



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2016 – 05:09 PM EST

PDB ID : 4ZTT
Title : Crystal structures of ferritin mutants reveal diferric-peroxo intermediates
Authors : Kim, S.; Park, Y.H.; Jung, S.W.; Seok, J.H.; Chung, Y.B.; Lee, D.B.; Gowda, G.; Lee, J.H.; Han, H.R.; Cho, A.E.; Lee, C.; Chung, M.S.; Kim, K.H.
Deposited on : 2015-05-15
Resolution : 1.83 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

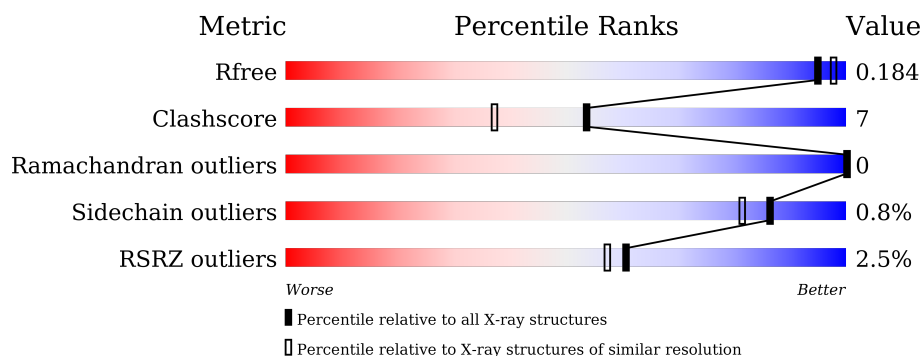
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
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) : rb-20028320

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X-RAY DIFFRACTION

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	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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 $\leq 5\%$. 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	166	<div> <div></div> <div>2%</div> <div>82%</div> <div>16%</div> <div></div> </div>	.
1	B	166	<div> <div></div> <div>4%</div> <div>82%</div> <div>16%</div> <div></div> </div>	..
1	C	166	<div> <div></div> <div>2%</div> <div>86%</div> <div>11%</div> <div></div> </div>	.
1	D	166	<div> <div></div> <div>2%</div> <div>83%</div> <div>13%</div> <div></div> </div>	..
1	E	166	<div> <div></div> <div>2%</div> <div>83%</div> <div>15%</div> <div></div> </div>	..
1	F	166	<div> <div></div> <div>4%</div> <div>91%</div> <div>8%</div> <div></div> </div>	.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FEO	E	201	-	-	X	-
3	OH	A	203	-	-	-	X
3	OH	B	202	-	-	-	X
3	OH	B	203	-	-	-	X
3	OH	C	204	-	-	-	X
3	OH	E	202	-	-	-	X
3	OH	F	206	-	-	-	X
4	GOL	A	204	-	-	X	X
4	GOL	C	205	-	-	X	-
4	GOL	C	206	-	-	-	X
4	GOL	C	207	-	-	-	X
4	GOL	C	208	-	-	X	-
4	GOL	E	203	-	-	-	X
4	GOL	E	204	-	-	-	X
8	PER	D	203	-	-	-	X
9	O	F	204	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9581 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 Bacterial non-heme ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	11	0
			1426	906	228	281	11			
1	B	164	Total	C	N	O	S	0	7	0
			1417	899	230	279	9			
1	C	162	Total	C	N	O	S	0	9	0
			1414	898	229	278	9			
1	D	162	Total	C	N	O	S	0	14	0
			1461	928	236	286	11			
1	E	163	Total	C	N	O	S	0	13	0
			1454	925	234	285	10			
1	F	164	Total	C	N	O	S	0	6	0
			1411	897	228	276	10			

There are 18 discrepancies between the modelled and reference sequences:

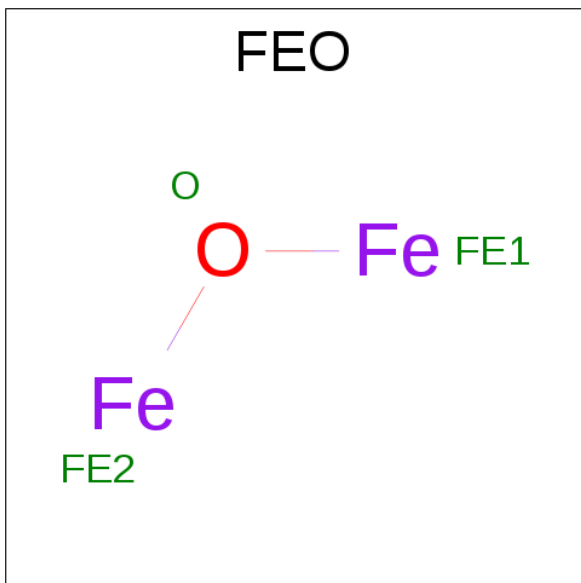
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP C9QT34
A	1	HIS	-	expression tag	UNP C9QT34
A	20	ALA	SER	engineered mutation	UNP C9QT34
B	0	HIS	-	expression tag	UNP C9QT34
B	1	HIS	-	expression tag	UNP C9QT34
B	20	ALA	SER	engineered mutation	UNP C9QT34
C	0	HIS	-	expression tag	UNP C9QT34
C	1	HIS	-	expression tag	UNP C9QT34
C	20	ALA	SER	engineered mutation	UNP C9QT34
D	0	HIS	-	expression tag	UNP C9QT34
D	1	HIS	-	expression tag	UNP C9QT34
D	20	ALA	SER	engineered mutation	UNP C9QT34
E	0	HIS	-	expression tag	UNP C9QT34
E	1	HIS	-	expression tag	UNP C9QT34
E	20	ALA	SER	engineered mutation	UNP C9QT34
F	0	HIS	-	expression tag	UNP C9QT34
F	1	HIS	-	expression tag	UNP C9QT34

