Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:28 PM GMT

PDB ID	:	4F4D
Title	:	F337R variant of human ferrochelatase
Authors	:	Lanzilotta, W.N.; Medlock, A.E.; Dailey, T.E.; Dailey, H.A.
Deposited on	:	2012-05-10
Resolution	:	1.80 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:

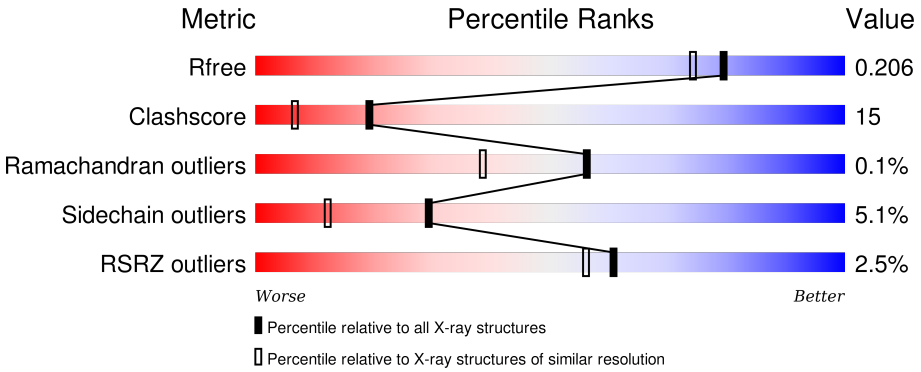
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	359	3% 77% 18%
1	B	359	3% 75% 20%

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
3	GOL	A	502[A]	-	-	-	X
3	GOL	A	502[B]	-	-	-	X
5	CHD	A	505	-	-	-	X
5	CHD	A	506	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6787 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 Ferrochelatase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	17	0
			2982	1904	516	544	18			
1	B	359	Total	C	N	O	S	0	22	0
			3005	1921	519	543	22			

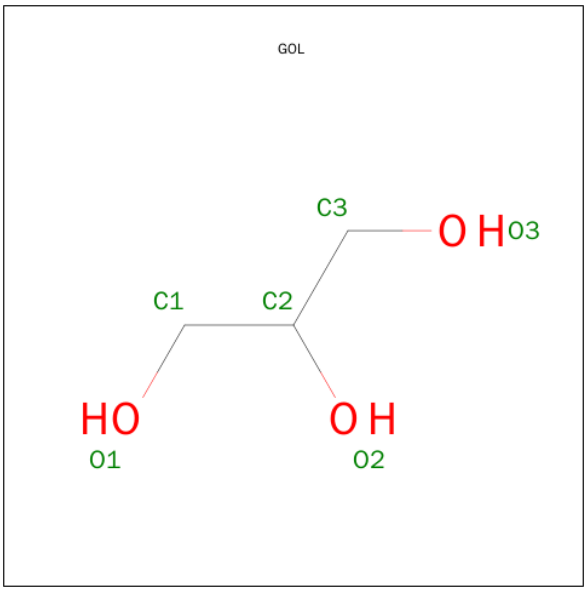
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	337	ARG	PHE	ENGINEERED MUTATION	UNP P22830
B	337	ARG	PHE	ENGINEERED MUTATION	UNP P22830

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

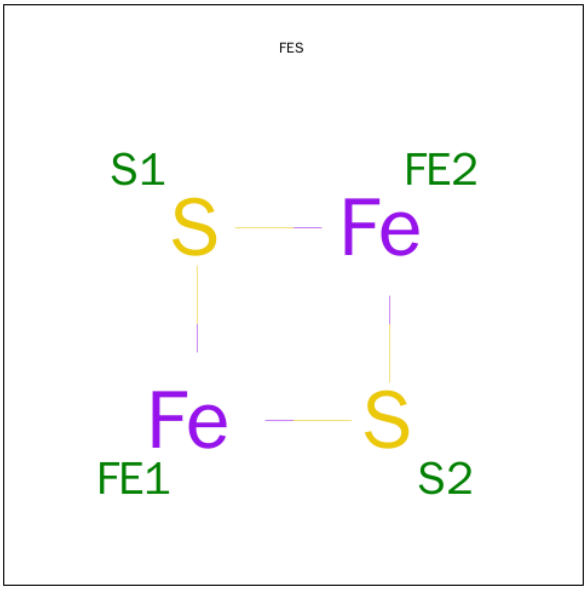
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



