Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 06:35 PM GMT

PDB ID	:	4M2E
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

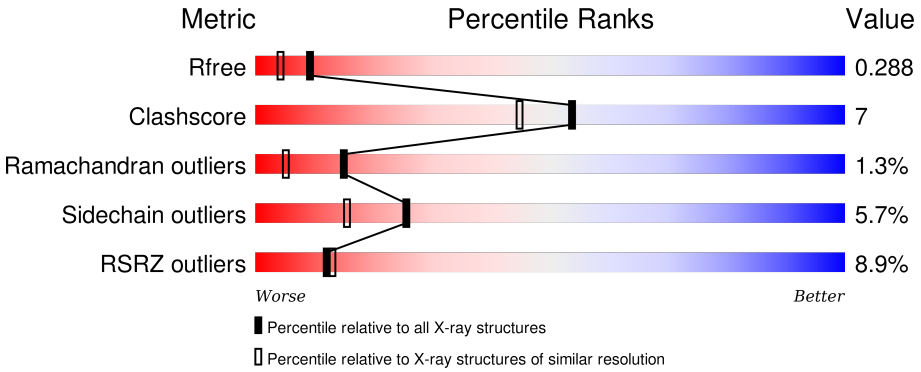
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (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 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	7% 81% 10% • 8%
1	B	364	16% 74% 11% • • 12%
1	C	364	4% 77% 13% • 8%
1	D	364	6% 76% 14% • 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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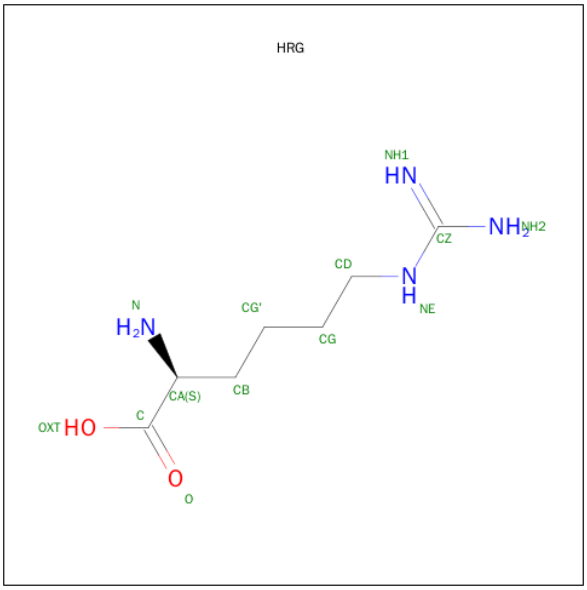
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP G9MBV2
D	-15	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-14	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-13	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-12	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-11	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-10	HIS	-	EXPRESSION TAG	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 (three-letter code: HRG) (formula: $C_7H_{16}N_4O_2$).



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

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 4 is water.

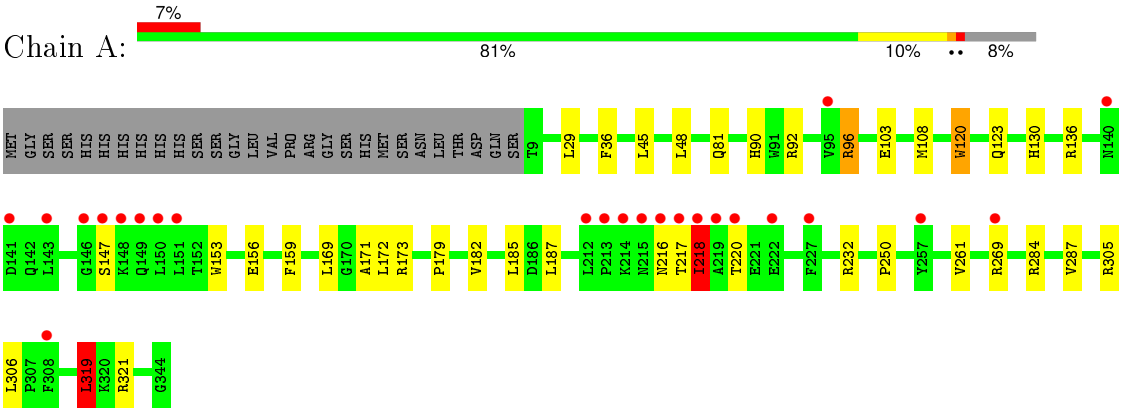
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	242	Total O 242 242	0	0
4	B	198	Total O 198 198	0	0
4	C	241	Total O 241 241	0	0
4	D	204	Total O 204 204	0	0