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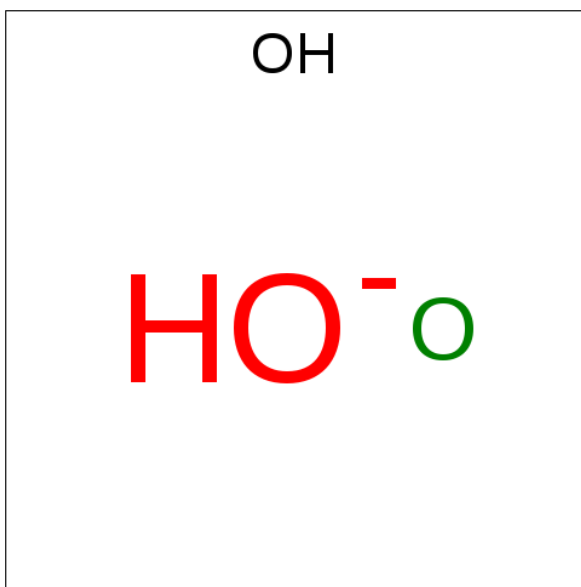
Chain	Residue	Modelled	Actual	Comment	Reference
F	20	ALA	SER	engineered mutation	UNP C9QT34

- Molecule 2 is MU-OXO-DIIRON (three-letter code: FEO) (formula: Fe_2O).



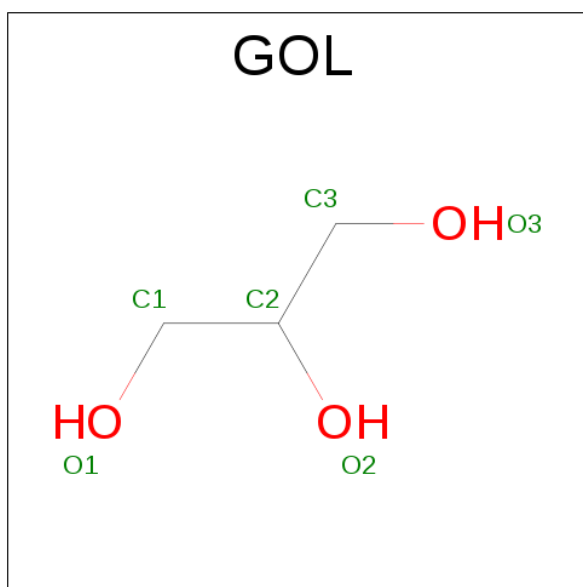
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	O	0	0
			3	2	1		
2	B	1	Total	Fe	O	0	0
			3	2	1		
2	E	1	Total	Fe	O	0	0
			3	2	1		

- Molecule 3 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0
3	E	1	Total O 1 1	0	0
3	F	1	Total O 1 1	0	0
3	F	1	Total O 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

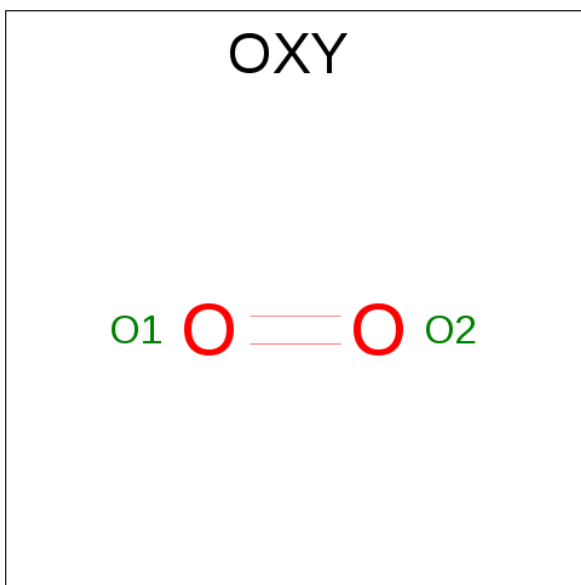
- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	2	Total	Fe	0	0
			2	2		
5	C	1	Total	Fe	0	0
			1	1		
5	F	2	Total	Fe	0	0
			2	2		

- Molecule 6 is FE (II) ION (three-letter code: FE2) (formula: Fe).

