



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:07 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 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

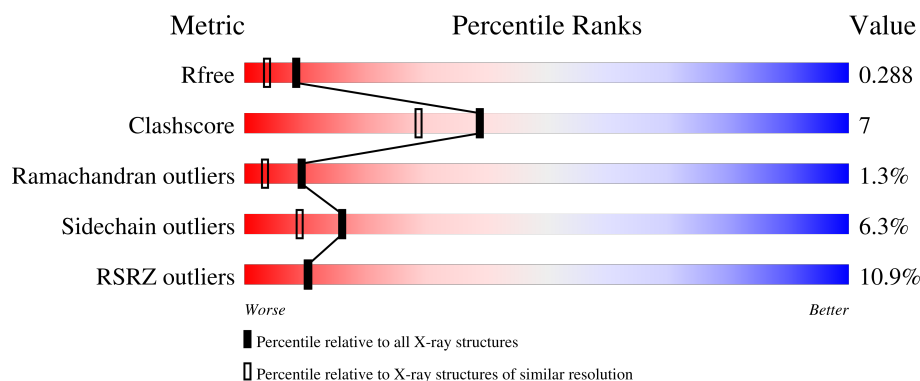
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	9% 81% 10% • 8%
1	B	364	20% 74% 10% •• 12%
1	C	364	6% 77% 13% • 8%
1	D	364	5% 74% 15% • 8%

2 Entry composition

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
1	A	336	Total	C	N	O	S	0	0	0
			2690	1693	487	503	7			
1	B	319	Total	C	N	O	S	0	0	0
			2565	1621	465	473	6			
1	C	336	Total	C	N	O	S	0	0	0
			2690	1693	487	503	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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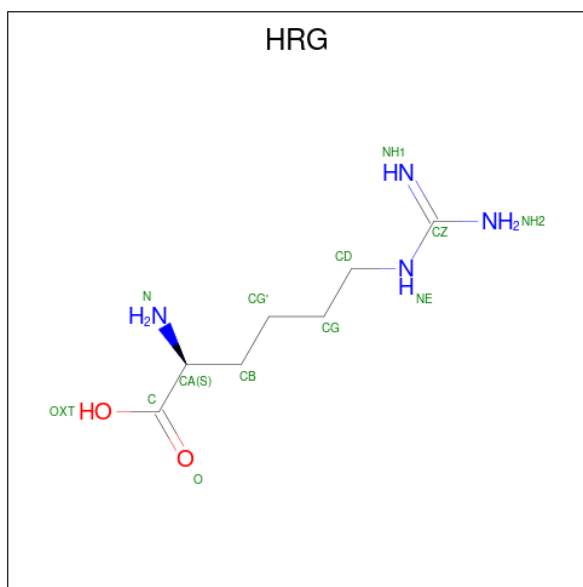
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP G9MBV2
B	-17	SER	-	expression tag	UNP G9MBV2
B	-16	SER	-	expression tag	UNP G9MBV2
B	-15	HIS	-	expression tag	UNP G9MBV2
B	-14	HIS	-	expression tag	UNP G9MBV2
B	-13	HIS	-	expression tag	UNP G9MBV2
B	-12	HIS	-	expression tag	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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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: $C_7H_{16}N_4O_2$).



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 1	Fe 1	0	0
3	C	1	Total 1	Fe 1	0	0
3	D	1	Total 1	Fe 1	0	0

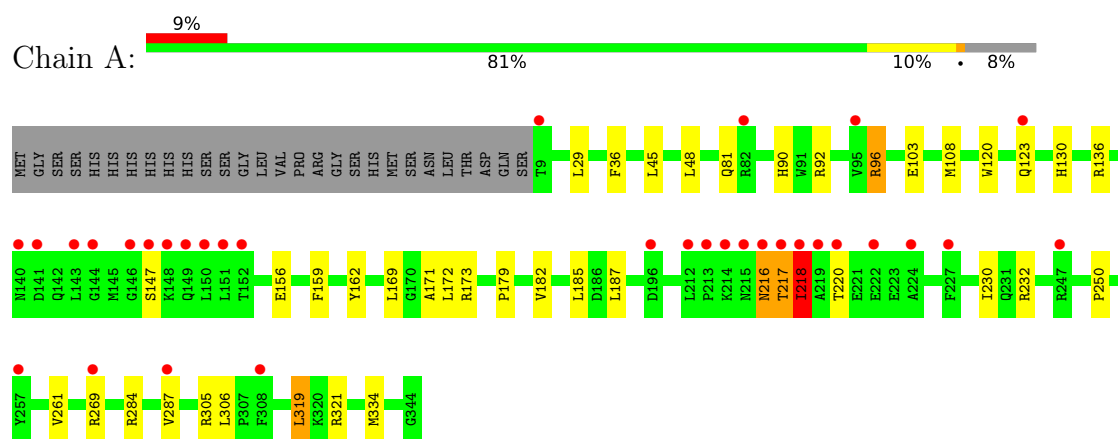
- Molecule 4 is water.

