



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 07:10 PM EDT

PDB ID : 4M2G  
Title : Crystal structure of non-heme iron oxygenase OrfP in complex with Fe, succinate, and (3R,4R)-dihydroxy-L-Arg  
Authors : Chang, C.Y.; Liu, Y.C.; Lyu, S.Y.; Wu, C.C.; Li, T.L.  
Deposited on : 2013-08-05  
Resolution : 2.39 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

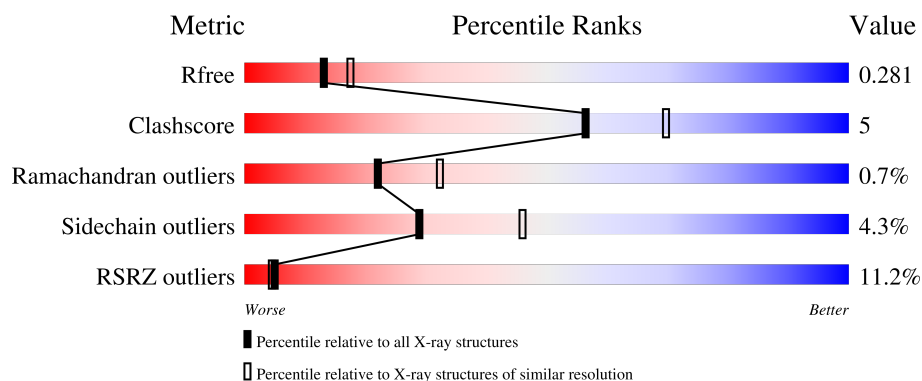
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	<div> <div>6%</div> <div>82% 10% • 8%</div> </div>
1	B	364	<div> <div>9%</div> <div>74% 10% • 15%</div> </div>
1	C	364	<div> <div>11%</div> <div>80% 10% • 9%</div> </div>
1	D	364	<div> <div>14%</div> <div>82% 10% 8%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11022 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	309	Total	C	N	O	S	0	0	0
			2487	1571	450	460	6			
1	C	331	Total	C	N	O	S	0	0	0
			2651	1671	482	491	7			
1	D	336	Total	C	N	O	S	0	0	0
			2690	1693	487	503	7			

There are 80 discrepancies between the modelled and reference sequences:

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

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

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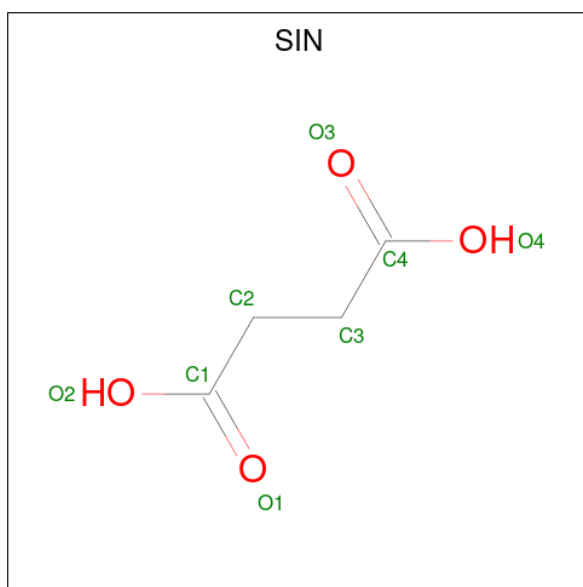
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP G9MBV2
D	-15	HIS	-	expression tag	UNP G9MBV2
D	-14	HIS	-	expression tag	UNP G9MBV2
D	-13	HIS	-	expression tag	UNP G9MBV2
D	-12	HIS	-	expression tag	UNP G9MBV2
D	-11	HIS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