3 Residue-property plots (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.

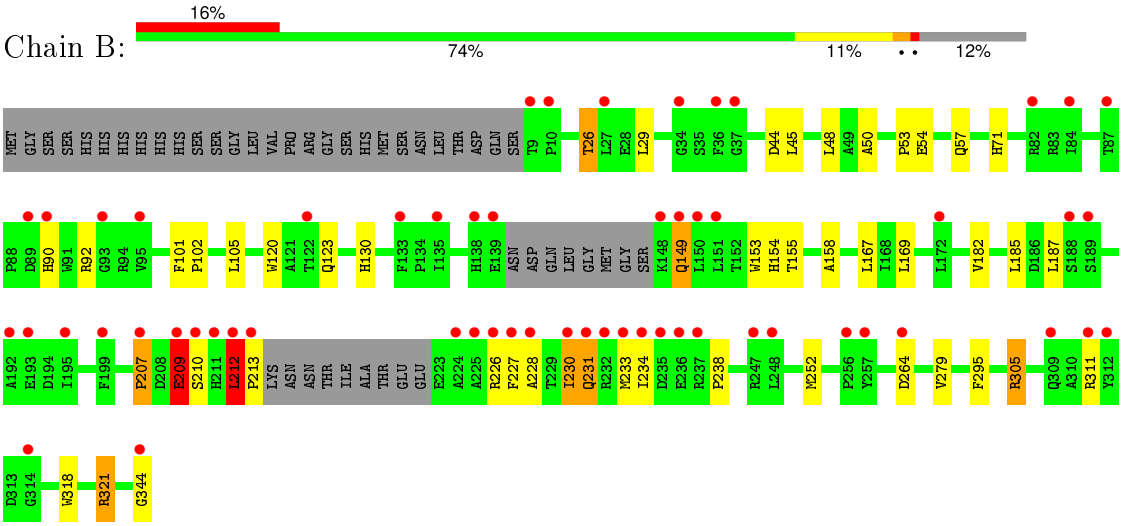
- Molecule 1: L-arginine beta-hydroxylase

Chain A:



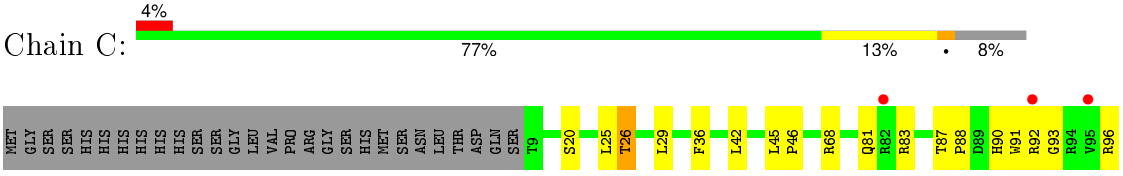
- Molecule 1: L-arginine beta-hydroxylase

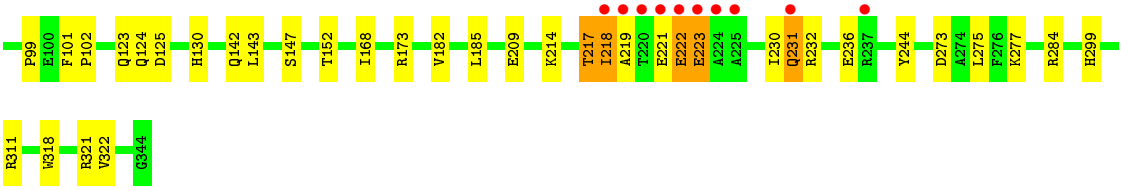
Chain B:



- Molecule 1: L-arginine beta-hydroxylase

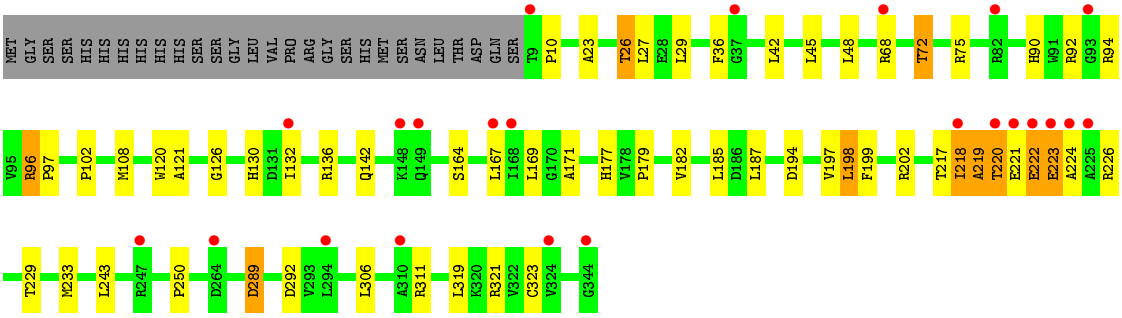
Chain C:





• Molecule 1: L-arginine beta-hydroxylase

Chain D:



4 Data and refinement statistics (i)

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 29.30 – 2.06	Depositor EDS
% Data completeness (in resolution range)	86.5 (30.00-2.06) 86.6 (29.30-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	4062 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.8	EDS
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 81006 reflections (0.001%)	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.*

[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: 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	0.49	2/2760 (0.1%)	0.62	1/3754 (0.0%)
1	B	0.50	2/2633 (0.1%)	0.58	0/3580
1	C	0.49	1/2760 (0.0%)	0.63	0/3754
1	D	0.49	0/2760	0.62	0/3754
All	All	0.49	5/10913 (0.0%)	0.61	1/14842 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	TRP	CD2-CE2	5.67	1.48	1.41
1	B	318	TRP	CD2-CE2	5.28	1.47	1.41
1	A	153	TRP	CD2-CE2	5.27	1.47	1.41
1	C	318	TRP	CD2-CE2	5.13	1.47	1.41
1	B	153	TRP	CD2-CE2	5.01	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	319	LEU	CA-CB-CG	5.07	126.96	115.30

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	2690	0	2606	23	0
1	B	2565	0	2488	31	0
1	C	2690	0	2606	39	0
1	D	2690	0	2606	44	0
2	A	13	0	14	0	0
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	137	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 (137) 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: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:D:219:ALA:C	1:D:220:THR:HG23	2.08	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:252:MET:HE1	1:B:279:VAL:HG21	1.87	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:PRO:HD3	4:B:571:HOH:O	2.09	0.52
1:A:217:THR:HB	1:A:218:ILE:O	2.10	0.51
1:D:26:THR:HG23	1:D:102:PRO:CB	2.34	0.51
1:B:305:ARG:HB3	4:B:653:HOH:O	2.11	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: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:C:223:GLU:OE1	1:C:223:GLU:HA	2.11	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:A:156:GLU:CD	1:A:321:ARG:HH22	2.17	0.48
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:HD13	1:B:230:ILE:H	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:C:92:ARG:O	1:C:92:ARG:CG	2.63	0.45
1:D:90:HIS:HD2	1:D:92:ARG:H	1.63	0.45
1:C:223:GLU:OE1	1:C:223:GLU:CA	2.65	0.45
1:B:120:TRP:HB2	1:B:123:GLN:HB2	1.99	0.45
1:A:261:VAL:HG11	1:A:269:ARG:HA	1.97	0.45
1:C:45:LEU:HB3	1:C:46:PRO:HD3	1.98	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:321:ARG:HG2	1:C:322:VAL:N	2.32	0.45
1:D:221:GLU:HG3	1:D:222:GLU:N	2.31	0.45
1:D:36:PHE:CE1	1:D:108:MET:HG3	2.52	0.45
1:C:81:GLN:HE22	1:C:173:ARG:HE	1.65	0.45
1:D:224:ALA:C	1:D:226:ARG:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ARG:O	1:C:99:PRO:HB2	2.16	0.44
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: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:71:HIS:HA	1:B:295:PHE:O	2.18	0.42
1:B:54:GLU:HG3	4:B:656:HOH:O	2.20	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: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:C:90:HIS:CD2	1:C:91:TRP:H	2.38	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:D:198:LEU:HB3	1:D:243:LEU:HG	2.03	0.41
1:D:217:THR:O	1:D:218:ILE:CG1	2.59	0.40
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: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

