B:82:ARG:HH11	1:B:82:ARG:CG	1.77	0.96
1:C:229:THR:HA	1:C:230:ILE:CB	1.96	0.95
1:A:26:THR:HG23	1:A:102:PRO:HB3	1.46	0.94
1:C:232:ARG:HE	1:C:236:GLU:HB2	1.31	0.94
1:B:237:ARG:HB3	1:B:238:PRO:CD	1.97	0.93
1:D:169:LEU:CD2	1:D:321:ARG:HG3	1.99	0.92
1:C:90:HIS:HD2	1:C:92:ARG:H	1.18	0.91
1:B:82:ARG:NH1	1:B:82:ARG:HG2	1.84	0.91
1:A:130:HIS:HE1	1:A:321:ARG:NH1	1.67	0.90
1:C:130:HIS:HE1	1:C:321:ARG:HE	1.19	0.89
1:A:130:HIS:HE1	1:A:321:ARG:HH11	0.86	0.86
1:A:8:SER:OG	1:A:9:THR:N	2.08	0.85
1:C:130:HIS:CE1	1:C:321:ARG:HE	1.95	0.85
1:D:26:THR:HG23	1:D:102:PRO:CB	2.10	0.82
1:A:26:THR:HG21	5:A:525:HOH:O	1.80	0.81
1:A:130:HIS:CE1	1:A:321:ARG:NH1	2.42	0.81
1:D:82:ARG:CG	1:D:82:ARG:HH21	1.90	0.80
1:B:38:ASP:OD1	1:B:40:VAL:HG12	1.81	0.79
1:A:209:GLU:HA	1:A:212:LEU:HD22	1.66	0.78
1:D:169:LEU:HD23	1:D:321:ARG:CG	2.14	0.77
1:B:261:VAL:HG11	1:B:269:ARG:HG2	1.68	0.75
1:C:142:GLN:NE2	1:C:152:THR:H	1.86	0.74
1:B:237:ARG:CB	1:B:238:PRO:CD	2.63	0.72
1:C:139:GLU:HG2	1:C:312:TYR:OH	1.89	0.72
1:D:130:HIS:NE2	1:D:321:ARG:HD2	2.03	0.72
1:C:229:THR:CA	1:C:230:ILE:HB	2.17	0.71
1:A:142:GLN:OE1	1:A:150:LEU:O	2.09	0.71
1:A:90:HIS:CD2	1:A:92:ARG:H	2.08	0.71
1:D:90:HIS:HD2	1:D:92:ARG:H	1.39	0.71
1:B:331:SER:HB2	1:B:343:LEU:HD11	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:THR:HA	1:C:230:ILE:CG1	2.20	0.70
1:B:235:ASP:H	1:B:237:ARG:HH21	1.39	0.70
1:D:176:ASP:OD2	1:D:311:ARG:NH2	2.26	0.68
1:C:90:HIS:CD2	1:C:92:ARG:H	2.07	0.67
1:C:232:ARG:HE	1:C:236:GLU:CB	2.06	0.67
1:C:184:GLU:HG3	1:C:284:ARG:HH22	1.59	0.67
1:A:26:THR:HG23	1:A:102:PRO:CB	2.23	0.66
1:C:36:PHE:HE2	1:C:104:GLU:OE2	1.78	0.66
1:A:90:HIS:HD2	1:A:92:ARG:H	1.41	0.66
1:A:36:PHE:CE1	1:A:108:MET:HG3	2.30	0.66
1:A:280:ASP:OD1	5:A:636:HOH:O	2.13	0.65
1:C:327:ASP:OD1	5:C:529:HOH:O	2.13	0.64
1:C:196:ASP:OD1	1:C:247:ARG:NH1	2.32	0.62
1:A:211:HIS:O	1:A:213:PRO:HD3	1.98	0.62
1:B:171:ALA:HA	1:B:319:LEU:HD22	1.82	0.62
1:A:26:THR:CG2	1:A:102:PRO:HB3	2.28	0.61
1:C:130:HIS:HE1	1:C:321:ARG:NE	1.94	0.61
1:C:229:THR:HA	1:C:230:ILE:HD12	1.82	0.61