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

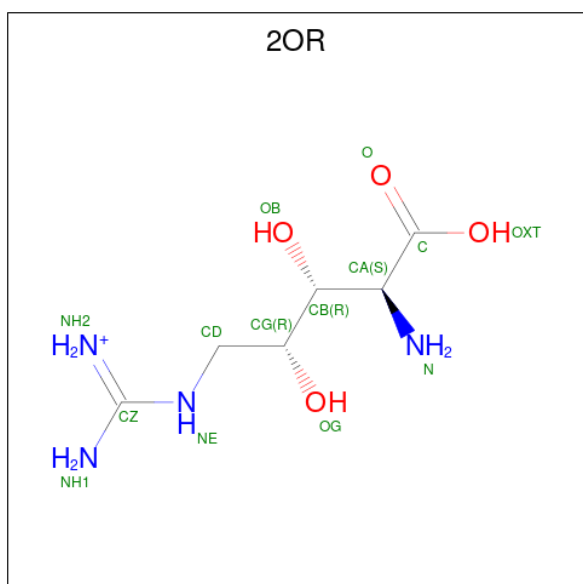
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0

- Molecule 3 is SUCCINIC ACID (three-letter code: SIN) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>4</sub>).



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

- Molecule 4 is amino{[(2R,3R,4S)-4-amino-2,3,5-trihydroxy-5-oxopentyl]amino}methaniminium (three-letter code: 2OR) (formula:  $C_6H_{15}N_4O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	6	4	4		
4	D	1	Total	C	N	O	0	0
			14	6	4	4		

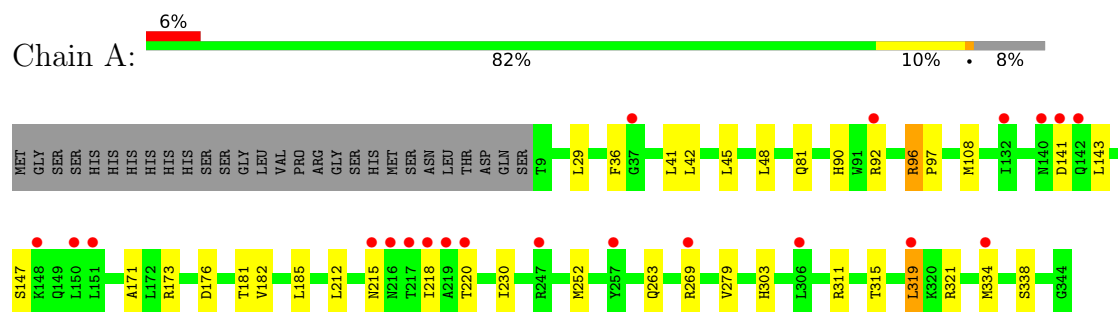
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	142	Total	O	0	0
			142	142		
5	B	106	Total	O	0	0
			106	106		
5	C	113	Total	O	0	0
			113	113		
5	D	79	Total	O	0	0
			79	79		

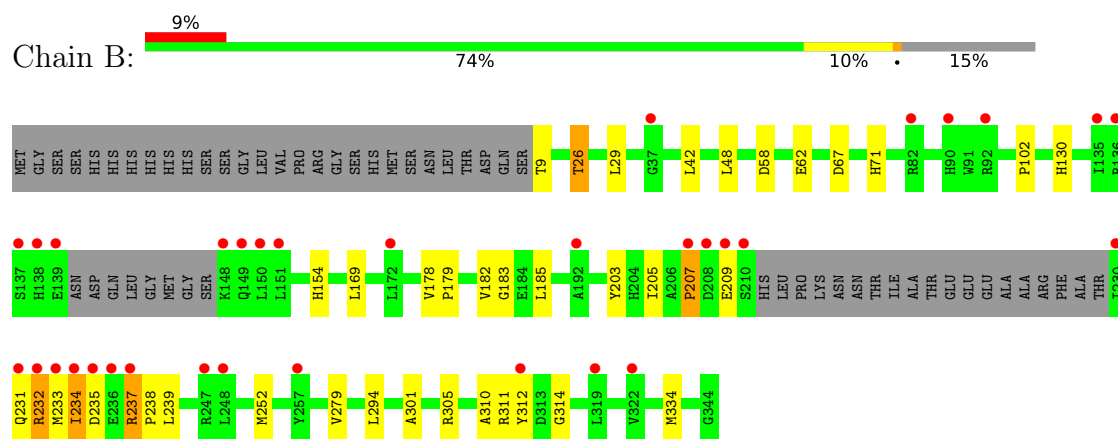
### 3 Residue-property plots [i](#)

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.