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%)	21 10
1	B	313/364 (86%)	302 (96%)	7 (2%)	4 (1%)	15 5
1	C	334/364 (92%)	322 (96%)	8 (2%)	4 (1%)	16 6
1	D	334/364 (92%)	318 (95%)	10 (3%)	6 (2%)	11 2
All	All	1315/1456 (90%)	1265 (96%)	33 (2%)	17 (1%)	15 5

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%)	34 25
1	B	272/311 (88%)	252 (93%)	20 (7%)	17 8
1	C	286/311 (92%)	271 (95%)	15 (5%)	29 18
1	D	286/311 (92%)	270 (94%)	16 (6%)	26 16
All	All	1130/1244 (91%)	1066 (94%)	64 (6%)	25 15

All (64) 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	105	LEU
1	B	130	HIS
1	B	149	GLN
1	B	154	HIS
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	264	ASP
1	B	305	ARG
1	B	311	ARG
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	214	LYS
1	C	217	THR
1	C	222	GLU
1	C	223	GLU
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	96	ARG
1	D	136	ARG
1	D	167	LEU
1	D	182	VAL
1	D	185	LEU
1	D	187	LEU
1	D	198	LEU
1	D	289	ASP
1	D	311	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	81	GLN

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Mol	Chain	Res	Type
1	A	90	HIS
1	A	138	HIS
1	A	142	GLN
1	A	149	GLN
1	A	216	ASN
1	A	231	GLN
1	B	57	GLN
1	B	90	HIS
1	B	231	GLN
1	B	309	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	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	263	GLN

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 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	A	401	-	6,12,12	0.42	0	4,14,14	0.59	0
2	HRG	C	402	-	6,12,12	0.33	0	4,14,14	1.21	0
2	HRG	D	402	-	6,12,12	0.42	0	4,14,14	1.02	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
2	HRG	A	401	-	-	0/6/12/12	0/0/0/0
2	HRG	C	402	-	-	0/6/12/12	0/0/0/0
2	HRG	D	402	-	-	0/6/12/12	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