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

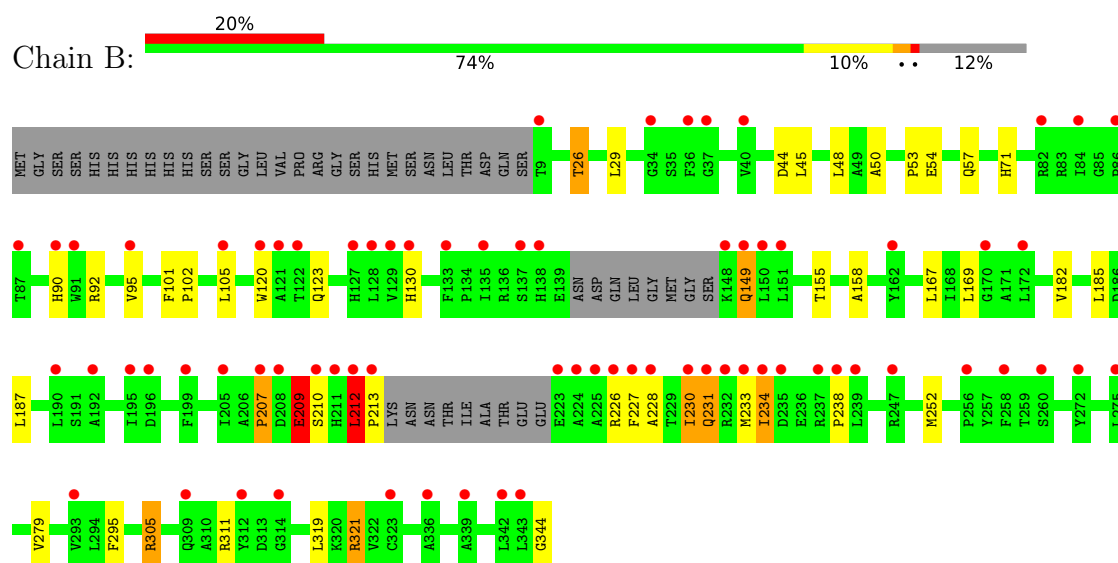
3 Residue-property plots [i](#)

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.

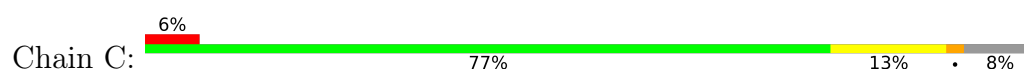
• Molecule 1: L-arginine beta-hydroxylase