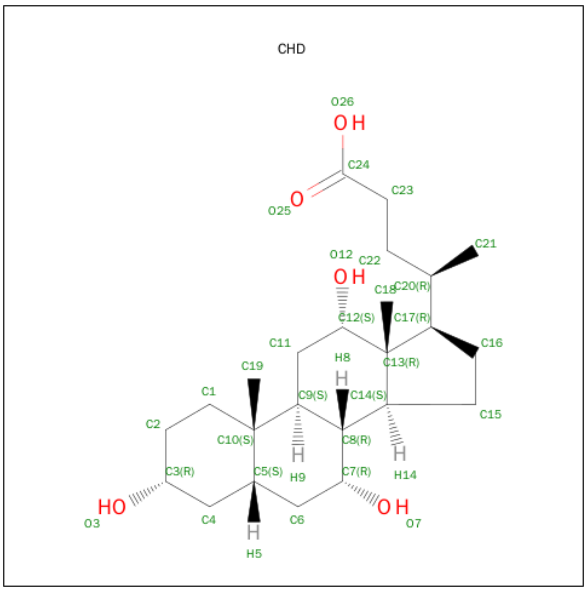
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			12	6	6		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 29 24 5	0	0
5	A	1	Total C O 29 24 5	0	0
5	A	1	Total C O 29 24 5	0	0
5	B	1	Total C O 29 24 5	0	0
5	B	1	Total C O 29 24 5	0	0
5	B	1	Total C O 29 24 5	0	0

- Molecule 6 is water.

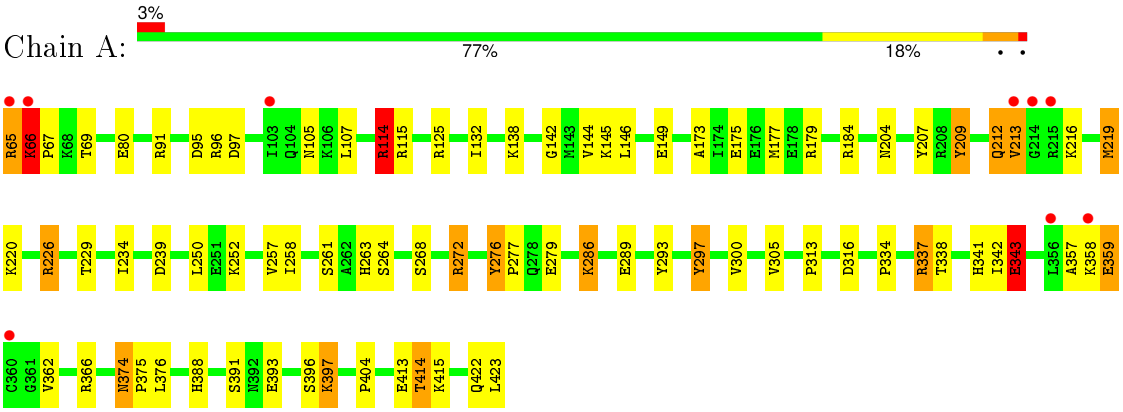
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	324	Total O 324 324	0	0
6	B	280	Total O 280 280	0	0

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.