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	336/364 (92%)	0.40	24 (7%) 19 21	13, 28, 60, 88	4 (1%)
1	B	319/364 (87%)	1.22	58 (18%) 2 2	22, 38, 98, 129	3 (0%)
1	C	336/364 (92%)	0.30	13 (3%) 43 47	14, 26, 49, 95	4 (1%)
1	D	336/364 (92%)	0.46	23 (6%) 20 22	17, 32, 53, 84	3 (0%)
All	All	1327/1456 (91%)	0.59	118 (8%) 12 13	13, 31, 62, 129	14 (1%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	ALA	18.3
1	B	233	MET	11.0
1	B	224	ALA	8.8
1	B	234	ILE	8.4
1	B	235	ASP	8.3
1	B	212	LEU	8.0
1	A	217	THR	7.5
1	B	228	ALA	7.5
1	B	213	PRO	7.4
1	B	237	ARG	7.3
1	B	236	GLU	7.2
1	B	150	LEU	7.1
1	D	220	THR	6.3
1	B	211	HIS	6.1
1	C	92	ARG	6.0
1	C	224	ALA	5.9
1	B	192	ALA	5.8
1	B	226	ARG	5.7
1	A	140	ASN	5.7
1	D	224	ALA	5.7
1	A	150	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	C	218	ILE	5.4
1	B	151	LEU	5.2
1	B	138	HIS	5.1
1	A	214	LYS	5.0
1	B	95	VAL	5.0
1	C	220	THR	5.0
1	C	221	GLU	4.9
1	A	218	ILE	4.7
1	B	232	ARG	4.5
1	A	141	ASP	4.4
1	D	223	GLU	4.3
1	D	221	GLU	4.2
1	B	149	GLN	4.1
1	B	37	GLY	4.1
1	B	210	SER	4.1
1	C	82	ARG	4.0
1	A	143	LEU	3.9
1	D	9	THR	3.9
1	C	219	ALA	3.9
1	A	148	LYS	3.9
1	B	148	LYS	3.8
1	D	344	GLY	3.8
1	B	89	ASP	3.8
1	B	90	HIS	3.8
1	B	230	ILE	3.8
1	D	222	GLU	3.6
1	A	212	LEU	3.6
1	B	209	GLU	3.6
1	C	231	GLN	3.4
1	A	149	GLN	3.4
1	D	148	LYS	3.3
1	B	188	SER	3.3
1	D	82	ARG	3.3
1	B	312	TYR	3.2
1	C	225	ALA	3.2
1	C	223	GLU	3.1
1	D	218	ILE	3.1
1	B	82	ARG	3.1
1	D	168	ILE	3.1
1	B	247	ARG	3.0
1	B	122	THR	3.0
1	B	34	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	84	ILE	2.9
1	A	215	ASN	2.9
1	B	199	PHE	2.9
1	B	309	GLN	2.8
1	D	310	ALA	2.8
1	A	220	THR	2.8
1	B	257	TYR	2.7
1	A	219	ALA	2.7
1	C	95	VAL	2.7
1	D	37	GLY	2.6
1	B	227	PHE	2.6
1	B	36	PHE	2.6
1	B	344	GLY	2.6
1	D	167	LEU	2.6
1	D	225	ALA	2.6
1	A	151	LEU	2.5
1	D	247	ARG	2.5
1	A	222	GLU	2.5
1	A	146	GLY	2.5
1	B	256	PRO	2.5
1	B	248	LEU	2.5
1	C	222	GLU	2.4
1	D	264	ASP	2.4
1	B	311	ARG	2.4
1	D	324	VAL	2.4
1	B	195	ILE	2.4
1	A	216	ASN	2.4
1	D	294	LEU	2.4
1	A	147	SER	2.4
1	A	95	VAL	2.4
1	A	257	TYR	2.4
1	A	308	PHE	2.3
1	C	237	ARG	2.3
1	B	27	LEU	2.3
1	B	9	THR	2.2
1	B	139	GLU	2.2
1	B	231	GLN	2.2
1	B	264	ASP	2.2
1	B	135	ILE	2.2
1	B	93	GLY	2.2
1	B	189	SER	2.2
1	B	172	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	87	THR	2.1
1	B	10	PRO	2.1
1	B	207	PRO	2.1
1	D	149	GLN	2.1
1	B	314	GLY	2.1
1	D	93	GLY	2.1
1	D	132	ILE	2.1
1	A	213	PRO	2.1
1	D	68	ARG	2.1
1	A	227	PHE	2.1
1	B	193	GLU	2.0
1	A	269	ARG	2.0
1	B	133	PHE	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
2	HRG	D	402	13/13	0.88	0.20	1.38	31,34,36,36	0
2	HRG	C	402	13/13	0.91	0.17	1.04	31,33,34,35	0
2	HRG	A	401	13/13	0.81	0.16	0.24	45,48,54,54	0
3	FE	C	401	1/1	0.96	0.07	-	67,67,67,67	0
3	FE	B	401	1/1	0.87	0.13	-	89,89,89,89	0
3	FE	D	401	1/1	0.99	0.05	-	70,70,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.