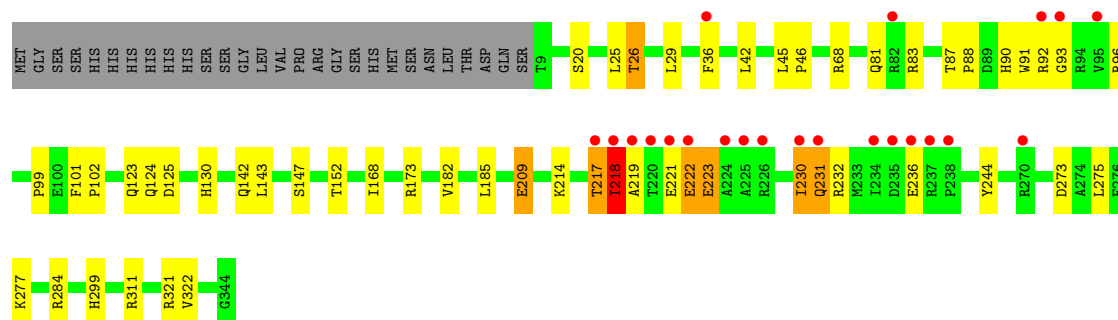


• Molecule 1: L-arginine beta-hydroxylase

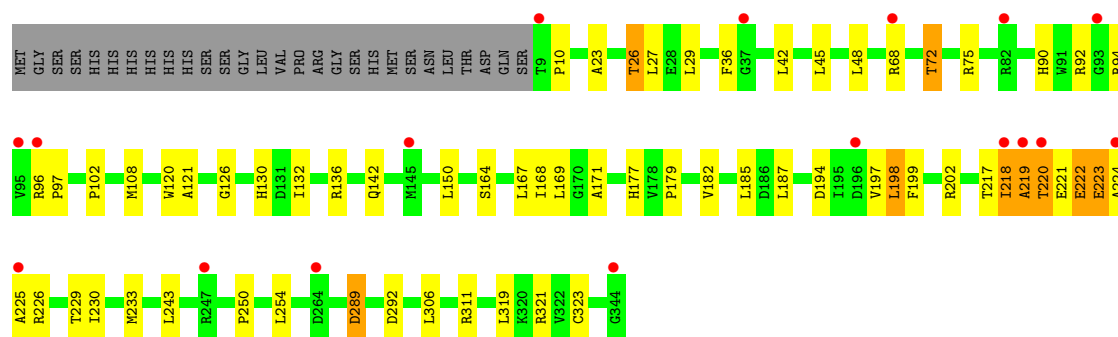
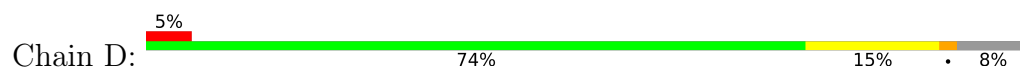


• Molecule 1: L-arginine beta-hydroxylase





- 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	68.32Å 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)	Xtriage
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	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
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

Xtriage'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.