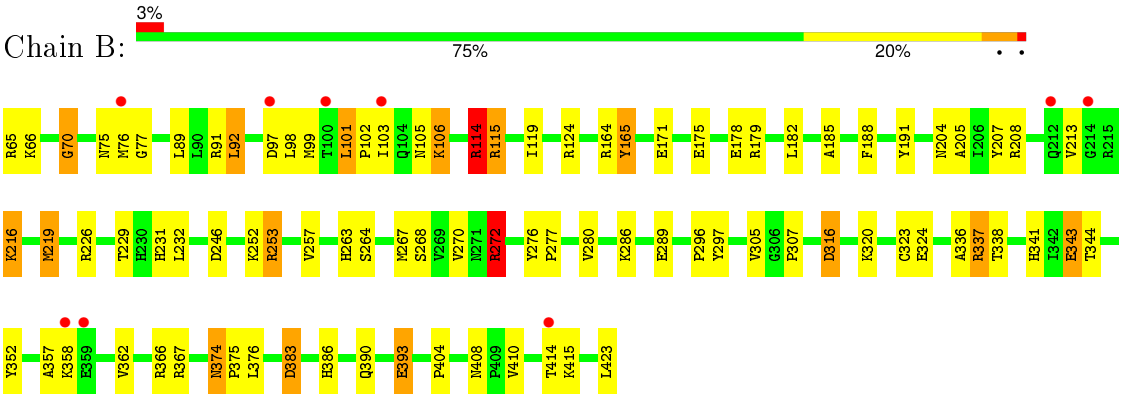
- Molecule 1: Ferrochelatase, mitochondrial

Chain A:



- Molecule 1: Ferrochelatase, mitochondrial

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.21Å 93.51Å 111.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.80 42.18 – 1.79	Depositor EDS
% Data completeness (in resolution range)	100.0 ((Not available)-1.80) 99.3 (42.18-1.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.177 , 0.207 0.176 , 0.206	Depositor DCC
R_{free} test set	4399 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	19.6	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	3 of 87466 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6787	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.86 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6578e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GOL, CHD, FES, CL

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	1.44	13/3103 (0.4%)	1.26	21/4197 (0.5%)
1	B	1.44	16/3143 (0.5%)	1.28	30/4253 (0.7%)
All	All	1.44	29/6246 (0.5%)	1.27	51/8450 (0.6%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	LYS	N-CA	9.02	1.64	1.46
1	A	297	TYR	CD2-CE2	8.59	1.52	1.39
1	A	114	ARG	CG-CD	7.88	1.71	1.51
1	B	280	VAL	CB-CG2	7.04	1.67	1.52
1	B	297	TYR	CD2-CE2	6.96	1.49	1.39
1	A	209	TYR	CD1-CE1	6.62	1.49	1.39
1	B	393	GLU	CG-CD	6.53	1.61	1.51
1	A	144	VAL	CB-CG2	6.27	1.66	1.52
1	A	397	LYS	CD-CE	-6.23	1.35	1.51
1	A	366	ARG	CB-CG	5.86	1.68	1.52
1	B	343[A]	GLU	CD-OE2	5.79	1.32	1.25
1	B	343[B]	GLU	CD-OE2	5.79	1.32	1.25
1	A	257	VAL	CB-CG2	-5.70	1.40	1.52
1	A	91	ARG	CZ-NH1	5.63	1.40	1.33
1	B	171	GLU	CB-CG	5.57	1.62	1.52
1	B	178	GLU	CG-CD	-5.51	1.43	1.51
1	B	188	PHE	CD1-CE1	5.46	1.50	1.39
1	B	280	VAL	CB-CG1	5.43	1.64	1.52
1	B	343[A]	GLU	CB-CG	-5.43	1.41	1.52
1	B	343[B]	GLU	CB-CG	-5.43	1.41	1.52
1	A	276	TYR	CD2-CE2	5.42	1.47	1.39
1	B	165	TYR	CB-CG	5.35	1.59	1.51
1	A	261	SER	CA-CB	5.29	1.60	1.52
1	A	396	SER	CB-OG	5.20	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	165	TYR	CD2-CE2	5.20	1.47	1.39
1	B	70	GLY	N-CA	5.18	1.53	1.46
1	B	205	ALA	CA-CB	5.09	1.63	1.52
1	A	397	LYS	CE-NZ	5.06	1.61	1.49
1	B	114	ARG	CG-CD	5.06	1.64	1.51