1:A:148:LYS:O	1:A:307:PRO:HB3	2.00	0.60
1:B:237:ARG:HB2	1:B:238:PRO:HD3	1.83	0.60
1:B:261:VAL:CG1	1:B:269:ARG:HG2	2.31	0.60
1:D:142:GLN:HE22	1:D:152:THR:H	1.50	0.59
1:B:82:ARG:NH1	1:B:82:ARG:CG	2.48	0.59
1:C:236:GLU:CG	1:C:238:PRO:HD3	2.24	0.59
1:C:142:GLN:HE22	1:C:152:THR:H	1.49	0.59
1:C:236:GLU:HG3	1:C:238:PRO:CD	2.25	0.59
1:C:232:ARG:HH11	1:C:232:ARG:CG	2.15	0.58
1:B:235:ASP:H	1:B:237:ARG:NH2	2.01	0.58
1:C:177:HIS:HD2	1:C:289:ASP:OD1	1.87	0.57
1:C:229:THR:HA	1:C:230:ILE:CD1	2.35	0.57
1:A:141:ASP:HB2	1:A:143:LEU:HD21	1.87	0.56
1:D:74:ILE:HG22	1:D:77:HIS:CE1	2.40	0.56
1:C:232:ARG:C	1:C:232:ARG:CD	2.74	0.56
1:B:311:ARG:NH1	1:B:315:THR:OG1	2.39	0.56
1:D:171:ALA:HA	1:D:319:LEU:HD22	1.87	0.55
1:A:222:GLU:HG3	1:A:223:GLU:H	1.71	0.55
1:C:311:ARG:NH1	1:C:315:THR:OG1	2.39	0.55
1:B:101:PHE:HB3	1:B:102:PRO:HD3	1.89	0.55
1:A:130:HIS:CE1	1:A:321:ARG:HD3	2.43	0.54
1:A:176:ASP:OD2	1:A:311:ARG:NH2	2.41	0.54
1:C:229:THR:CA	1:C:230:ILE:CB	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:ARG:NE	1:C:236:GLU:HB2	2.12	0.54
1:B:257:TYR:HD2	1:B:258:PHE:CE1	2.26	0.54
1:B:160:HIS:ND1	1:B:161:PRO:HD2	2.23	0.53
1:C:68:ARG:NH2	1:C:249:ASP:OD1	2.42	0.53
1:D:132:ILE:HD13	3:D:402:SIN:H31	1.89	0.53
1:D:26:THR:CG2	1:D:102:PRO:HB3	2.25	0.53
1:C:143:LEU:HA	4:C:403:ZZU:HN2	1.73	0.53
1:C:91:TRP:CH2	1:C:125:ASP:OD1	2.63	0.52
1:A:141:ASP:CB	1:A:143:LEU:HD21	2.40	0.52
1:C:208:ASP:HA	1:C:258:PHE:CE1	2.44	0.52
1:D:66:ALA:O	1:D:67:ASP:C	2.47	0.51
1:D:142:GLN:OE1	1:D:150:LEU:O	2.27	0.51
1:C:91:TRP:HH2	1:C:125:ASP:OD1	1.94	0.51
1:B:201:PRO:O	1:B:239:LEU:HB3	2.10	0.51
1:B:58:ASP:O	1:B:62:GLU:HG3	2.10	0.51
1:B:90:HIS:CD2	1:B:92:ARG:HD2	2.46	0.51
1:C:126:GLY:O	1:C:342:LEU:HD21	2.11	0.50
1:B:12:TYR:OH	1:C:237:ARG:NH1	2.45	0.49
1:C:230:ILE:O	1:C:232:ARG:N	2.43	0.49
1:B:150:LEU:O	1:B:151:LEU:HB2	2.11	0.49
1:D:83:ARG:O	1:D:99:PRO:HB2	2.13	0.49
1:A:130:HIS:HE1	1:A:321:ARG:HD3	1.78	0.49
1:C:91:TRP:CH2	1:C:124:GLN:HA	2.47	0.49
1:B:36:PHE:CE1	1:B:108:MET:HG3	2.48	0.49
1:C:232:ARG:NE	1:C:236:GLU:CB	2.74	0.48