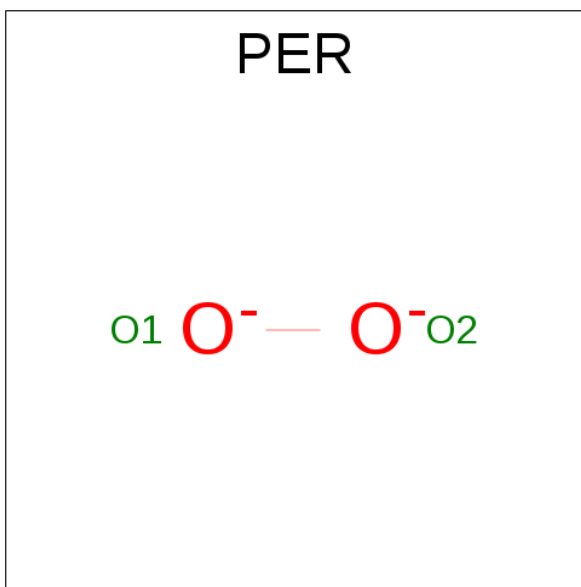
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Fe	0	0
			1	1		
6	E	1	Total	Fe	0	0
			1	1		

- Molecule 7 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	O	0	0
			2	2		

- Molecule 8 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total O 2 2	0	0

- Molecule 9 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	2	Total O 2 2	0	0

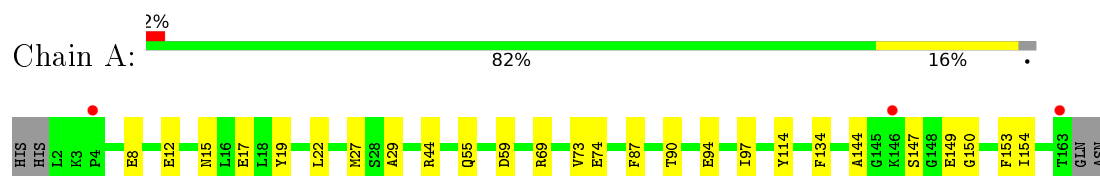
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	151	Total O 151 151	0	0
10	B	153	Total O 153 153	0	0
10	C	140	Total O 140 140	0	0
10	D	141	Total O 141 141	0	0
10	E	153	Total O 153 153	0	0
10	F	145	Total O 145 145	0	0

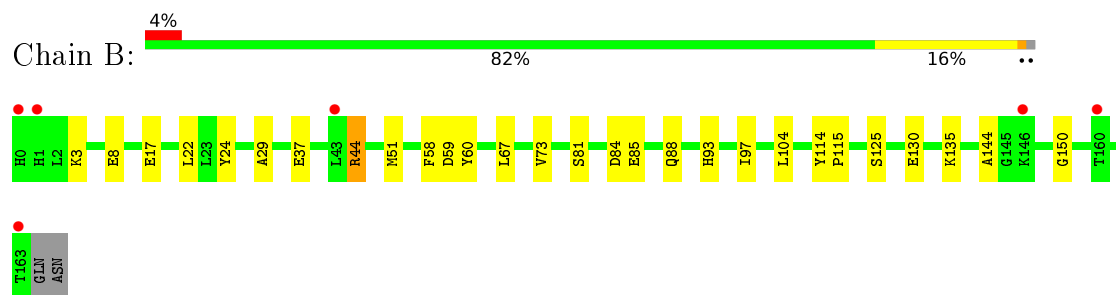
3 Residue-property plots [i](#)

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.

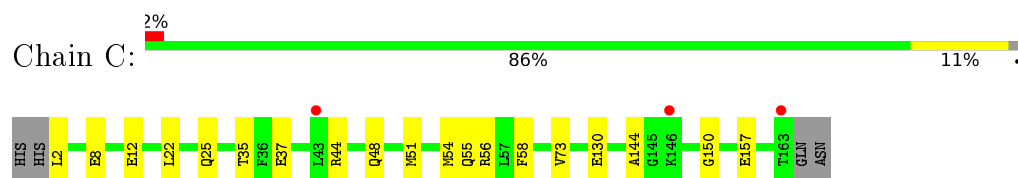
- Molecule 1: Bacterial non-heme ferritin



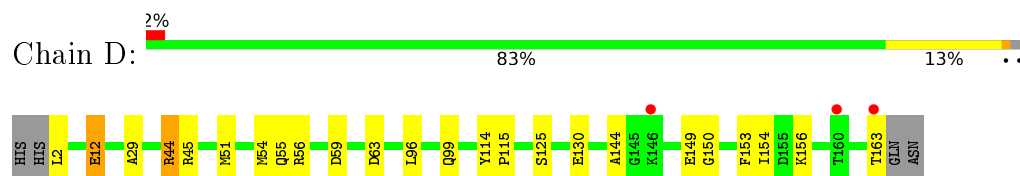
- Molecule 1: Bacterial non-heme ferritin



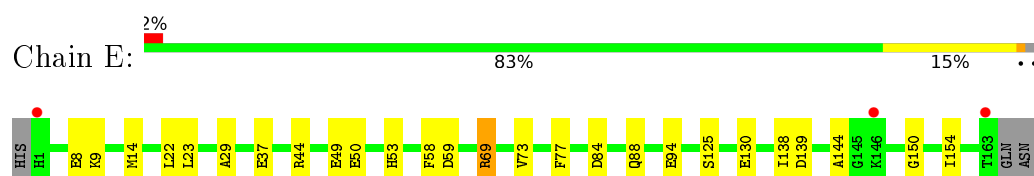
- Molecule 1: Bacterial non-heme ferritin