All (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
1:B:212:LEU:HB3	1:B:213:PRO:CD	2.02	0.89
1:D:130:HIS:CD2	1:D:321:ARG:HH12	1.91	0.88
1:C:142:GLN:HE22	1:C:152:THR:H	1.20	0.88
1:D:26:THR:HG23	1:D:102:PRO:HB3	1.54	0.87
1:D:219:ALA:O	1:D:220:THR:CG2	2.18	0.87
1:B:26:THR:HG23	1:B:102:PRO:HB3	1.58	0.85
1:D:130:HIS:CD2	1:D:321:ARG:NH1	2.45	0.82
1:D:217:THR:O	1:D:218:ILE:HG12	1.77	0.82
1:B:209:GLU:HG2	1:B:210:SER:H	1.43	0.82
1:D:219:ALA:C	1:D:220:THR:HG23	2.08	0.79
1:C:142:GLN:NE2	1:C:152:THR:H	1.81	0.78
1:D:169:LEU:HD23	1:D:321:ARG:HG3	1.65	0.77
1:C:26:THR:HG23	1:C:102:PRO:HB3	1.67	0.77
1:B:44:ASP:HB3	1:B:48:LEU:HD13	1.66	0.76
1:A:217:THR:HA	1:A:218:ILE:CG1	2.15	0.75
1:C:26:THR:HG21	4:C:549:HOH:O	1.88	0.74
1:D:218:ILE:HA	4:D:662:HOH:O	1.87	0.74
1:C:90:HIS:CD2	1:C:92:ARG:H	2.06	0.73
1:B:26:THR:CG2	1:B:102:PRO:HB3	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:HIS:HD2	1:C:92:ARG:H	1.40	0.69
1:D:130:HIS:HE1	4:D:559:HOH:O	1.75	0.68
1:A:96:ARG:NH1	4:A:639:HOH:O	2.24	0.67
1:A:217:THR:CA	1:A:218:ILE:HG13	2.22	0.66
1:C:123:GLN:HE22	2:C:402:HRG:HN2	1.44	0.66
1:D:121:ALA:O	1:D:226:ARG:HD3	1.96	0.65
1:A:90:HIS:HD2	1:A:92:ARG:H	1.43	0.64
1:C:130:HIS:HD2	1:C:321:ARG:HH11	1.46	0.64
1:B:209:GLU:CG	1:B:210:SER:H	2.09	0.63
1:A:130:HIS:NE2	1:A:321:ARG:HD3	2.13	0.63
1:C:123:GLN:NE2	2:C:402:HRG:HN2	1.98	0.62
1:D:75:ARG:NH1	1:D:292:ASP:OD2	2.33	0.61
1:A:36:PHE:CE1	1:A:108:MET:HG3	2.36	0.61
1:A:120:TRP:HB2	1:A:123:GLN:HG3	1.83	0.60
1:A:90:HIS:CD2	1:A:92:ARG:HG3	2.37	0.60
1:B:26:THR:HG23	1:B:102:PRO:CB	2.32	0.60
1:C:130:HIS:CD2	1:C:321:ARG:HH11	2.19	0.60
1:B:231:GLN:HA	1:B:234:ILE:HB	1.85	0.59
1:A:230:ILE:HD11	1:A:334:MET:HE1	1.84	0.59
1:D:10:PRO:O	1:D:72:THR:HG22	2.03	0.58
1:D:26:THR:HG21	4:D:595:HOH:O	2.04	0.58
1:A:187:LEU:HD22	1:A:250:PRO:HD3	1.86	0.58
1:D:120:TRP:O	1:D:126:GLY:HA2	2.04	0.58
1:A:90:HIS:CD2	1:A:92:ARG:H	2.22	0.57
1:C:26:THR:HG23	1:C:102:PRO:CB	2.34	0.57
1:C:26:THR:CG2	1:C:102:PRO:HB3	2.32	0.57
1:D:169:LEU:CD2	1:D:321:ARG:HG3	2.33	0.57
1:D:26:THR:CG2	1:D:102:PRO:HB3	2.32	0.57
1:D:221:GLU:HG3	1:D:222:GLU:H	1.71	0.56
1:A:171:ALA:HA	1:A:319:LEU:HD22	1.85	0.56
1:B:233:MET:HA	1:B:238:PRO:HD3	1.88	0.56
1:C:244:TYR:OH	1:C:299:HIS:ND1	2.37	0.56
1:B:101:PHE:HB3	1:B:102:PRO:HD3	1.87	0.55
1:B:209:GLU:HG2	1:B:210:SER:N	2.19	0.55
1:A:162:TYR:CE2	1:A:334:MET:HE3	2.42	0.54
1:D:219:ALA:C	1:D:220:THR:CG2	2.77	0.54
1:A:156:GLU:CD	1:A:321:ARG:HH22	2.17	0.53
1:C:143:LEU:HD21	1:C:209:GLU:HG2	1.90	0.52
1:C:36:PHE:HZ	1:C:96:ARG:NH1	2.08	0.52
1:D:221:GLU:O	1:D:223:GLU:N	2.43	0.52
1:B:53:PRO:HD3	4:B:571:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:THR:HB	1:A:218:ILE:O	2.10	0.51
1:B:305:ARG:HB3	4:B:653:HOH:O	2.11	0.51
1:D:26:THR:HG23	1:D:102:PRO:CB	2.34	0.51
1:C:221:GLU:HA	1:C:222:GLU:HG3	1.93	0.51
1:B:305:ARG:HG2	4:B:661:HOH:O	2.10	0.50
1:A:162:TYR:CD2	1:A:334:MET:HE3	2.46	0.50
1:B:230:ILE:HB	1:B:234:ILE:HD13	1.91	0.50
1:C:91:TRP:CE3	1:C:92:ARG:HA	2.47	0.50
1:D:23:ALA:O	1:D:27:LEU:HD23	2.11	0.49
1:D:171:ALA:HA	1:D:319:LEU:HD22	1.94	0.49