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	226	ARG	NE-CZ-NH1	17.02	128.81	120.30
1	A	226	ARG	NE-CZ-NH1	12.95	126.77	120.30
1	B	226	ARG	NE-CZ-NH2	-10.29	115.15	120.30
1	B	92	LEU	CA-CB-CG	10.12	138.58	115.30
1	A	337	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	A	316	ASP	CB-CG-OD2	9.54	126.88	118.30
1	B	253[A]	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	B	253[B]	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	A	226	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	A	337	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	272[A]	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	A	272[B]	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	B	246	ASP	CB-CG-OD2	8.03	125.52	118.30
1	A	125	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	A	125	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	B	272[A]	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	272[B]	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	316	ASP	CB-CG-OD2	7.65	125.19	118.30
1	B	253[A]	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	B	253[B]	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	A	366	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	A	219	MET	CG-SD-CE	-7.22	88.64	100.20
1	A	91	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	B	343[A]	GLU	OE1-CD-OE2	6.31	130.87	123.30
1	B	343[B]	GLU	OE1-CD-OE2	6.31	130.87	123.30
1	B	343[A]	GLU	CG-CD-OE1	-6.20	105.89	118.30
1	B	343[B]	GLU	CG-CD-OE1	-6.20	105.89	118.30
1	B	91	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	367	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	316	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	A	66	LYS	C-N-CD	5.72	140.41	128.40
1	B	91	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	178	GLU	CA-CB-CG	-5.60	101.08	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	344	THR	CA-CB-CG2	-5.42	104.82	112.40
1	A	239	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	124	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	366	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	92	LEU	CB-CG-CD2	-5.37	101.87	111.00
1	A	297	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	A	97	ASP	CB-CA-C	5.24	120.87	110.40
1	B	164	ARG	CG-CD-NE	-5.22	100.83	111.80
1	B	383[A]	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	383[B]	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	92	LEU	CB-CG-CD1	5.08	119.64	111.00
1	A	286[A]	LYS	CD-CE-NZ	-5.06	100.06	111.70
1	A	286[B]	LYS	CD-CE-NZ	-5.06	100.06	111.70
1	A	114	ARG	CG-CD-NE	5.05	122.40	111.80
1	A	343[A]	GLU	CA-CB-CG	5.03	124.47	113.40
1	A	343[B]	GLU	CA-CB-CG	5.03	124.47	113.40
1	B	272[A]	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	B	272[B]	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	2982	0	3044	86	1
1	B	3005	0	3083	92	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	12	0	15	2	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	87	0	117	12	0
5	B	87	0	117	12	0
6	A	324	0	0	17	1
6	B	280	0	0	20	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6787	0	6376	189	5

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 15.