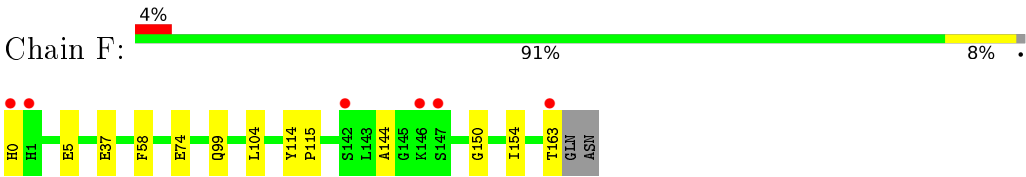
- Molecule 1: Bacterial non-heme ferritin



- Molecule 1: Bacterial non-heme ferritin



● Molecule 1: Bacterial non-heme ferritin



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	128.82Å 128.82Å 172.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.66 – 1.83 19.66 – 1.83	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.66-1.83) 98.9 (19.66-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.156 , 0.192 0.154 , 0.184	Depositor DCC
R_{free} test set	5691 reflections (4.94%)	DCC
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9581	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: GOL, OXY, OH, FEO, PER, FE2, O, 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	1.22	1/1457 (0.1%)	1.10	4/1965 (0.2%)
1	B	1.23	5/1450 (0.3%)	1.05	4/1957 (0.2%)
1	C	1.21	3/1445 (0.2%)	1.00	1/1949 (0.1%)
1	D	1.21	5/1492 (0.3%)	1.12	12/2010 (0.6%)
1	E	1.22	3/1486 (0.2%)	1.14	7/2004 (0.3%)
1	F	1.18	1/1444 (0.1%)	1.04	0/1948
All	All	1.21	18/8774 (0.2%)	1.08	28/11833 (0.2%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	125	SER	CB-OG	-8.70	1.30	1.42
1	B	125	SER	CB-OG	-8.35	1.31	1.42
1	E	49	GLU	CD-OE2	6.77	1.33	1.25
1	E	94	GLU	CD-OE1	6.38	1.32	1.25
1	D	130	GLU	CD-OE1	6.29	1.32	1.25
1	B	130	GLU	CD-OE1	6.28	1.32	1.25
1	E	125	SER	CB-OG	-5.88	1.34	1.42
1	C	130	GLU	CD-OE1	5.85	1.32	1.25
1	D	96	LEU	C-O	5.49	1.33	1.23
1	B	81	SER	CB-OG	5.45	1.49	1.42
1	A	114	TYR	CB-CG	-5.43	1.43	1.51
1	F	5	GLU	CD-OE2	-5.23	1.20	1.25
1	D	12[A]	GLU	CD-OE1	5.21	1.31	1.25
1	D	12[B]	GLU	CD-OE1	5.21	1.31	1.25
1	C	157	GLU	CD-OE2	-5.18	1.20	1.25
1	B	17	GLU	CD-OE2	5.02	1.31	1.25
1	B	24	TYR	CZ-OH	5.01	1.46	1.37
1	C	8	GLU	CG-CD	5.00	1.59	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	44	ARG	NE-CZ-NH2	12.58	126.59	120.30
1	A	44	ARG	NE-CZ-NH2	10.35	125.47	120.30
1	D	44	ARG	NE-CZ-NH2	10.21	125.40	120.30
1	A	69	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	D	59	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	D	12[A]	GLU	CG-CD-OE2	-7.74	102.82	118.30
1	D	12[B]	GLU	CG-CD-OE2	-7.74	102.82	118.30
1	A	17	GLU	OE1-CD-OE2	-7.11	114.77	123.30
1	E	69[A]	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	E	69[B]	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	D	12[A]	GLU	CG-CD-OE1	6.54	131.37	118.30
1	D	12[B]	GLU	CG-CD-OE1	6.54	131.37	118.30
1	D	44	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	D	56	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	D	45	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	B	44	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	D	59	ASP	CB-CG-OD1	6.01	123.71	118.30
1	E	44	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	A	44	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	D	44	ARG	CA-CB-CG	5.74	126.02	113.40
1	E	59	ASP	CB-CG-OD1	5.50	123.25	118.30
1	C	56	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	E	23	LEU	CB-CG-CD1	5.23	119.90	111.00
1	D	63	ASP	CB-CG-OD1	5.23	123.01	118.30