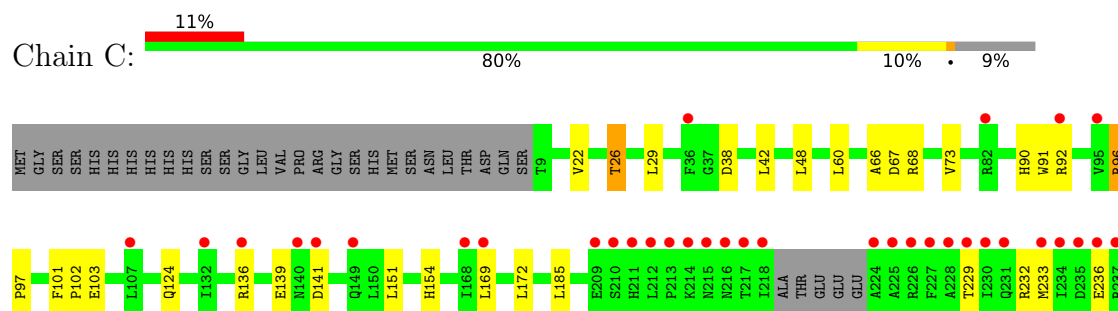
- Molecule 1: L-arginine beta-hydroxylase



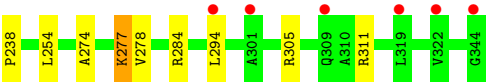
- Molecule 1: L-arginine beta-hydroxylase



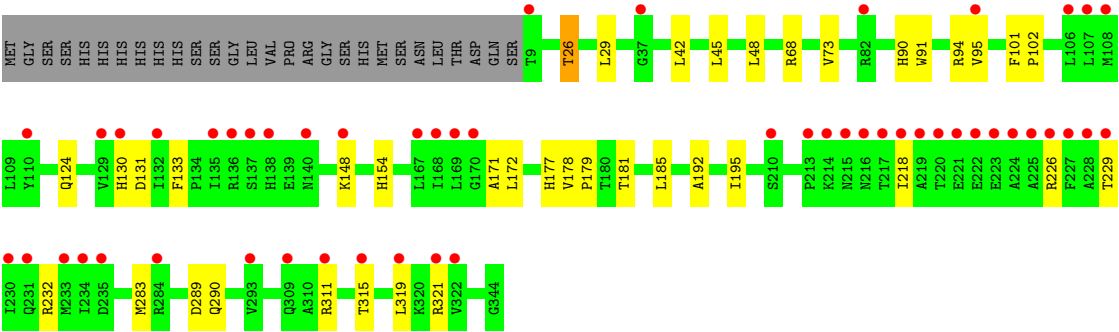
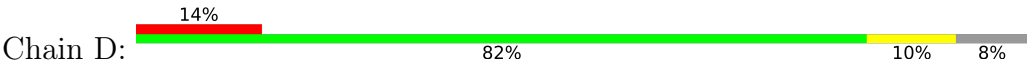
- Molecule 1: L-arginine beta-hydroxylase







● 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, $\alpha$ , $\beta$ , $\gamma$	67.29Å 116.21Å 96.16Å 90.00° 91.66° 90.00°	Depositor
Resolution (Å)	26.15 – 2.39 26.13 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (26.15-2.39) 99.8 (26.13-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.214 , 0.271 0.218 , 0.281	Depositor DCC
$R_{free}$ test set	2963 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 32.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11022	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FE, 2OR, 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	0.37	0/2760	0.59	0/3754
1	B	0.38	0/2552	0.59	1/3469 (0.0%)
1	C	0.36	0/2720	0.58	0/3698
1	D	0.34	0/2760	0.55	0/3754
All	All	0.36	0/10792	0.58	1/14675 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	ARG	C-N-CD	6.06	141.12	128.40

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	17	0
1	B	2487	0	2413	47	0
1	C	2651	0	2575	23	0
1	D	2690	0	2606	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	8	0	4	0	0
3	B	8	0	4	0	0
3	C	8	0	4	0	0
3	D	8	0	4	0	0
4	C	14	0	13	1	0
4	D	14	0	13	2	0
5	A	142	0	0	1	0
5	B	106	0	0	1	0
5	C	113	0	0	0	0
5	D	79	0	0	0	0
All	All	11022	0	10242	104	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 5.