1:D:232:ARG:HD2	1:D:232:ARG:C	2.34	0.48
1:C:181:THR:O	1:C:303:HIS:HA	2.14	0.48
1:B:265:ASP:O	1:B:269:ARG:HG3	2.13	0.48
1:A:131:ASP:HB3	1:A:133:PHE:CE2	2.48	0.48
1:C:228:ALA:O	1:C:229:THR:O	2.31	0.48
1:D:177:HIS:HD2	1:D:289:ASP:OD1	1.97	0.47
1:D:208:ASP:C	1:D:210:SER:H	2.18	0.47
1:A:22:VAL:O	1:A:26:THR:HB	2.14	0.47
1:B:156:GLU:CD	1:B:321:ARG:HH22	2.17	0.47
1:C:92:ARG:HH11	1:C:92:ARG:HG2	1.79	0.47
1:A:136:ARG:O	1:A:139:GLU:HB2	2.15	0.47
1:D:131:ASP:HB3	1:D:133:PHE:CE2	2.50	0.47
1:C:265:ASP:O	1:C:269:ARG:HG3	2.15	0.47
1:C:36:PHE:CE2	1:C:104:GLU:OE2	2.62	0.47
1:D:193:GLU:O	1:D:197:VAL:HG23	2.15	0.47
1:C:92:ARG:HH11	1:C:92:ARG:CG	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:VAL:HG13	1:B:202:ARG:NH1	2.30	0.46
1:D:37:GLY:O	1:D:39:PRO:HD3	2.15	0.46
1:C:147:SER:HA	1:C:308:PHE:CE1	2.51	0.46
1:C:229:THR:CA	1:C:230:ILE:HD12	2.44	0.46
1:A:141:ASP:HB3	1:A:143:LEU:CD2	2.45	0.46
1:C:253:ARG:O	1:C:253:ARG:HG3	2.14	0.46
1:B:155:THR:HB	1:B:158:ALA:HB2	1.97	0.46
1:D:343:LEU:N	1:D:343:LEU:HD12	2.31	0.46
1:B:199:PHE:CE2	1:B:247:ARG:HG2	2.51	0.46
1:B:252:MET:CE	1:B:275:LEU:HD11	2.46	0.46
1:A:141:ASP:CB	1:A:143:LEU:CD2	2.95	0.45
1:A:178:VAL:HA	1:A:179:PRO:HD3	1.88	0.45
1:A:212:LEU:HB2	1:A:215:ASN:HD21	1.81	0.45
1:D:179:PRO:HB3	1:D:285:GLU:HB3	1.98	0.45
1:C:209:GLU:O	1:C:212:LEU:HB2	2.17	0.45
1:C:232:ARG:HD2	1:C:233:MET:N	2.32	0.45
1:A:136:ARG:HA	1:A:312:TYR:CE1	2.52	0.45
1:B:236:GLU:O	1:B:237:ARG:HG3	2.16	0.45
1:C:200:GLU:OE2	1:C:202:ARG:NH1	2.45	0.45
1:D:15:THR:HG21	5:D:555:HOH:O	2.16	0.45
1:D:232:ARG:HD2	1:D:232:ARG:O	2.18	0.44
1:A:132:ILE:HD11	1:A:321:ARG:HD2	1.99	0.44
1:A:223:GLU:O	1:A:227:PHE:HD2	2.01	0.44
1:D:79:PHE:CD2	1:D:291:GLY:HA2	2.53	0.44
1:C:100:GLU:HG3	1:C:320:LYS:CE	2.48	0.43
1:A:71:HIS:HA	1:A:295:PHE:O	2.18	0.43
1:B:306:LEU:HD23	1:B:306:LEU:HA	1.78	0.43
1:D:82:ARG:NH2	1:D:82:ARG:CG	2.52	0.43
1:D:101:PHE:HB3	1:D:102:PRO:HD3	2.00	0.43
1:C:313:ASP:OD1	1:C:315:THR:HG23	2.18	0.43
1:B:200:GLU:HB3	1:B:201:PRO:HD2	2.00	0.43
1:C:184:GLU:CG	1:C:284:ARG:HH22	2.27	0.43