1:B:252:MET:HE1	1:B:279:VAL:HG21	1.95	0.49
1:D:224:ALA:C	1:D:226:ARG:H	2.19	0.49
1:B:207:PRO:HD3	4:B:614:HOH:O	2.13	0.49
1:D:222:GLU:O	1:D:223:GLU:O	2.30	0.49
1:C:223:GLU:HA	1:C:223:GLU:OE1	2.11	0.49
1:D:142:GLN:O	2:D:402:HRG:HD2	2.13	0.48
1:D:194:ASP:O	1:D:198:LEU:HD22	2.14	0.47
1:A:169:LEU:HD23	1:A:321:ARG:HG3	1.95	0.47
1:B:230:ILE:H	1:B:230:ILE:HD13	1.80	0.47
1:C:36:PHE:CZ	1:C:96:ARG:NH1	2.82	0.47
1:D:132:ILE:HB	1:D:319:LEU:HB2	1.95	0.47
1:D:229:THR:O	1:D:233:MET:HG3	2.15	0.47
1:B:50:ALA:HA	1:B:57:GLN:NE2	2.31	0.46
1:D:179:PRO:HG2	1:D:306:LEU:HD12	1.96	0.46
1:B:155:THR:HB	1:B:158:ALA:HB2	1.97	0.46
1:D:164:SER:OG	1:D:323:CYS:HB3	2.15	0.46
1:D:90:HIS:HD2	1:D:92:ARG:H	1.63	0.45
1:A:261:VAL:HG11	1:A:269:ARG:HA	1.97	0.45
1:B:120:TRP:HB2	1:B:123:GLN:HB2	1.99	0.45
1:C:45:LEU:HB3	1:C:46:PRO:HD3	1.98	0.45
1:C:223:GLU:OE1	1:C:223:GLU:CA	2.65	0.45
1:A:179:PRO:HG2	1:A:306:LEU:HD12	1.98	0.45
1:B:209:GLU:CG	1:B:210:SER:N	2.79	0.45
1:C:230:ILE:HG13	1:C:231:GLN:N	2.31	0.45
1:C:81:GLN:HE22	1:C:173:ARG:HE	1.65	0.45
1:C:321:ARG:HG2	1:C:322:VAL:N	2.32	0.45
1:D:36:PHE:CE1	1:D:108:MET:HG3	2.52	0.45
1:D:221:GLU:HG3	1:D:222:GLU:N	2.31	0.45
1:C:218:ILE:HB	1:C:219:ALA:H	1.66	0.44
1:A:169:LEU:CD2	1:A:321:ARG:HG3	2.47	0.44
1:C:83:ARG:O	1:C:99:PRO:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:VAL:HG13	1:D:202:ARG:NH1	2.33	0.44
1:B:226:ARG:NH1	1:B:344:GLY:O	2.51	0.44
1:C:168:ILE:O	1:C:321:ARG:HA	2.17	0.43
1:D:221:GLU:CG	1:D:222:GLU:H	2.30	0.43
1:C:90:HIS:HD2	1:C:92:ARG:N	2.13	0.43
1:C:25:LEU:O	1:C:29:LEU:HG	2.18	0.43
1:D:199:PHE:HZ	1:D:250:PRO:HB3	1.84	0.43
1:D:224:ALA:C	1:D:226:ARG:N	2.76	0.43
1:B:44:ASP:HB3	1:B:48:LEU:CD1	2.44	0.42
1:D:199:PHE:CZ	1:D:250:PRO:HB3	2.53	0.42
1:B:54:GLU:HG3	4:B:656:HOH:O	2.20	0.42
1:B:71:HIS:HA	1:B:295:PHE:O	2.18	0.42
1:C:125:ASP:OD2	1:C:217:THR:HG23	2.20	0.42
1:C:81:GLN:NE2	1:C:173:ARG:HE	2.18	0.42
1:B:90:HIS:HD2	1:B:92:ARG:H	1.67	0.42
1:B:169:LEU:HD23	1:B:321:ARG:HB2	2.02	0.42
1:C:273:ASP:O	1:C:277:LYS:HG2	2.19	0.42
1:B:149:GLN:HB3	1:B:305:ARG:HH22	1.83	0.41
1:D:96:ARG:HA	1:D:97:PRO:HA	1.90	0.41
1:A:81:GLN:NE2	1:A:173:ARG:HE	2.18	0.41
1:A:103:GLU:HG2	1:A:172:LEU:HD22	2.02	0.41
1:D:90:HIS:CD2	1:D:92:ARG:H	2.37	0.41
1:A:216:ASN:C	1:A:216:ASN:HD22	2.29	0.41
1:B:90:HIS:NE2	1:B:92:ARG:HD2	2.35	0.41
1:C:101:PHE:HB3	1:C:102:PRO:HD3	2.03	0.41
1:A:179:PRO:HB3	1:A:287:VAL:HG22	2.03	0.41
1:A:305:ARG:HD3	4:A:744:HOH:O	2.21	0.41
1:C:90:HIS:CD2	1:C:91:TRP:H	2.38	0.41
1:D:198:LEU:HB3	1:D:243:LEU:HG	2.03	0.41
1:A:81:GLN:HE22	1:A:173:ARG:HE	1.69	0.40
1:D:177:HIS:HD2	1:D:289:ASP:OD1	2.04	0.40
1:D:217:THR:O	1:D:218:ILE:CG1	2.59	0.40
1:C:87:THR:HA	1:C:88:PRO:HD3	1.92	0.40
1:C:91:TRP:CH2	1:C:124:GLN:HA	2.56	0.40
1:C:90:HIS:CD2	1:C:91:TRP:N	2.89	0.40
1:C:130:HIS:HE1	4:C:649:HOH:O	2.03	0.40
1:D:223:GLU:C	1:D:225:ALA:H	2.30	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	334/364 (92%)	323 (97%)	8 (2%)	3 (1%)	14	7
1	B	313/364 (86%)	302 (96%)	7 (2%)	4 (1%)	9	3
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