All (104) 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:B:207:PRO:HD3	1:B:237:ARG:NH1	1.21	1.48
1:B:207:PRO:CD	1:B:237:ARG:NH1	2.00	1.23
1:B:233:MET:CG	1:B:334:MET:HG2	1.78	1.12
1:B:233:MET:HE2	1:B:334:MET:CE	1.86	1.04
1:B:233:MET:CE	1:B:334:MET:HE2	1.88	1.03
1:B:207:PRO:CG	1:B:237:ARG:CZ	2.41	0.99
1:B:233:MET:HE2	1:B:334:MET:HE2	0.99	0.98
1:B:233:MET:HG3	1:B:334:MET:CG	1.94	0.97
1:B:233:MET:HG3	1:B:334:MET:HG2	1.00	0.96
1:B:233:MET:O	1:B:235:ASP:N	1.99	0.95
1:B:207:PRO:CD	1:B:237:ARG:CZ	2.47	0.92
1:B:207:PRO:HD3	1:B:237:ARG:HH12	1.14	0.90
1:D:154:HIS:CE1	4:D:402:2OR:H9	1.88	0.90
1:B:207:PRO:HG2	1:B:237:ARG:CZ	2.05	0.86
1:A:92:ARG:NH1	5:A:552:HOH:O	2.14	0.81
1:B:233:MET:CE	1:B:233:MET:HA	2.17	0.74
1:D:154:HIS:CE1	4:D:402:2OR:OG	2.40	0.72
1:C:26:THR:HG23	1:C:102:PRO:HB3	1.71	0.70
1:B:207:PRO:HD3	1:B:237:ARG:HH11	1.50	0.66
1:C:26:THR:CG2	1:C:102:PRO:HB3	2.25	0.66
1:D:26:THR:HG23	1:D:102:PRO:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ILE:HD12	1:D:218:ILE:H	1.62	0.64
1:B:232:ARG:O	1:B:234:ILE:N	2.28	0.64
1:B:233:MET:SD	1:B:334:MET:CG	2.86	0.64
1:B:233:MET:SD	1:B:334:MET:HG2	2.38	0.64
1:B:233:MET:HA	1:B:233:MET:HE3	1.79	0.63
1:D:26:THR:CG2	1:D:102:PRO:HB3	2.29	0.62
1:A:36:PHE:CE1	1:A:108:MET:HG3	2.35	0.61
1:B:233:MET:CG	1:B:334:MET:CG	2.68	0.60
1:B:26:THR:CG2	1:B:102:PRO:HB3	2.31	0.59
1:B:232:ARG:O	1:B:234:ILE:HD12	2.01	0.59
1:B:232:ARG:C	1:B:234:ILE:H	2.06	0.59
1:B:207:PRO:CG	1:B:237:ARG:NH1	2.58	0.59
1:B:234:ILE:HG22	1:B:234:ILE:O	2.02	0.59
1:A:90:HIS:CD2	1:A:92:ARG:H	2.20	0.58
1:B:26:THR:HG23	1:B:102:PRO:HB3	1.86	0.58
1:B:203:TYR:C	1:B:239:LEU:HD22	2.24	0.57
1:B:233:MET:SD	1:B:334:MET:HG3	2.44	0.57
1:A:81:GLN:HE22	1:A:173:ARG:HE	1.54	0.56
1:B:203:TYR:O	1:B:239:LEU:HA	2.06	0.56
1:B:169:LEU:HD12	1:B:294:LEU:HD23	1.90	0.53
1:A:171:ALA:HA	1:A:319:LEU:HD22	1.89	0.53
1:B:233:MET:HB3	1:B:334:MET:HE2	1.90	0.53
1:B:207:PRO:CD	1:B:237:ARG:HH12	1.92	0.52
1:B:207:PRO:CG	1:B:237:ARG:NE	2.73	0.52
1:D:171:ALA:HA	1:D:319:LEU:HD22	1.93	0.51
1:B:233:MET:CE	1:B:334:MET:CE	2.68	0.50
1:A:263:GLN:O	1:A:269:ARG:NH2	2.44	0.49
1:B:207:PRO:HG2	1:B:237:ARG:NH2	2.28	0.49
1:A:181:THR:O	1:A:303:HIS:HA	2.13	0.49
1:A:81:GLN:NE2	1:A:173:ARG:HE	2.10	0.49