1:B:154:HIS:O	1:B:154:HIS:HD2	2.01	0.43
1:A:130:HIS:CE1	1:A:321:ARG:HB3	2.54	0.43
1:C:231:GLN:HB2	1:C:233:MET:HG2	1.99	0.43
1:B:235:ASP:HB3	1:B:236:GLU:H	1.62	0.43
1:D:36:PHE:HZ	1:D:104:GLU:HB3	1.84	0.43
1:B:199:PHE:CZ	1:B:247:ARG:HA	2.54	0.43
1:D:91:TRP:CH2	1:D:124:GLN:HA	2.54	0.42
1:D:236:GLU:CD	1:D:236:GLU:H	2.21	0.42
1:D:140:ASN:O	1:D:149:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ARG:NH1	1:C:104:GLU:OE1	2.44	0.42
1:C:35:SER:O	1:C:38:ASP:HB3	2.19	0.42
1:A:175:PRO:HG3	1:A:315:THR:O	2.19	0.42
1:B:289:ASP:O	1:B:292:ASP:HB2	2.18	0.42
1:A:212:LEU:O	1:A:215:ASN:ND2	2.53	0.42
1:B:136:ARG:O	1:B:139:GLU:HB2	2.20	0.42
1:C:297:ASP:OD2	1:D:329:ARG:NH1	2.46	0.42
1:B:33:TYR:CD1	1:B:41:LEU:HB2	2.54	0.42
1:A:222:GLU:HG3	1:A:223:GLU:N	2.34	0.42
1:B:97:PRO:HD2	5:B:532:HOH:O	2.19	0.42
1:A:141:ASP:O	1:A:149:GLN:HG3	2.20	0.41
1:B:253:ARG:O	1:B:253:ARG:HG2	2.20	0.41
1:A:38:ASP:HA	1:A:39:PRO:HD3	1.96	0.41
1:D:90:HIS:CD2	1:D:92:ARG:H	2.28	0.41
1:A:177:HIS:HD2	5:A:539:HOH:O	2.02	0.41
1:B:111:SER:HB2	1:B:324:VAL:HG22	2.01	0.41
1:A:136:ARG:HA	1:A:312:TYR:CZ	2.56	0.41
1:A:195:ILE:H	1:A:195:ILE:HG13	1.71	0.41
1:D:81:GLN:NE2	1:D:173:ARG:HH11	2.18	0.41
1:A:103:GLU:HG2	1:A:172:LEU:HD22	2.02	0.41
1:C:236:GLU:O	1:C:237:ARG:HB2	2.21	0.41
1:A:116:GLU:OE2	1:B:61:ARG:NH1	2.28	0.41
1:A:226:ARG:HD2	1:A:336:ALA:HA	2.03	0.41
1:C:313:ASP:OD1	1:C:313:ASP:C	2.59	0.41
1:A:181:THR:O	1:A:303:HIS:HA	2.21	0.41
1:C:232:ARG:HH11	1:C:232:ARG:HG3	1.85	0.40
1:C:232:ARG:NH1	1:C:232:ARG:HG2	2.36	0.40
1:C:232:ARG:C	1:C:232:ARG:HD3	2.41	0.40
1:C:232:ARG:NH1	1:C:232:ARG:CG	2.75	0.40
1:C:168:ILE:O	1:C:321:ARG:HA	2.21	0.40
1:D:233:MET:O	1:D:236:GLU:OE2	2.39	0.40
1:C:87:THR:HA	1:C:88:PRO:HD3	1.92	0.40
1:A:62:GLU:HG3	1:B:43:ARG:HD2	2.02	0.40
1:C:209:GLU:O	1:C:212:LEU:N	2.51	0.40
1:B:154:HIS:CD2	1:B:154:HIS:O	2.75	0.40
1:C:92:ARG:NH1	1:C:92:ARG:CG	2.83	0.40
1:C:337:THR:H	1:C:340:THR:HG22	1.86	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:510:HOH:O	5:D:521:HOH:O[1_455]	1.59	0.61
5:A:510:HOH:O	5:D:592:HOH:O[1_455]	2.06	0.14