1	E	125	SER	N-CA-CB	5.17	118.26	110.50
1	B	17	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	B	60	TYR	CD1-CE1-CZ	-5.05	115.26	119.80
1	B	59	ASP	CB-CG-OD2	-5.02	113.78	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1426	0	1355	29	0
1	B	1417	0	1339	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1414	0	1346	15	0
1	D	1461	0	1390	21	0
1	E	1454	0	1379	20	0
1	F	1411	0	1336	10	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	E	3	0	0	2	0
3	A	2	0	0	1	0
3	B	2	0	0	1	0
3	C	1	0	0	0	0
3	D	1	0	0	1	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
4	A	12	0	16	11	0
4	B	12	0	15	0	0
4	C	30	0	39	9	0
4	D	12	0	16	2	0
4	E	12	0	15	2	0
4	F	6	0	8	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	F	2	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
7	C	2	0	0	0	0
8	D	2	0	0	0	0
9	F	2	0	0	1	0
10	A	151	0	0	8	0
10	B	153	0	0	9	1
10	C	140	0	0	3	1
10	D	141	0	0	4	0
10	E	153	0	0	15	0
10	F	145	0	0	5	2
All	All	9581	0	8254	111	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (111) 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)
9:F:203:O:O	9:F:204:O:O	1.63	1.16
1:E:37:GLU:OE1	10:E:302:HOH:O	1.69	1.11
4:C:205:GOL:H32	1:D:51:MET:HE1	1.20	1.11
2:E:201:FEO:FE2	10:E:303:HOH:O	1.06	1.07
1:C:37:GLU:OE1	10:C:302:HOH:O	1.73	1.05
1:E:130:GLU:OE2	10:E:303:HOH:O	1.75	1.04
2:E:201:FEO:O	10:E:303:HOH:O	1.76	1.02
4:C:205:GOL:H32	1:D:51:MET:CE	1.91	0.99
1:B:44:ARG:HD3	10:B:346:HOH:O	1.63	0.98
3:D:204:OH:O	10:D:301:HOH:O	1.84	0.96
1:E:53:HIS:CB	10:E:301:HOH:O	2.25	0.82
1:F:37:GLU:OE1	10:F:302:HOH:O	1.99	0.80
1:B:8:GLU:OE1	10:B:302:HOH:O	2.00	0.80
1:A:97:ILE:HD13	3:A:203:OH:O	1.81	0.79
1:A:15:ASN:O	4:A:204:GOL:H11	1.82	0.79
1:E:50:GLU:OE2	10:E:303:HOH:O	1.98	0.79
1:A:73:VAL:HA	4:A:204:GOL:H31	1.66	0.77
1:A:94:GLU:OE1	10:A:301:HOH:O	2.01	0.77
1:A:147:SER:OG	1:A:149[B]:GLU:OE1	2.03	0.76
1:E:84[B]:ASP:OD1	10:E:304:HOH:O	2.04	0.75
1:C:12:GLU:OE2	10:C:303:HOH:O	2.05	0.74
1:E:53:HIS:CG	10:E:301:HOH:O	2.36	0.73
4:C:208:GOL:O2	10:C:304:HOH:O	2.07	0.73
4:C:205:GOL:C3	1:D:51:MET:CE	2.66	0.73
1:A:8:GLU:OE1	10:A:302:HOH:O	2.08	0.72
1:B:37:GLU:OE1	10:B:303:HOH:O	2.08	0.71
1:D:156:LYS:HE3	10:D:315:HOH:O	1.90	0.69
1:A:147:SER:OG	1:A:149[B]:GLU:CD	2.32	0.68
1:C:25:GLN:HE22	1:D:55[B]:GLN:HE22	1.42	0.68
4:A:204:GOL:H2	10:A:305:HOH:O	1.95	0.66
1:E:139:ASP:OD2	10:E:305:HOH:O	2.14	0.66
4:A:204:GOL:C2	10:A:305:HOH:O	2.42	0.66
1:B:93:HIS:NE2	10:B:305:HOH:O	2.18	0.65
1:E:69[A]:ARG:NH1	4:E:204:GOL:O3	2.28	0.65
1:A:147:SER:HG	1:A:149[B]:GLU:CD	2.00	0.64
1:C:44:ARG:NE	4:C:208:GOL:O3	2.26	0.64
1:E:8:GLU:OE1	10:E:306:HOH:O	2.14	0.63
1:C:44:ARG:HE	4:C:208:GOL:HO3	1.46	0.63
1:F:163:THR:C	10:F:337:HOH:O	2.36	0.63
4:A:204:GOL:H12	10:A:309:HOH:O	1.99	0.62
1:C:55[A]:GLN:OE1	1:D:44:ARG:HD2	2.01	0.60
1:E:144:ALA:O	1:E:150:GLY:HA3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149[B]:GLU:HG3	1:D:149:GLU:OE1	2.01	0.60
1:B:51:MET:HE2	10:E:399:HOH:O	2.01	0.60
1:B:84[A]:ASP:OD2	10:B:304:HOH:O	2.16	0.59