1:C:154:HIS:NE2	4:C:402:2OR:OG	2.46	0.49
1:C:229:THR:HG22	1:C:232:ARG:HH21	1.78	0.49
1:D:172:LEU:O	1:D:290:GLN:HG3	2.13	0.48
1:A:90:HIS:HD2	1:A:92:ARG:H	1.61	0.48
1:B:203:TYR:C	1:B:239:LEU:CD2	2.82	0.48
1:D:177:HIS:HD2	1:D:289:ASP:OD1	1.97	0.47
1:C:90:HIS:CD2	1:C:92:ARG:H	2.33	0.47
1:C:91:TRP:CH2	1:C:124:GLN:HA	2.49	0.47
1:C:151:LEU:HB3	1:C:305:ARG:H	1.79	0.47
1:C:274:ALA:O	1:C:278:VAL:HG23	2.15	0.47
1:C:90:HIS:HD2	1:C:92:ARG:H	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LEU:HD12	1:C:294:LEU:HD23	1.95	0.47
1:C:26:THR:HG23	1:C:102:PRO:CB	2.42	0.47
1:D:181:THR:HB	1:D:283:MET:HE3	1.97	0.47
1:C:236:GLU:HG3	1:C:238:PRO:HD3	1.97	0.47
1:B:58:ASP:O	1:B:62:GLU:HG3	2.16	0.45
1:A:252:MET:HE1	1:A:279:VAL:HG21	1.98	0.45
1:C:232:ARG:HG3	1:C:233:MET:HG3	1.97	0.45
1:C:277:LYS:HA	1:C:277:LYS:HD2	1.77	0.45
1:C:73:VAL:HG22	1:C:294:LEU:HD12	2.00	0.44
1:A:41:LEU:O	1:A:45:LEU:HG	2.17	0.44
1:C:101:PHE:HB3	1:C:102:PRO:HD3	2.00	0.43
1:B:237:ARG:NE	5:B:584:HOH:O	2.30	0.43
1:D:101:PHE:HB3	1:D:102:PRO:HD3	1.99	0.43
1:A:338:SER:HB3	1:B:67:ASP:HB3	2.00	0.43
1:C:103:GLU:HG2	1:C:172:LEU:HD22	1.99	0.43
1:D:229:THR:HG22	1:D:232:ARG:HH22	1.84	0.43
1:A:212:LEU:O	1:A:215:ASN:HB2	2.19	0.43
1:C:136:ARG:O	1:C:139:GLU:HG3	2.18	0.43
1:B:207:PRO:HG3	1:B:237:ARG:HD2	2.01	0.43
1:D:91:TRP:CD2	1:D:124:GLN:HG3	2.54	0.43
1:D:26:THR:HG23	1:D:102:PRO:CB	2.45	0.42
1:D:90:HIS:CD2	1:D:91:TRP:H	2.37	0.42
1:B:183:GLY:O	1:B:301:ALA:HA	2.19	0.42
1:B:252:MET:HE1	1:B:279:VAL:HG21	2.01	0.42
1:B:232:ARG:C	1:B:234:ILE:N	2.70	0.42
1:A:176:ASP:OD2	1:A:311:ARG:NH2	2.53	0.42
1:C:96:ARG:HA	1:C:97:PRO:HA	1.84	0.42
1:B:310:ALA:HB3	1:B:312:TYR:CE1	2.55	0.41
1:A:230:ILE:HG12	1:A:334:MET:HE2	2.02	0.41
1:A:311:ARG:NH1	1:A:315:THR:OG1	2.53	0.41
1:C:38:ASP:OD1	1:C:38:ASP:C	2.59	0.41
1:C:22:VAL:O	1:C:26:THR:HB	2.20	0.41
1:D:130:HIS:HB2	1:D:321:ARG:HB3	2.03	0.41
1:D:178:VAL:HA	1:D:179:PRO:HD3	1.91	0.41
1:D:192:ALA:HA	1:D:195:ILE:HD12	2.03	0.41
1:A:96:ARG:HA	1:A:97:PRO:HA	1.89	0.40
1:B:178:VAL:HA	1:B:179:PRO:HD3	1.88	0.40
1:B:207:PRO:HG2	1:B:237:ARG:NE	2.33	0.40
1:D:131:ASP:HB3	1:D:133:PHE:CE2	2.57	0.40
1:C:66:ALA:O	1:C:67:ASP:C	2.59	0.40
1:B:9:THR:HG21	1:B:71:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LEU:HD23	1:C:60:LEU:HA	1.95	0.40

