



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 12:05 AM UTC

PDB ID : 4M2E / pdb_00004m2e
Title : Crystal structure of non-heme iron oxygenase OrfP in complex with Fe and L-homoarginine
Authors : Chang, C.Y.; Liu, Y.C.; Lyu, S.Y.; Wu, C.C.; Li, T.L.
Deposited on : 2013-08-05
Resolution : 2.06 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

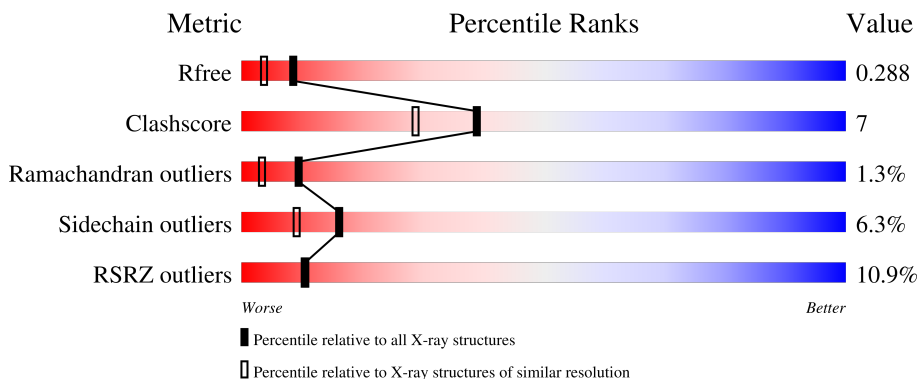
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	
1	B	364	
1	C	364	
1	D	364	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 11562 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
			Total	C	N	O	S			
1	A	336	Total 2690	C 1693	N 487	O 503	S 7	0	0	0
1	B	319	Total 2565	C 1621	N 465	O 473	S 6	0	0	0
1	C	336	Total 2690	C 1693	N 487	O 503	S 7	0	0	0
1	D	336	Total 2690	C 1693	N 487	O 503	S 7	0	0	0

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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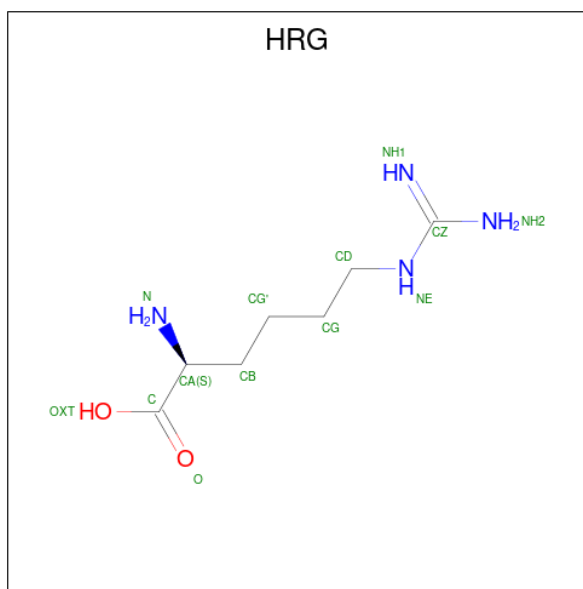
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP G9MBV2
B	-17	SER	-	expression tag	UNP G9MBV2
B	-16	SER	-	expression tag	UNP G9MBV2
B	-15	HIS	-	expression tag	UNP G9MBV2
B	-14	HIS	-	expression tag	UNP G9MBV2
B	-13	HIS	-	expression tag	UNP G9MBV2
B	-12	HIS	-	expression tag	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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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 L-HOMOARGININE (CCD ID: HRG) (formula: C₇H₁₆N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	7	4	2		
2	C	1	Total	C	N	O	0	0
			13	7	4	2		
2	D	1	Total	C	N	O	0	0
			13	7	4	2		