1:C:51:MET:O	1:C:55[B]:GLN:HG3	2.04	0.58
1:A:149[B]:GLU:CG	1:D:149:GLU:OE1	2.52	0.58
1:A:147:SER:CB	1:A:149[B]:GLU:OE1	2.51	0.57
1:A:144:ALA:HB3	1:A:154:ILE:HD11	1.85	0.57
1:C:144:ALA:O	1:C:150:GLY:HA3	2.03	0.57
1:F:144:ALA:HB3	1:F:154:ILE:HD11	1.86	0.57
1:C:44:ARG:HH21	4:C:208:GOL:H32	1.69	0.56
1:B:44:ARG:CG	10:B:346:HOH:O	2.53	0.55
1:D:144:ALA:O	1:D:150:GLY:HA3	2.07	0.55
4:A:205:GOL:O1	10:A:303:HOH:O	2.18	0.55
1:A:12:GLU:OE1	10:A:304:HOH:O	2.18	0.54
1:E:53:HIS:HB3	10:E:301:HOH:O	1.98	0.54
1:F:144:ALA:O	1:F:150:GLY:HA3	2.08	0.54
4:C:205:GOL:C3	1:D:51:MET:HE2	2.37	0.53
1:E:9:LYS:HE2	10:E:420:HOH:O	2.08	0.53
1:B:44:ARG:CD	10:B:346:HOH:O	2.37	0.53
1:C:48[A]:GLN:HG2	4:C:205:GOL:O1	2.10	0.52
1:D:156:LYS:CE	10:D:315:HOH:O	2.55	0.52
1:B:3:LYS:NZ	10:B:307:HOH:O	2.34	0.52
1:A:19:TYR:HB2	4:A:204:GOL:C1	2.41	0.51
1:B:144:ALA:O	1:B:150:GLY:HA3	2.11	0.51
1:D:2:LEU:N	10:D:314:HOH:O	2.44	0.50
1:A:144:ALA:O	1:A:150:GLY:HA3	2.12	0.50
1:A:147:SER:HB2	1:A:149[B]:GLU:OE1	2.11	0.49
1:B:29:ALA:HB2	1:E:58:PHE:CZ	2.47	0.49
1:B:135:LYS:NZ	10:B:308:HOH:O	2.35	0.49
1:A:73:VAL:HG22	10:A:339:HOH:O	2.12	0.49
1:E:88:GLN:N	1:E:138[B]:ILE:HD11	2.28	0.49
1:D:54[B]:MET:SD	1:D:54[B]:MET:C	2.91	0.48
1:C:25:GLN:NE2	1:D:55[B]:GLN:HE22	2.11	0.48
1:A:15:ASN:O	4:A:204:GOL:C1	2.58	0.47
1:C:54[B]:MET:C	1:C:54[B]:MET:SD	2.93	0.47
1:E:22:LEU:HD12	1:E:73:VAL:HG11	1.95	0.47
1:F:99[A]:GLN:NE2	10:F:312:HOH:O	2.48	0.47
1:C:25:GLN:HE22	1:D:55[B]:GLN:NE2	2.09	0.47
1:C:58:PHE:CZ	1:D:29:ALA:HB2	2.51	0.46
1:D:144:ALA:HB3	1:D:154[A]:ILE:HD11	1.97	0.46
1:A:149[B]:GLU:HG2	1:A:150:GLY:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LEU:HD12	1:B:73:VAL:HG11	1.99	0.45
1:D:114:TYR:N	1:D:115:PRO:CD	2.80	0.45
4:E:203:GOL:H32	10:E:306:HOH:O	2.17	0.44
1:F:74:GLU:OE2	10:F:303:HOH:O	2.21	0.44
1:A:73:VAL:HG13	4:A:204:GOL:O1	2.17	0.44
1:C:22:LEU:HD12	1:C:73:VAL:HG11	1.99	0.44
1:F:0:HIS:NE2	10:F:305:HOH:O	2.34	0.44
1:B:114:TYR:N	1:B:115:PRO:CD	2.81	0.43
1:A:74:GLU:HG3	4:A:204:GOL:O3	2.18	0.43
1:E:138[B]:ILE:HG23	10:E:307:HOH:O	2.18	0.43
1:D:99[A]:GLN:NE2	4:D:205:GOL:O1	2.43	0.43
1:F:114:TYR:N	1:F:115:PRO:CD	2.82	0.43
1:B:84[A]:ASP:O	1:B:88:GLN:HG2	2.18	0.43
1:D:99[A]:GLN:HE22	4:D:205:GOL:HO1	1.65	0.43
1:A:153:PHE:CD2	1:D:153:PHE:HZ	2.37	0.42
1:A:29:ALA:HB2	1:F:58:PHE:CZ	2.54	0.42
1:A:90[B]:THR:HG23	1:A:134:PHE:CD1	2.55	0.42
1:A:55[B]:GLN:NE2	1:A:59:ASP:OD1	2.35	0.42
1:B:58:PHE:CZ	1:E:29:ALA:HB2	2.55	0.42
1:F:99[B]:GLN:O	1:F:99[B]:GLN:HG3	2.19	0.42
1:B:67:LEU:HD21	1:E:77[A]:PHE:CZ	2.56	0.41
1:E:154[B]:ILE:HD13	1:E:154[B]:ILE:HA	1.80	0.41
1:E:14[B]:MET:C	1:E:14[B]:MET:SD	2.99	0.41
1:B:97:ILE:HD13	3:B:203:OH:O	2.21	0.41
1:A:22:LEU:HD12	1:A:73:VAL:HG11	2.03	0.40
1:A:27:MET:SD	1:A:90[A]:THR:HG22	2.61	0.40
1:A:15:ASN:HB3	4:A:204:GOL:H12	2.03	0.40
1:A:87:PHE:O	1:A:90[B]:THR:HG22	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:395:HOH:O	10:F:324:HOH:O[3_755]	2.13	0.07
10:B:343:HOH:O	10:F:392:HOH:O[6_775]	2.17	0.03