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%)	325 (97%)	6 (2%)	3 (1%)	17	25
1	B	303/364 (83%)	284 (94%)	15 (5%)	4 (1%)	12	17
1	C	327/364 (90%)	311 (95%)	16 (5%)	0	100	100
1	D	334/364 (92%)	317 (95%)	15 (4%)	2 (1%)	25	36
All	All	1298/1456 (89%)	1237 (95%)	52 (4%)	9 (1%)	22	32

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	234	ILE
1	B	238	PRO
1	B	314	GLY
1	D	94	ARG
1	A	147	SER
1	B	207	PRO
1	D	95	VAL
1	A	220	THR
1	A	218	ILE

### 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%)	276 (96%)	10 (4%)	36	55
1	B	265/311 (85%)	251 (95%)	14 (5%)	22	37
1	C	282/311 (91%)	270 (96%)	12 (4%)	29	46
1	D	286/311 (92%)	274 (96%)	12 (4%)	30	47
All	All	1119/1244 (90%)	1071 (96%)	48 (4%)	29	46

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	42	LEU
1	A	48	LEU
1	A	96	ARG
1	A	141	ASP
1	A	143	LEU
1	A	182	VAL
1	A	185	LEU
1	A	319	LEU
1	A	321	ARG
1	B	26	THR
1	B	29	LEU
1	B	42	LEU
1	B	48	LEU
1	B	130	HIS
1	B	154	HIS
1	B	182	VAL
1	B	185	LEU
1	B	205	ILE
1	B	209	GLU
1	B	231	GLN
1	B	232	ARG
1	B	305	ARG
1	B	311	ARG
1	C	26	THR
1	C	29	LEU
1	C	42	LEU
1	C	48	LEU

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Mol	Chain	Res	Type
1	C	68	ARG
1	C	96	ARG
1	C	141	ASP
1	C	185	LEU
1	C	254	LEU
1	C	277	LYS
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	73	VAL
1	D	148	LYS
1	D	185	LEU
1	D	226	ARG
1	D	311	ARG
1	D	315	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	81	GLN
1	A	90	HIS
1	A	138	HIS
1	A	142	GLN
1	B	57	GLN
1	B	90	HIS
1	B	138	HIS
1	B	231	GLN
1	C	57	GLN
1	C	81	GLN
1	C	90	HIS
1	C	123	GLN
1	C	142	GLN
1	C	177	HIS
1	C	216	ASN
1	D	57	GLN
1	D	142	GLN

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Mol	Chain	Res	Type
1	D	177	HIS
1	D	216	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	2OR	D	402	2	12,13,13	0.86	0	13,17,17	0.79	0
3	SIN	A	402	-	7,7,7	1.09	0	8,8,8	1.14	0
3	SIN	D	403	2	7,7,7	1.03	0	8,8,8	1.16	0
3	SIN	C	403	2	7,7,7	1.07	0	8,8,8	1.05	0
3	SIN	B	402	-	7,7,7	0.99	0	8,8,8	1.71	1 (12%)
4	2OR	C	402	2	12,13,13	0.80	0	13,17,17	0.87	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
4	2OR	D	402	2	-	0/17/17/17	-
3	SIN	A	402	-	-	5/5/5/5	-
3	SIN	D	403	2	-	5/5/5/5	-
3	SIN	C	403	2	-	2/5/5/5	-
3	SIN	B	402	-	-	5/5/5/5	-
4	2OR	C	402	2	-	8/17/17/17	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	SIN	C3-C2-C1	-3.15	106.82	113.60