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

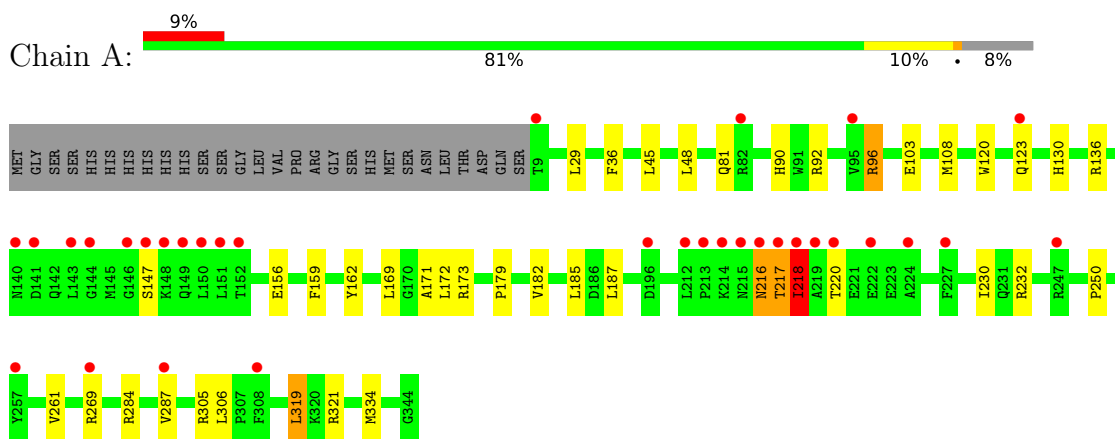
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	242	Total O 242 242	0	0
4	B	198	Total O 198 198	0	0
4	C	241	Total O 241 241	0	0
4	D	204	Total O 204 204	0	0

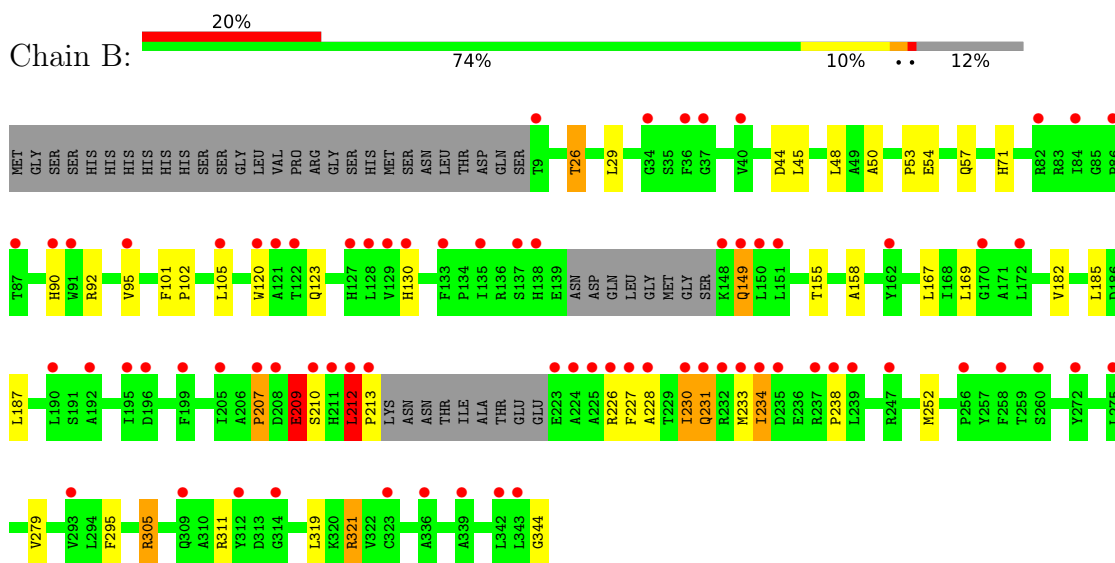
3 Residue-property plots

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.