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	171/166 (103%)	168 (98%)	3 (2%)	0	100	100
1	B	169/166 (102%)	164 (97%)	5 (3%)	0	100	100
1	C	169/166 (102%)	167 (99%)	2 (1%)	0	100	100
1	D	174/166 (105%)	170 (98%)	4 (2%)	0	100	100
1	E	174/166 (105%)	171 (98%)	3 (2%)	0	100	100
1	F	168/166 (101%)	168 (100%)	0	0	100	100
All	All	1025/996 (103%)	1008 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	157/150 (105%)	157 (100%)	0	100	100
1	B	155/150 (103%)	153 (99%)	2 (1%)	76	65
1	C	155/150 (103%)	153 (99%)	2 (1%)	76	65
1	D	160/150 (107%)	157 (98%)	3 (2%)	65	50
1	E	159/150 (106%)	159 (100%)	0	100	100
1	F	154/150 (103%)	153 (99%)	1 (1%)	90	87
All	All	940/900 (104%)	932 (99%)	8 (1%)	86	78

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	85	GLU
1	B	104	LEU
1	C	2	LEU
1	C	35	THR
1	D	12[A]	GLU
1	D	12[B]	GLU
1	D	163	THR
1	F	104	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	112	GLN
1	C	127	GLN
1	F	34	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 9 are monoatomic and 9 are modelled with single atom - leaving 19 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	FEO	A	201	1,10,3	0,2,2	0.00	-	0,1,1	0.00	-
4	GOL	A	204	-	5,5,5	0.68	0	5,5,5	0.96	0
4	GOL	A	205	-	5,5,5	0.55	0	5,5,5	0.92	0
2	FEO	B	201	1,10,3	0,2,2	0.00	-	0,1,1	0.00	-
4	GOL	B	204	-	5,5,5	1.17	0	5,5,5	1.49	1 (20%)
4	GOL	B	205	-	5,5,5	0.60	0	5,5,5	0.68	0
7	OXY	C	203	5,6	1,1,1	0.27	0	0,0,0	0.00	-
4	GOL	C	205	-	5,5,5	0.91	0	5,5,5	1.43	0
4	GOL	C	206	-	5,5,5	0.51	0	5,5,5	1.21	0
4	GOL	C	207	-	5,5,5	0.29	0	5,5,5	0.64	0
4	GOL	C	208	-	5,5,5	0.31	0	5,5,5	0.64	0
4	GOL	C	209	-	5,5,5	0.33	0	5,5,5	0.57	0
8	PER	D	203	5	0,1,1	0.00	-	0,0,0	0.00	-
4	GOL	D	205	-	5,5,5	0.70	0	5,5,5	1.10	1 (20%)
4	GOL	D	206	-	5,5,5	0.22	0	5,5,5	0.81	0
2	FEO	E	201	1,3	0,2,2	0.00	-	0,1,1	0.00	-
4	GOL	E	203	-	5,5,5	0.30	0	5,5,5	0.86	0
4	GOL	E	204	-	5,5,5	2.76	2 (40%)	5,5,5	1.92	2 (40%)
4	GOL	F	207	-	5,5,5	1.18	1 (20%)	5,5,5	0.98	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	FEO	A	201	1,10,3	-	0/0/0/0	0/0/0/0
4	GOL	A	204	-	-	0/4/4/4	0/0/0/0
4	GOL	A	205	-	-	0/4/4/4	0/0/0/0
2	FEO	B	201	1,10,3	-	0/0/0/0	0/0/0/0
4	GOL	B	204	-	-	0/4/4/4	0/0/0/0
4	GOL	B	205	-	-	0/4/4/4	0/0/0/0
7	OXY	C	203	5,6	-	0/0/0/0	0/0/0/0
4	GOL	C	205	-	-	0/4/4/4	0/0/0/0
4	GOL	C	206	-	-	0/4/4/4	0/0/0/0
4	GOL	C	207	-	-	0/4/4/4	0/0/0/0
4	GOL	C	208	-	-	0/4/4/4	0/0/0/0
4	GOL	C	209	-	-	0/4/4/4	0/0/0/0
8	PER	D	203	5	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	205	-	-	0/4/4/4	0/0/0/0
4	GOL	D	206	-	-	0/4/4/4	0/0/0/0
2	FEO	E	201	1,3	-	0/0/0/0	0/0/0/0
4	GOL	E	203	-	-	0/4/4/4	0/0/0/0
4	GOL	E	204	-	-	0/4/4/4	0/0/0/0
4	GOL	F	207	-	-	0/4/4/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	204	GOL	O2-C2	-5.70	1.26	1.43
4	E	204	GOL	C1-C2	-2.00	1.44	1.52
4	F	207	GOL	O2-C2	2.50	1.50	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	204	GOL	O2-C2-C1	-3.09	93.62	108.47
4	B	204	GOL	O3-C3-C2	-2.55	97.06	109.97
4	D	205	GOL	O1-C1-C2	-2.04	99.62	109.97
4	E	204	GOL	O1-C1-C2	-2.02	99.76	109.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	204	GOL	10	0
4	A	205	GOL	1	0
4	C	205	GOL	5	0
4	C	208	GOL	4	0
4	D	205	GOL	2	0
2	E	201	FEO	2	0
4	E	203	GOL	1	0
4	E	204	GOL	1	0