All (189) 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:A:65:ARG:CG	6:A:733:HOH:O	1.78	1.28
1:A:334[B]:PRO:HG3	6:A:816:HOH:O	1.45	1.17
1:A:65:ARG:HG2	6:A:733:HOH:O	1.35	1.12
5:B:505:CHD:H22	6:B:852:HOH:O	1.49	1.12
1:B:323[B]:CYS:SG	1:B:362[B]:VAL:HG12	1.93	1.08
1:A:204:ASN:ND2	1:A:414[A]:THR:HG21	1.69	1.07
1:A:204:ASN:HD22	1:A:414[B]:THR:HG21	1.14	1.06
1:A:204:ASN:HD22	1:A:414[A]:THR:HG21	0.95	1.06
1:A:334[B]:PRO:HG2	6:A:663:HOH:O	1.54	1.05
1:B:204:ASN:HD22	1:B:414:THR:HG21	1.25	1.01
1:A:286[A]:LYS:NZ	6:A:726:HOH:O	1.95	1.00
1:B:208:ARG:NH2	1:B:410[A]:VAL:HG21	1.83	0.92
1:A:96:ARG:HH22	1:A:105:ASN:ND2	1.66	0.92
1:B:272[A]:ARG:HD2	6:B:733:HOH:O	1.68	0.91
1:B:338:THR:HG21	6:B:802:HOH:O	1.70	0.90
1:B:76[A]:MET:HG2	1:B:191:TYR:OH	1.72	0.90
1:B:99:MET:CE	1:B:101:LEU:HD21	2.01	0.90
1:A:66:LYS:HD2	1:A:66:LYS:N	1.86	0.89
1:A:204:ASN:HD22	1:A:414[A]:THR:CG2	1.84	0.88
1:A:204:ASN:ND2	1:A:414[B]:THR:HG21	1.90	0.86
1:A:96:ARG:HH22	1:A:105:ASN:HD21	1.19	0.85
1:B:99:MET:HE3	1:B:101:LEU:HD21	1.59	0.84
1:A:338:THR:HG21	6:A:699:HOH:O	1.77	0.84
1:A:234:ILE:HG13	1:A:286[B]:LYS:HE3	1.59	0.83
1:B:267:MET:HA	1:B:270[B]:VAL:HG12	1.60	0.83
1:B:204:ASN:ND2	1:B:414:THR:HG21	1.92	0.83
1:A:305[A]:VAL:HG21	5:A:504:CHD:H161	1.62	0.81
1:B:76[C]:MET:HG2	1:B:191:TYR:OH	1.82	0.79
3:A:502[B]:GOL:H11	1:B:277:PRO:HB2	1.66	0.78
1:B:286:LYS:NZ	6:B:831:HOH:O	2.18	0.75
1:B:357:ALA:HB1	1:B:362[B]:VAL:HG21	1.67	0.75
1:A:204:ASN:ND2	1:A:414[A]:THR:CG2	2.47	0.75
1:A:142:GLY:HA2	1:A:145[B]:LYS:HD3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ARG:HH21	1:B:410[A]:VAL:HG21	1.49	0.74
1:B:323[B]:CYS:SG	1:B:362[B]:VAL:CG1	2.75	0.72
1:A:145[B]:LYS:HE2	1:A:146:LEU:HG	1.71	0.71
1:A:220:LYS:HG3	6:A:793:HOH:O	1.89	0.71
1:B:383[B]:ASP:OD2	6:B:683:HOH:O	2.08	0.70
1:B:76[C]:MET:HG2	1:B:191:TYR:HH	1.55	0.70
1:B:182:LEU:HD12	1:B:219[A]:MET:HE1	1.73	0.70
1:A:204:ASN:HA	1:A:414[B]:THR:HG21	1.73	0.70
1:A:65:ARG:HG3	6:A:733:HOH:O	1.63	0.70
5:A:504:CHD:O25	6:A:832:HOH:O	2.10	0.69
5:B:505:CHD:O3	6:B:812:HOH:O	2.12	0.68
1:A:341:HIS:CE1	1:A:343[A]:GLU:HG2	2.29	0.68
1:A:209:TYR:O	1:A:212[A]:GLN:HG3	1.93	0.68
1:A:341:HIS:ND1	1:A:343[A]:GLU:HG2	2.09	0.68
1:B:114:ARG:HH11	1:B:114:ARG:CG	2.08	0.67
1:B:175:GLU:HG2	1:B:179[B]:ARG:NH1	2.09	0.67
1:B:204:ASN:HA	1:B:414:THR:HG21	1.76	0.67
1:A:96:ARG:NH2	1:A:105:ASN:ND2	2.41	0.66
1:B:99:MET:HE2	1:B:101:LEU:HD21	1.78	0.66
1:A:66:LYS:HB2	1:A:67:PRO:HD2	1.78	0.66
5:B:505:CHD:C2	6:B:852:HOH:O	2.22	0.66
1:B:114:ARG:HG3	1:B:114:ARG:HH11	1.60	0.66
1:A:66:LYS:HD2	1:A:66:LYS:H	1.61	0.65
1:A:229:THR:HB	1:A:286[B]:LYS:HE2	1.77	0.65
1:A:357:ALA:HB1	1:A:362:VAL:HG11	1.77	0.65
1:B:75[A]:ASN:HD21	1:B:337[A]:ARG:HH22	1.43	0.65
1:B:103:ILE:HG23	1:B:106:LYS:HE2	1.78	0.64
1:B:115:ARG:NH1	5:B:505:CHD:O25	2.30	0.64