All (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
1	D	223	GLU
1	B	209	GLU
1	C	236	GLU
1	D	94	ARG
1	A	147	SER
1	A	220	THR
1	B	228	ALA
1	C	147	SER
1	D	219	ALA
1	B	207	PRO
1	C	93	GLY
1	C	218	ILE

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	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

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	45	LEU
1	A	48	LEU
1	A	96	ARG
1	A	136	ARG
1	A	159	PHE
1	A	182	VAL
1	A	185	LEU
1	A	216	ASN
1	A	218	ILE
1	A	232	ARG
1	A	284	ARG
1	A	319	LEU
1	B	26	THR
1	B	29	LEU
1	B	45	LEU
1	B	95	VAL
1	B	105	LEU
1	B	130	HIS
1	B	149	GLN
1	B	167	LEU
1	B	182	VAL
1	B	185	LEU
1	B	187	LEU
1	B	209	GLU
1	B	212	LEU
1	B	227	PHE
1	B	230	ILE

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Mol	Chain	Res	Type
1	B	231	GLN
1	B	234	ILE
1	B	305	ARG
1	B	311	ARG
1	B	319	LEU
1	B	321	ARG
1	C	20	SER
1	C	26	THR
1	C	42	LEU
1	C	68	ARG
1	C	182	VAL
1	C	185	LEU
1	C	209	GLU
1	C	214	LYS
1	C	217	THR
1	C	218	ILE
1	C	222	GLU
1	C	223	GLU
1	C	230	ILE
1	C	231	GLN
1	C	232	ARG
1	C	275	LEU
1	C	284	ARG
1	C	311	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	72	THR
1	D	136	ARG
1	D	150	LEU
1	D	167	LEU
1	D	168	ILE
1	D	182	VAL
1	D	185	LEU
1	D	187	LEU
1	D	198	LEU
1	D	230	ILE
1	D	254	LEU
1	D	289	ASP

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Mol	Chain	Res	Type
1	D	311	ARG

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	69	HIS
1	A	81	GLN
1	A	90	HIS
1	A	138	HIS
1	A	290	GLN
1	B	57	GLN
1	B	69	HIS
1	B	90	HIS
1	B	149	GLN
1	B	154	HIS
1	B	231	GLN
1	C	57	GLN
1	C	69	HIS
1	C	81	GLN
1	C	90	HIS
1	C	123	GLN
1	C	130	HIS
1	C	142	GLN
1	C	290	GLN
1	D	57	GLN
1	D	81	GLN
1	D	90	HIS
1	D	127	HIS
1	D	130	HIS
1	D	142	GLN
1	D	177	HIS
1	D	231	GLN
1	D	263	GLN
1	D	290	GLN

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 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.

All (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'
2	C	402	HRG	CA-CB-CG'-CG
2	A	401	HRG	CD-CG-CG'-CB
2	C	402	HRG	OXT-C-CA-N
2	C	402	HRG	N-CA-CB-CG'
2	C	402	HRG	O-C-CA-N

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 [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%)	0.47	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%)