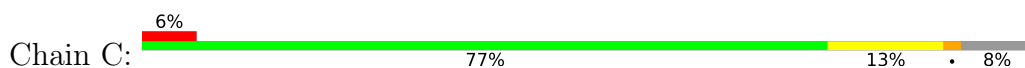
- Molecule 1: L-arginine beta-hydroxylase

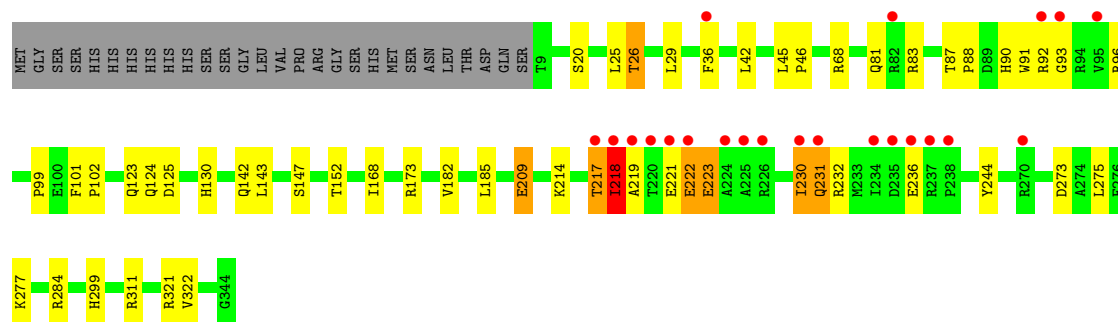


- Molecule 1: L-arginine beta-hydroxylase

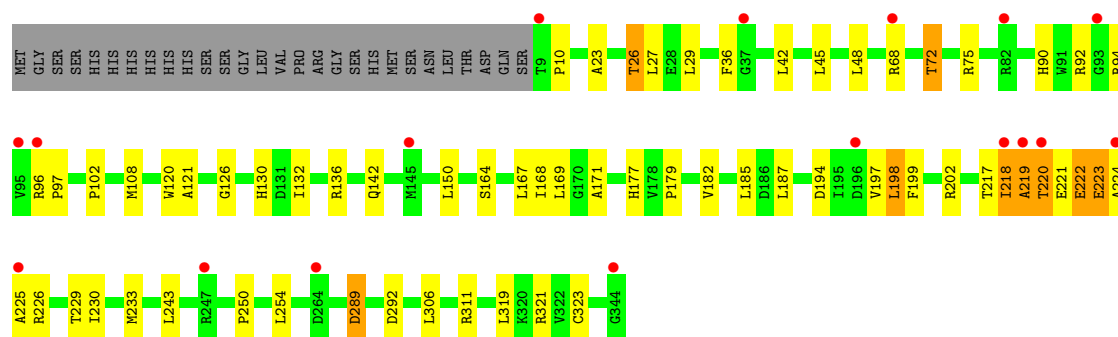
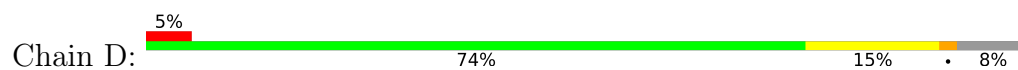


- Molecule 1: L-arginine beta-hydroxylase





- 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	68.32Å 117.16Å 96.04Å 90.00° 91.62° 90.00°	Depositor
Resolution (Å)	30.00 – 2.06 30.00 – 2.06	Depositor EDS
% Data completeness (in resolution range)	86.5 (30.00-2.06) 86.8 (30.00-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.01 (at 2.06Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.223 , 0.288 0.223 , 0.288	Depositor DCC
R_{free} test set	4063 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtrriage
Anisotropy	0.054	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11562	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: HRG, FE

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	0.69	0/2760	0.84	2/3754 (0.1%)
1	B	0.69	0/2633	0.81	0/3580
1	C	0.71	0/2760	0.83	0/3754
1	D	0.70	0/2760	0.82	0/3754
All	All	0.70	0/10913	0.82	2/14842 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	THR	CA-C-N	5.17	131.00	121.70
1	A	217	THR	C-N-CA	5.17	131.00	121.70

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	2690	0	2606	27	0
1	B	2565	0	2488	31	0
1	C	2690	0	2606	38	0
1	D	2690	0	2606	47	0
2	A	13	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	13	0	14	2	0
2	D	13	0	14	1	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	242	0	0	2	0
4	B	198	0	0	5	0
4	C	241	0	0	2	0
4	D	204	0	0	3	0
All	All	11562	0	10348	143	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.