1:A:66:LYS:N	1:A:66:LYS:CD	2.61	0.64
1:A:277:PRO:HB2	3:A:502[A]:GOL:H31	1.79	0.64
1:B:76[B]:MET:HG3	1:B:165:TYR:HD1	1.63	0.64
1:A:337:ARG:HH11	1:A:343[B]:GLU:CD	2.02	0.63
1:B:374:ASN:HD22	1:B:376:LEU:H	1.47	0.63
1:B:374:ASN:ND2	1:B:376:LEU:H	1.97	0.62
1:B:76[C]:MET:HG2	6:B:761:HOH:O	1.98	0.62
1:B:182:LEU:HB2	1:B:219[A]:MET:HE3	1.80	0.62
1:B:341:HIS:ND1	1:B:343[B]:GLU:HG2	2.14	0.62
1:B:76[B]:MET:HG3	1:B:165:TYR:CD1	2.34	0.62
1:A:145[B]:LYS:HG2	1:A:146:LEU:N	2.15	0.62
1:A:337:ARG:NH1	1:A:343[B]:GLU:OE2	2.33	0.62
1:B:272[B]:ARG:HG2	6:B:774:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:505:CHD:H12	5:A:505:CHD:H212	1.84	0.60
1:B:103:ILE:O	1:B:103:ILE:HG22	2.02	0.59
1:A:374:ASN:ND2	1:A:376:LEU:H	2.01	0.59
1:A:80:GLU:HG3	6:A:817:HOH:O	2.03	0.58
1:A:138[A]:LYS:NZ	6:A:864:HOH:O	2.35	0.58
1:A:115:ARG:HD2	5:A:505:CHD:H222	1.85	0.58
1:B:320:LYS:HE2	1:B:324:GLU:OE2	2.03	0.58
1:A:114:ARG:HH11	1:A:114:ARG:CB	2.16	0.58
1:A:207:TYR:HB3	1:A:414[B]:THR:HG22	1.86	0.57
1:A:334[B]:PRO:CG	6:A:816:HOH:O	2.24	0.57
1:B:76[C]:MET:SD	6:B:761:HOH:O	2.58	0.56
1:B:98:LEU:HD11	5:B:505:CHD:H192	1.86	0.56
1:B:323[B]:CYS:HG	1:B:362[B]:VAL:HG12	1.69	0.56
1:A:374:ASN:HD22	1:A:375:PRO:N	2.05	0.55
1:B:75[A]:ASN:ND2	1:B:337[A]:ARG:HH22	2.04	0.55
1:B:267:MET:SD	1:B:270[B]:VAL:HG11	2.47	0.55
1:B:182:LEU:HB2	1:B:219[A]:MET:CE	2.36	0.55
1:A:250:LEU:HD12	6:A:767:HOH:O	2.07	0.54
1:A:391:SER:OG	1:A:393[B]:GLU:HG2	2.07	0.54
1:A:69:THR:HG23	1:A:184:ARG:HG2	1.90	0.54
1:A:175:GLU:HG2	1:A:179[A]:ARG:NH1	2.22	0.54
1:A:115:ARG:NH1	5:A:504:CHD:H221	2.23	0.54
1:A:115:ARG:NH1	5:A:504:CHD:C22	2.71	0.53
1:B:357:ALA:HB1	1:B:362[B]:VAL:CG2	2.37	0.53
1:B:89:LEU:HD11	1:B:119[A]:ILE:HD12	1.90	0.53
1:A:220:LYS:CG	6:A:793:HOH:O	2.53	0.53
1:B:305:VAL:HG21	5:B:505:CHD:H161	1.91	0.53
1:B:337[A]:ARG:NH2	6:B:770:HOH:O	2.42	0.52
1:B:257[A]:VAL:HG12	1:B:296:PRO:HG2	1.91	0.52
1:A:422:GLN:HG2	1:A:423:LEU:HG	1.91	0.52
1:A:268:SER:O	1:A:272[B]:ARG:HG3	2.08	0.52
1:A:145[B]:LYS:HG2	1:A:146:LEU:H	1.75	0.52
1:B:267:MET:CE	1:B:270[B]:VAL:HG11	2.40	0.51
1:A:204:ASN:HA	1:A:414[A]:THR:HG21	1.92	0.51
1:A:357:ALA:HB1	1:A:362:VAL:CG1	2.41	0.51
1:A:374:ASN:HD22	1:A:374:ASN:C	2.14	0.50
1:B:374:ASN:C	1:B:374:ASN:HD22	2.15	0.50
1:B:268:SER:O	1:B:272[B]:ARG:HG3	2.11	0.50
1:A:374:ASN:HD22	1:A:376:LEU:H	1.58	0.50
1:B:207:TYR:HB3	1:B:414:THR:HG22	1.93	0.49
1:B:263:HIS:HD2	1:B:264:SER:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:HIS:CE1	1:B:343[B]:GLU:HG2	2.47	0.49
1:B:305:VAL:HG11	5:B:505:CHD:H232	1.94	0.49
1:B:89:LEU:HD21	1:B:119[A]:ILE:CD1	2.43	0.49
1:B:253[A]:ARG:NH1	6:B:678:HOH:O	2.46	0.49
1:B:263:HIS:HE1	6:B:795:HOH:O	1.95	0.49
1:A:114:ARG:CB	1:A:114:ARG:NH1	2.75	0.48
1:B:75[B]:ASN:ND2	1:B:77:GLY:H	2.11	0.48