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	335/364 (92%)	315 (94%)	17 (5%)	3 (1%)	21	17
1	B	298/364 (82%)	281 (94%)	13 (4%)	4 (1%)	15	10
1	C	318/364 (87%)	301 (95%)	12 (4%)	5 (2%)	12	7
1	D	312/364 (86%)	299 (96%)	10 (3%)	3 (1%)	19	15
All	All	1263/1456 (87%)	1196 (95%)	52 (4%)	15 (1%)	16	11

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	237	ARG
1	C	229	THR
1	C	230	ILE
1	C	233	MET
1	D	94	ARG
1	A	147	SER
1	A	220	THR
1	B	207	PRO
1	C	231	GLN
1	C	232	ARG
1	D	209	GLU
1	B	151	LEU
1	A	217	THR
1	B	317	ARG
1	D	233	MET

5.3.2 Protein sidechains (i)

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	286/310 (92%)	263 (92%)	23 (8%)	15 13
1	B	259/310 (84%)	232 (90%)	27 (10%)	9 7
1	C	274/310 (88%)	258 (94%)	16 (6%)	25 26
1	D	269/310 (87%)	254 (94%)	15 (6%)	26 27
All	All	1088/1240 (88%)	1007 (93%)	81 (7%)	17 16

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	9	THR
1	A	26	THR
1	A	29	LEU
1	A	41	LEU
1	A	42	LEU
1	A	48	LEU
1	A	60	LEU
1	A	96	ARG
1	A	123	GLN
1	A	128	LEU
1	A	143	LEU
1	A	149	GLN
1	A	167	LEU
1	A	179	PRO
1	A	185	LEU
1	A	189	SER
1	A	209	GLU
1	A	212	LEU
1	A	216	ASN
1	A	220	THR
1	A	246	SER
1	A	284	ARG
1	B	10	PRO

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Mol	Chain	Res	Type
1	B	29	LEU
1	B	42	LEU
1	B	45	LEU
1	B	68	ARG
1	B	82	ARG
1	B	92	ARG
1	B	105	LEU
1	B	133	PHE
1	B	136	ARG
1	B	137	SER
1	B	151	LEU
1	B	152	THR
1	B	154	HIS
1	B	167	LEU
1	B	182	VAL
1	B	185	LEU
1	B	187	LEU
1	B	189	SER
1	B	208	ASP
1	B	209	GLU
1	B	234	ILE
1	B	236	GLU
1	B	239	LEU
1	B	305	ARG
1	B	311	ARG
1	B	321	ARG
1	C	29	LEU
1	C	42	LEU
1	C	48	LEU
1	C	68	ARG
1	C	92	ARG
1	C	96	ARG
1	C	125	ASP
1	C	147	SER
1	C	185	LEU
1	C	212	LEU
1	C	232	ARG
1	C	236	GLU
1	C	254	LEU
1	C	277	LYS
1	C	311	ARG
1	C	338	SER

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Mol	Chain	Res	Type
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	82	ARG
1	D	106	LEU
1	D	136	ARG
1	D	185	LEU
1	D	187	LEU
1	D	232	ARG
1	D	233	MET
1	D	254	LEU
1	D	311	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	81	GLN
1	A	90	HIS
1	A	130	HIS
1	A	149	GLN
1	A	215	ASN
1	B	57	GLN
1	B	81	GLN
1	B	90	HIS
1	B	138	HIS
1	B	154	HIS
1	B	290	GLN
1	C	57	GLN
1	C	81	GLN
1	C	90	HIS
1	C	123	GLN
1	C	130	HIS
1	C	142	GLN
1	C	177	HIS
1	C	211	HIS
1	D	57	GLN
1	D	81	GLN
1	D	90	HIS

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Mol	Chain	Res	Type
1	D	142	GLN
1	D	177	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	SIN	C	402	2	1,7,7	0.46	0	2,8,8	2.34	2 (100%)
4	ZZU	C	403	2	5,12,12	1.05	0	3,15,15	2.96	1 (33%)
3	SIN	D	402	2	1,7,7	0.13	0	2,8,8	0.46	0
4	ZZU	D	403	-	5,12,12	0.62	0	3,15,15	0.75	0