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	402	2OR	O-C-CA-CB
4	C	402	2OR	OXT-C-CA-CB
4	C	402	2OR	CA-CB-CG-OG
4	C	402	2OR	CA-CB-CG-CD
4	C	402	2OR	OB-CB-CG-OG
4	C	402	2OR	OB-CB-CG-CD
3	A	402	SIN	C1-C2-C3-C4
3	D	403	SIN	C1-C2-C3-C4
4	C	402	2OR	OXT-C-CA-N
3	B	402	SIN	C1-C2-C3-C4
4	C	402	2OR	O-C-CA-N
3	B	402	SIN	C2-C3-C4-O3
3	A	402	SIN	O1-C1-C2-C3
3	D	403	SIN	C2-C3-C4-O3
3	D	403	SIN	C2-C3-C4-O4
3	B	402	SIN	C2-C3-C4-O4
3	A	402	SIN	C2-C3-C4-O3
3	A	402	SIN	O2-C1-C2-C3
3	A	402	SIN	C2-C3-C4-O4
3	D	403	SIN	O2-C1-C2-C3
3	C	403	SIN	O2-C1-C2-C3
3	D	403	SIN	O1-C1-C2-C3
3	B	402	SIN	O2-C1-C2-C3
3	C	403	SIN	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	402	SIN	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	402	2OR	2	0
4	C	402	2OR	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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	336/364 (92%)	0.15	21 (6%)	20 18	26, 42, 83, 158	6 (1%)
1	B	309/364 (84%)	0.48	33 (10%)	6 5	24, 52, 90, 131	3 (0%)
1	C	331/364 (90%)	0.49	41 (12%)	4 3	31, 45, 127, 178	4 (1%)
1	D	336/364 (92%)	0.80	52 (15%)	2 1	35, 60, 127, 155	3 (0%)
All	All	1312/1456 (90%)	0.48	147 (11%)	5 4	24, 49, 112, 178	16 (1%)