5.7 Other polymers ⓘ

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, 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	162/166 (97%)	-0.03	3 (1%) 70 67	19, 25, 40, 58	0
1	B	164/166 (98%)	-0.15	6 (3%) 45 41	17, 24, 38, 55	1 (0%)
1	C	162/166 (97%)	-0.07	3 (1%) 70 67	18, 26, 39, 53	1 (0%)
1	D	162/166 (97%)	-0.09	3 (1%) 70 67	18, 26, 40, 55	1 (0%)
1	E	163/166 (98%)	-0.07	3 (1%) 71 69	17, 25, 40, 55	2 (1%)
1	F	164/166 (98%)	-0.14	6 (3%) 45 41	17, 24, 42, 59	1 (0%)
All	All	977/996 (98%)	-0.09	24 (2%) 61 57	17, 25, 41, 59	6 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	163	THR	4.7
1	F	0	HIS	4.4
1	D	163	THR	3.9
1	C	163	THR	3.7
1	F	146	LYS	3.6
1	B	0	HIS	3.5
1	B	163	THR	3.5
1	E	1	HIS	3.3
1	F	163	THR	3.2
1	D	146	LYS	2.9
1	F	142	SER	2.8
1	B	146	LYS	2.8
1	A	163	THR	2.7
1	C	146	LYS	2.7
1	C	43	LEU	2.7
1	A	146	LYS	2.4
1	B	43	LEU	2.4
1	E	146	LYS	2.4
1	F	1	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	147	SER	2.2
1	B	1	HIS	2.1
1	B	160	THR	2.1
1	A	4	PRO	2.1
1	D	160	THR	2.1

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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	OH	B	203	1/1	0.96	0.24	10.83	26,26,26,26	1
3	OH	A	203	1/1	1.00	0.24	5.83	19,19,19,19	1
4	GOL	A	204	6/6	0.96	0.26	5.38	35,39,40,57	6
4	GOL	E	203	6/6	0.88	0.22	5.26	42,43,47,53	6
3	OH	F	206	1/1	1.00	0.15	4.68	27,27,27,27	1
9	O	F	204	1/1	0.93	0.22	4.38	39,39,39,39	1
4	GOL	E	204	6/6	0.94	0.21	4.33	26,27,46,47	6
8	PER	D	203	2/2	0.99	0.16	3.48	10,10,10,17	2
3	OH	B	202	1/1	0.98	0.13	2.98	17,17,17,17	0
3	OH	E	202	1/1	0.99	0.16	2.77	16,16,16,16	0
4	GOL	C	206	6/6	0.92	0.20	2.67	44,45,50,51	6
4	GOL	C	207	6/6	0.90	0.13	2.58	41,48,53,54	6
3	OH	C	204	1/1	0.94	0.13	2.48	22,22,22,22	0
4	GOL	C	205	6/6	0.93	0.18	1.98	28,31,36,38	6
4	GOL	D	205	6/6	0.92	0.18	1.90	32,47,54,67	6
3	OH	F	205	1/1	0.95	0.14	1.71	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	OH	D	204	1/1	0.98	0.13	1.49	22,22,22,22	0
3	OH	A	202	1/1	0.97	0.12	1.47	16,16,16,16	0
4	GOL	B	205	6/6	0.90	0.18	0.74	36,42,49,59	6
4	GOL	A	205	6/6	0.93	0.14	0.68	33,42,45,54	6
4	GOL	B	204	6/6	0.94	0.13	0.54	23,26,30,31	6
7	OXY	C	203	2/2	0.99	0.09	0.50	10,10,10,18	2
4	GOL	D	206	6/6	0.78	0.19	0.49	39,49,52,63	6
9	O	F	203	1/1	1.00	0.10	0.16	21,21,21,21	0
4	GOL	F	207	6/6	0.96	0.09	-0.34	23,26,28,30	6
5	FE	C	201	1/1	1.00	0.07	-0.61	17,17,17,17	0
5	FE	F	202	1/1	1.00	0.07	-0.75	16,16,16,16	0
5	FE	D	201	1/1	1.00	0.07	-0.77	17,17,17,17	0
5	FE	D	202	1/1	1.00	0.07	-0.90	20,20,20,20	0
2	FEO	B	201	3/3	1.00	0.07	-0.95	15,15,17,17	0
2	FEO	A	201	3/3	1.00	0.07	-0.95	17,17,17,18	0
5	FE	F	201	1/1	1.00	0.07	-1.12	18,18,18,18	0
6	FE2	C	202	1/1	1.00	0.06	-1.56	18,18,18,18	0
2	FEO	E	201	3/3	1.00	0.07	-1.59	16,16,18,18	0
4	GOL	C	209	6/6	0.82	0.24	-	27,44,49,55	6
6	FE2	E	205	1/1	0.99	0.66	-	500,500,500,500	1
4	GOL	C	208	6/6	0.85	0.25	-	28,51,56,57	6

6.5 Other polymers

There are no such residues in this entry.