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	SIN	C	402	2	-	0/1/5/5	0/0/0/0
4	ZZU	C	403	2	-	0/8/14/14	0/0/0/0
3	SIN	D	402	2	-	0/1/5/5	0/0/0/0
4	ZZU	D	403	-	-	0/8/14/14	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	SIN	C3-C2-C1	-2.44	108.27	112.75
3	C	402	SIN	C2-C3-C4	2.24	116.85	112.75
4	C	403	ZZU	OB-CB-CG	5.04	120.57	109.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403	ZZU	1	0
3	D	402	SIN	1	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, 95^{th} 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	337/364 (92%)	0.06	18 (5%) 30 32	21, 35, 72, 130	6 (1%)
1	B	304/364 (83%)	0.40	32 (10%) 8 9	26, 45, 74, 105	3 (0%)
1	C	322/364 (88%)	0.06	13 (4%) 42 44	22, 33, 65, 105	4 (1%)
1	D	316/364 (86%)	0.12	13 (4%) 41 42	23, 40, 63, 95	3 (0%)
All	All	1279/1456 (87%)	0.15	76 (5%) 26 28	21, 38, 71, 130	16 (1%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	THR	9.0
1	C	212	LEU	6.2
1	C	230	ILE	5.9
1	B	93	GLY	5.8
1	A	218	ILE	5.7
1	A	214	LYS	5.4
1	B	192	ALA	5.3
1	B	202	ARG	5.2
1	A	219	ALA	5.1
1	A	216	ASN	5.1
1	D	234	ILE	5.0
1	B	90	HIS	4.6
1	C	319	LEU	4.6
1	B	92	ARG	4.3
1	B	82	ARG	4.2
1	D	9	THR	4.1
1	A	334	MET	4.0
1	A	213	PRO	3.8
1	C	228	ALA	3.6
1	B	344	GLY	3.6
1	D	319	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	140	ASN	3.5
1	C	234	ILE	3.5
1	B	135	ILE	3.4
1	B	237	ARG	3.4
1	A	8	SER	3.4
1	B	151	LEU	3.3
1	B	138	HIS	3.3
1	D	93	GLY	3.3
1	B	248	LEU	3.2
1	B	188	SER	3.1
1	B	233	MET	3.1
1	C	236	GLU	3.1
1	A	37	GLY	3.1
1	B	234	ILE	3.1
1	D	247	ARG	3.1
1	A	95	VAL	3.0
1	C	171	ALA	3.0
1	C	170	GLY	3.0
1	B	107	LEU	3.0
1	B	122	THR	2.9
1	B	322	VAL	2.9
1	B	239	LEU	2.8
1	C	169	LEU	2.8
1	C	213	PRO	2.8
1	B	273	ASP	2.8
1	B	187	LEU	2.8
1	B	137	SER	2.7
1	A	150	LEU	2.7
1	B	257	TYR	2.6
1	A	215	ASN	2.6
1	C	107	LEU	2.6
1	C	82	ARG	2.5
1	D	132	ILE	2.5
1	D	235	ASP	2.5
1	B	247	ARG	2.5
1	B	260	SER	2.5
1	D	254	LEU	2.5
1	B	95	VAL	2.4
1	B	108	MET	2.4
1	A	221	GLU	2.4
1	B	136	ARG	2.3
1	D	82	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	132	ILE	2.3
1	D	232	ARG	2.3
1	D	233	MET	2.3
1	A	141	ASP	2.2
1	D	112	ALA	2.2
1	D	20	SER	2.2
1	A	149	GLN	2.2
1	B	210	SER	2.1
1	A	107	LEU	2.1
1	B	319	LEU	2.1
1	A	106	LEU	2.1
1	B	168	ILE	2.1
1	B	89	ASP	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	ZZU	D	403	13/13	0.94	0.17	2.48	29,48,73,79	0
3	SIN	D	402	8/8	0.94	0.23	1.48	42,54,66,66	0
3	SIN	C	402	8/8	0.96	0.18	0.21	31,40,51,55	0
4	ZZU	C	403	13/13	0.93	0.13	0.04	31,47,66,79	0
2	FE	C	401	1/1	0.96	0.04	-2.08	68,68,68,68	0
2	FE	D	401	1/1	0.99	0.09	-2.26	76,76,76,76	0
2	FE	B	401	1/1	0.90	0.04	-	90,90,90,90	0
2	FE	A	401	1/1	0.97	0.06	-	73,73,73,73	0

6.5 Other polymers (i)

There are no such residues in this entry.