1:B:97[B]:ASP:HB2	1:B:408:ASN:HD21	1.78	0.48
1:B:374:ASN:HD22	1:B:375:PRO:N	2.12	0.48
1:A:263:HIS:HD2	1:A:264:SER:O	1.96	0.48
1:B:216:LYS:N	1:B:216:LYS:HD2	2.28	0.48
1:B:76[C]:MET:HG3	1:B:77:GLY:H	1.79	0.48
1:B:76[C]:MET:CE	6:B:761:HOH:O	2.61	0.47
1:A:66:LYS:HB2	1:A:67:PRO:CD	2.40	0.47
1:B:415:LYS:HD3	6:B:718:HOH:O	2.13	0.47
1:B:204:ASN:HA	1:B:414:THR:CG2	2.44	0.47
1:A:263:HIS:HE1	6:A:691:HOH:O	1.98	0.47
1:B:97[B]:ASP:HB2	1:B:408:ASN:ND2	2.30	0.47
1:A:173:ALA:O	1:A:177:MET:HG3	2.14	0.47
1:A:142:GLY:O	1:A:145[B]:LYS:HG2	2.14	0.46
5:B:505:CHD:C23	5:B:505:CHD:H161	2.45	0.46
1:A:114:ARG:HH11	1:A:114:ARG:CG	2.29	0.46
1:B:76[C]:MET:HG3	1:B:77:GLY:N	2.30	0.46
1:B:103:ILE:CG2	1:B:103:ILE:O	2.63	0.46
1:A:204:ASN:HA	1:A:414[B]:THR:CG2	2.42	0.45
1:A:138[B]:LYS:HG3	6:A:751:HOH:O	2.16	0.45
1:A:212[A]:GLN:HG3	1:A:213:VAL:H	1.81	0.45
5:B:505:CHD:H231	5:B:505:CHD:H17	1.59	0.45
1:B:307:PRO:HD2	6:B:740:HOH:O	2.15	0.45
1:B:336:ALA:C	1:B:337[A]:ARG:HG2	2.37	0.45
1:B:393:GLU:CD	6:B:666:HOH:O	2.55	0.45
1:A:341:HIS:CE1	1:A:342:ILE:HG22	2.52	0.45
1:A:226:ARG:HD3	1:A:279:GLU:OE2	2.17	0.45
1:A:96:ARG:NH2	1:A:105:ASN:HD21	1.99	0.45
1:B:92:LEU:HD13	1:B:165:TYR:CD1	2.52	0.45
1:B:229[A]:THR:HG23	1:B:286:LYS:HG3	1.98	0.45
1:A:289[A]:GLU:HG2	1:A:293:TYR:OH	2.16	0.45
1:B:101:LEU:HA	1:B:102:PRO:HD2	1.82	0.44
1:B:185:ALA:HB2	1:B:219[A]:MET:HE2	1.99	0.44
5:A:505:CHD:H193	5:A:505:CHD:H111	1.80	0.44
1:B:410[A]:VAL:HG12	1:B:414:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:GLU:O	1:A:359:GLU:HG3	2.16	0.44
1:A:142:GLY:O	1:A:145[B]:LYS:HE2	2.18	0.44
1:A:212[A]:GLN:HG3	1:A:213:VAL:N	2.33	0.44
1:A:115:ARG:HH11	5:A:504:CHD:H222	1.83	0.44
1:B:229[A]:THR:HG22	6:B:659:HOH:O	2.17	0.44
1:B:289[A]:GLU:OE2	6:B:756:HOH:O	2.21	0.43
5:B:504:CHD:H212	5:B:504:CHD:H12	2.00	0.43
1:A:145[B]:LYS:CG	1:A:146:LEU:N	2.82	0.43
1:B:98:LEU:HD21	5:B:505:CHD:C19	2.48	0.43
1:B:231:HIS:CE1	1:B:232:LEU:HG	2.54	0.43
1:A:305[B]:VAL:HG21	5:A:504:CHD:H232	2.00	0.43
1:B:386:HIS:O	1:B:390:GLN:HG3	2.18	0.43
5:A:504:CHD:H17	5:A:504:CHD:H231	1.57	0.42
1:A:300:VAL:HG12	1:A:313:PRO:HG2	2.02	0.42
1:B:70:GLY:HA3	1:B:182:LEU:HD13	2.00	0.42
1:B:337[A]:ARG:HD2	6:B:742:HOH:O	2.19	0.42
1:B:219[A]:MET:HE3	1:B:219[A]:MET:HB3	1.75	0.42
1:B:316:ASP:HB3	1:B:352:TYR:CE1	2.55	0.42
1:B:98:LEU:HD21	5:B:505:CHD:H193	2.01	0.42
1:B:99:MET:HE3	1:B:101:LEU:CD2	2.40	0.42
1:A:115:ARG:NH1	5:A:504:CHD:H222	2.35	0.42
1:A:95:ASP:OD1	1:A:95:ASP:C	2.58	0.42
1:A:207:TYR:CZ	1:A:413[A]:GLU:HB3	2.54	0.41
1:B:276:TYR:HB3	1:B:277:PRO:HD3	2.02	0.41
1:A:388:HIS:ND1	1:A:393[B]:GLU:HG3	2.35	0.41
5:A:505:CHD:H213	6:A:771:HOH:O	2.20	0.41
1:A:258:ILE:O	1:A:297:TYR:HA	2.20	0.41
1:A:276:TYR:HB3	1:A:277:PRO:HD3	2.03	0.40
1:A:132:ILE:HD11	1:A:341:HIS:CD2	2.56	0.40
1:A:107:LEU:HA	1:A:107:LEU:HD23	1.87	0.40