All (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
1	B	235	ASP	5.5
1	C	219	ALA	5.3
1	B	225	ALA	5.2
1	B	230	ILE	5.1
1	A	217	THR	5.0
1	B	82	ARG	4.9
1	B	212	LEU	4.8
1	A	269	ARG	4.8
1	D	220	THR	4.7
1	B	234	ILE	4.6
1	A	82	ARG	4.6
1	B	233	MET	4.5
1	B	226	ARG	4.3
1	D	82	ARG	4.3
1	A	218	ILE	4.2
1	B	228	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	225	ALA	4.1
1	B	150	LEU	4.1
1	B	213	PRO	4.1
1	C	95	VAL	4.0
1	D	218	ILE	4.0
1	A	150	LEU	3.8
1	B	224	ALA	3.7
1	D	247	ARG	3.7
1	B	238	PRO	3.6
1	A	146	GLY	3.6
1	C	220	THR	3.6
1	A	143	LEU	3.5
1	D	93	GLY	3.5
1	B	95	VAL	3.5
1	D	196	ASP	3.5
1	A	216	ASN	3.5
1	C	222	GLU	3.3
1	A	212	LEU	3.2
1	C	93	GLY	3.2
1	B	210	SER	3.2
1	B	339	ALA	3.2
1	B	36	PHE	3.2
1	B	312	TYR	3.1
1	D	264	ASP	3.1
1	B	34	GLY	3.0
1	C	36	PHE	3.0
1	A	141	ASP	3.0
1	A	220	THR	3.0
1	B	9	THR	3.0
1	B	207	PRO	3.0
1	C	221	GLU	2.9
1	B	128	LEU	2.9
1	C	238	PRO	2.9
1	B	231	GLN	2.9
1	C	224	ALA	2.9
1	B	239	LEU	2.9
1	A	214	LYS	2.8
1	B	314	GLY	2.8
1	B	138	HIS	2.8
1	A	308	PHE	2.8
1	B	133	PHE	2.8
1	B	223	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	37	GLY	2.7
1	B	190	LEU	2.7
1	C	217	THR	2.7
1	A	151	LEU	2.7
1	B	256	PRO	2.7
1	C	231	GLN	2.7
1	B	151	LEU	2.7
1	A	95	VAL	2.7
1	A	215	ASN	2.6
1	A	222	GLU	2.6
1	B	87	THR	2.6
1	D	219	ALA	2.6
1	A	196	ASP	2.6
1	B	172	LEU	2.6
1	B	199	PHE	2.6
1	B	195	ILE	2.6
1	A	140	ASN	2.5
1	A	247	ARG	2.5
1	B	343	LEU	2.5
1	B	247	ARG	2.5
1	B	135	ILE	2.5
1	B	121	ALA	2.5
1	D	9	THR	2.4
1	A	224	ALA	2.4
1	B	232	ARG	2.4
1	B	258	PHE	2.4
1	D	37	GLY	2.4
1	B	149	GLN	2.4
1	B	196	ASP	2.4
1	B	122	THR	2.4
1	C	225	ALA	2.4
1	B	90	HIS	2.4
1	B	342	LEU	2.4
1	C	226	ARG	2.4
1	A	257	TYR	2.4
1	A	144	GLY	2.4
1	B	237	ARG	2.4
1	D	68	ARG	2.4
1	A	147	SER	2.4
1	B	130	HIS	2.4
1	B	208	ASP	2.3
1	B	129	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	275	LEU	2.3
1	B	211	HIS	2.3
1	B	40	VAL	2.3
1	B	86	PRO	2.3
1	B	120	TRP	2.3
1	B	205	ILE	2.2
1	A	152	THR	2.2
1	A	148	LYS	2.2
1	B	127	HIS	2.2
1	B	260	SER	2.2
1	B	84	ILE	2.2
1	A	287	VAL	2.2
1	A	219	ALA	2.2
1	B	192	ALA	2.2
1	B	309	GLN	2.2
1	B	293	VAL	2.2
1	A	123	GLN	2.2
1	A	149	GLN	2.2
1	B	336	ALA	2.2
1	B	272	TYR	2.2
1	A	227	PHE	2.1
1	C	234	ILE	2.1
1	B	105	LEU	2.1
1	B	137	SER	2.1
1	D	145	MET	2.1
1	B	91	TRP	2.1
1	D	96	ARG	2.1
1	A	9	THR	2.1
1	A	213	PRO	2.1
1	B	170	GLY	2.1
1	C	270	ARG	2.1
1	D	95	VAL	2.1
1	B	148	LYS	2.1
1	B	162	TYR	2.1
1	C	237	ARG	2.1
1	C	236	GLU	2.0
1	C	235	ASP	2.0
1	D	344	GLY	2.0
1	C	230	ILE	2.0
1	B	323	CYS	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($\text{\AA}^2$)	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.