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	218	ILE	9.7
1	B	237	ARG	9.2
1	D	228	ALA	8.7
1	B	233	MET	8.5
1	A	217	THR	7.8
1	A	216	ASN	7.5
1	C	216	ASN	7.2
1	D	225	ALA	6.8
1	D	224	ALA	6.5
1	D	230	ILE	6.4
1	C	217	THR	6.3
1	A	215	ASN	6.2
1	D	219	ALA	5.8
1	C	227	PHE	5.7
1	A	218	ILE	5.7
1	D	218	ILE	5.7
1	D	214	LYS	5.6
1	C	226	ARG	5.6
1	C	230	ILE	5.5
1	C	228	ALA	5.5
1	D	233	MET	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	235	ASP	5.3
1	B	138	HIS	5.1
1	C	231	GLN	5.1
1	D	217	THR	5.1
1	D	210	SER	5.0
1	C	235	ASP	5.0
1	C	225	ALA	4.9
1	B	209	GLU	4.9
1	B	137	SER	4.8
1	B	37	GLY	4.8
1	C	212	LEU	4.7
1	C	224	ALA	4.7
1	C	229	THR	4.6
1	B	236	GLU	4.6
1	D	226	ARG	4.6
1	C	210	SER	4.5
1	A	142	GLN	4.5
1	B	231	GLN	4.1
1	C	233	MET	4.0
1	D	213	PRO	3.9
1	D	148	LYS	3.9
1	C	140	ASN	3.9
1	D	222	GLU	3.9
1	B	234	ILE	3.9
1	D	9	THR	3.8
1	D	82	ARG	3.8
1	D	221	GLU	3.8
1	C	236	GLU	3.8
1	B	192	ALA	3.8
1	C	132	ILE	3.7
1	C	136	ARG	3.7
1	C	82	ARG	3.6
1	A	92	ARG	3.6
1	D	216	ASN	3.6
1	D	215	ASN	3.5
1	C	214	LYS	3.5
1	B	149	GLN	3.5
1	D	223	GLU	3.4
1	B	151	LEU	3.4
1	C	169	LEU	3.4
1	D	169	LEU	3.4
1	D	95	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	229	THR	3.4
1	D	107	LEU	3.4
1	A	150	LEU	3.3
1	D	168	ILE	3.2
1	D	220	THR	3.2
1	D	309	GLN	3.2
1	C	309	GLN	3.2
1	A	306	LEU	3.1
1	C	168	ILE	3.1
1	A	140	ASN	3.1
1	B	150	LEU	3.1
1	C	215	ASN	3.1
1	D	321	ARG	3.0
1	C	95	VAL	3.0
1	D	136	ARG	3.0
1	C	209	GLU	2.9
1	B	90	HIS	2.9
1	B	207	PRO	2.8
1	D	322	VAL	2.8
1	C	319	LEU	2.7
1	D	37	GLY	2.7
1	D	106	LEU	2.7
1	D	231	GLN	2.7
1	C	213	PRO	2.7
1	A	334	MET	2.7
1	A	141	ASP	2.7
1	B	136	ARG	2.7
1	B	210	SER	2.6
1	B	208	ASP	2.6
1	D	234	ILE	2.6
1	C	149	GLN	2.6
1	D	311	ARG	2.5
1	D	315	THR	2.5
1	D	319	LEU	2.5
1	C	344	GLY	2.5
1	B	139	GLU	2.5
1	D	135	ILE	2.5
1	D	138	HIS	2.5
1	B	148	LYS	2.5
1	C	211	HIS	2.5
1	B	92	ARG	2.4
1	B	257	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	110	TYR	2.4
1	B	172	LEU	2.4
1	D	167	LEU	2.4
1	D	108	MET	2.4
1	A	132	ILE	2.4
1	D	130	HIS	2.4
1	D	170	GLY	2.4
1	A	151	LEU	2.4
1	A	37	GLY	2.3
1	C	294	LEU	2.3
1	C	322	VAL	2.3
1	C	237	ARG	2.3
1	C	234	ILE	2.3
1	A	219	ALA	2.3
1	D	235	ASP	2.3
1	B	135	ILE	2.3
1	B	247	ARG	2.3
1	B	312	TYR	2.3
1	B	248	LEU	2.3
1	C	36	PHE	2.3
1	B	82	ARG	2.3
1	D	132	ILE	2.2
1	A	257	TYR	2.2
1	C	141	ASP	2.2
1	D	293	VAL	2.2
1	C	92	ARG	2.2
1	B	322	VAL	2.1
1	A	319	LEU	2.1
1	D	129	VAL	2.1
1	A	247	ARG	2.1
1	B	232	ARG	2.1
1	D	284	ARG	2.1
1	D	227	PHE	2.1
1	A	269	ARG	2.1
1	D	140	ASN	2.1
1	B	319	LEU	2.0
1	A	148	LYS	2.0
1	A	220	THR	2.0
1	B	230	ILE	2.0
1	C	107	LEU	2.0
1	D	137	SER	2.0
1	C	301	ALA	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 monosaccharides 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, 95<sup>th</sup> 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
3	SIN	A	402	8/8	0.83	0.28	50,54,61,61	0
4	2OR	C	402	14/14	0.83	0.25	67,79,94,96	0
3	SIN	D	403	8/8	0.85	0.28	63,74,82,83	0
2	FE	D	401	1/1	0.88	0.14	76,76,76,76	0
3	SIN	B	402	8/8	0.88	0.18	56,59,62,63	0
4	2OR	D	402	14/14	0.89	0.20	74,80,88,89	0
2	FE	B	401	1/1	0.92	0.11	85,85,85,85	0
3	SIN	C	403	8/8	0.93	0.22	52,58,68,69	0
2	FE	C	401	1/1	0.93	0.18	73,73,73,73	0
2	FE	A	401	1/1	0.98	0.15	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.