The worst 5 of 143 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:D:219:ALA:O	1:D:220:THR:HG23	1.26	1.31
1:B:212:LEU:HB3	1:B:213:PRO:HD3	1.28	1.11
1:D:130:HIS:HD2	1:D:321:ARG:NH1	1.52	1.05
1:A:217:THR:HA	1:A:218:ILE:HG13	1.41	1.01
1:D:130:HIS:HD2	1:D:321:ARG:HH12	1.05	1.01

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	334/364 (92%)	323 (97%)	8 (2%)	3 (1%)	14 7
1	B	313/364 (86%)	302 (96%)	7 (2%)	4 (1%)	9 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	334/364 (92%)	322 (96%)	8 (2%)	4 (1%)	10	4
1	D	334/364 (92%)	318 (95%)	10 (3%)	6 (2%)	6	2
All	All	1315/1456 (90%)	1265 (96%)	33 (2%)	17 (1%)	9	3

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	ILE
1	B	212	LEU
1	D	218	ILE
1	D	220	THR
1	D	222	GLU

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	286/311 (92%)	273 (96%)	13 (4%)	24	18
1	B	272/311 (88%)	251 (92%)	21 (8%)	12	5
1	C	286/311 (92%)	268 (94%)	18 (6%)	16	9
1	D	286/311 (92%)	267 (93%)	19 (7%)	15	8
All	All	1130/1244 (91%)	1059 (94%)	71 (6%)	16	9

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	68	ARG
1	D	136	ARG
1	D	187	LEU
1	B	209	GLU
1	B	187	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	81	GLN
1	D	231	GLN
1	C	130	HIS
1	D	290	GLN
1	D	130	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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$
2	HRG	D	402	-	11,12,12	0.92	1 (9%)	10,14,14	1.35	1 (10%)
2	HRG	A	401	-	11,12,12	0.91	1 (9%)	10,14,14	1.19	1 (10%)
2	HRG	C	402	-	11,12,12	0.83	0	10,14,14	1.34	1 (10%)

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
2	HRG	D	402	-	-	3/12/12/12	-
2	HRG	A	401	-	-	2/12/12/12	-
2	HRG	C	402	-	-	5/12/12/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	402	HRG	OXT-C	-2.28	1.23	1.30
2	A	401	HRG	OXT-C	-2.27	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HRG	OXT-C-O	-3.15	116.93	124.08
2	C	402	HRG	OXT-C-O	-2.85	117.62	124.08
2	D	402	HRG	OXT-C-O	-2.48	118.45	124.08

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	402	HRG	N-CA-CB-CG'
2	D	402	HRG	C-CA-CB-CG'
2	C	402	HRG	NE-CD-CG-CG'
2	A	401	HRG	NE-CD-CG-CG'
2	D	402	HRG	NE-CD-CG-CG'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	402	HRG	1	0
2	C	402	HRG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.47	33 (9%) 13 13	7, 28, 60, 88	4 (1%)
1	B	319/364 (87%)	1.37	73 (22%) 2 2	20, 38, 98, 129	3 (0%)
1	C	336/364 (92%)	0.36	22 (6%) 25 24	14, 26, 49, 95	4 (1%)
1	D	336/364 (92%)	0.53	17 (5%) 33 33	17, 32, 53, 84	3 (0%)
All	All	1327/1456 (91%)	0.67	145 (10%) 10 10	7, 31, 62, 129	14 (1%)

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	92	ARG	7.5
1	C	218	ILE	6.6
1	C	82	ARG	6.0
1	B	227	PHE	5.7
1	D	224	ALA	5.7

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(\AA^2)	Q<0.9
2	HRG	A	401	13/13	0.72	0.18	45,48,54,54	0
2	HRG	D	402	13/13	0.82	0.13	31,34,36,36	0
3	FE	B	401	1/1	0.84	0.13	89,89,89,89	0
2	HRG	C	402	13/13	0.86	0.12	31,33,34,35	0
3	FE	C	401	1/1	0.96	0.19	67,67,67,67	0
3	FE	D	401	1/1	0.98	0.09	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.