All (5) 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)
6:A:695:HOH:O	6:A:707:HOH:O[3_555]	1.56	0.64
1:A:149[B]:GLU:OE1	6:B:787:HOH:O[4_455]	1.90	0.30
6:B:718:HOH:O	6:B:724:HOH:O[3_655]	2.04	0.16
6:B:851:HOH:O	6:B:866:HOH:O[3_645]	2.05	0.15
6:B:719:HOH:O	6:B:723:HOH:O[3_655]	2.10	0.10

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	374/359 (104%)	364 (97%)	9 (2%)	1 (0%)	46 29
1	B	380/359 (106%)	372 (98%)	8 (2%)	0	100 100
All	All	754/718 (105%)	736 (98%)	17 (2%)	1 (0%)	56 38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	LYS

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	341/324 (105%)	322 (94%)	19 (6%)	26 10
1	B	347/324 (107%)	327 (94%)	20 (6%)	25 9
All	All	688/648 (106%)	649 (94%)	39 (6%)	29 10

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	66	LYS
1	A	114	ARG
1	A	212[A]	GLN
1	A	212[B]	GLN

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Mol	Chain	Res	Type
1	A	213	VAL
1	A	216	LYS
1	A	219	MET
1	A	252	LYS
1	A	343[A]	GLU
1	A	343[B]	GLU
1	A	358	LYS
1	A	359	GLU
1	A	374	ASN
1	A	397	LYS
1	A	404	PRO
1	A	414[A]	THR
1	A	414[B]	THR
1	A	415	LYS
1	B	65	ARG
1	B	66	LYS
1	B	101	LEU
1	B	105	ASN
1	B	106	LYS
1	B	114	ARG
1	B	115	ARG
1	B	213	VAL
1	B	216	LYS
1	B	219[A]	MET
1	B	219[B]	MET
1	B	252	LYS
1	B	272[A]	ARG
1	B	272[B]	ARG
1	B	337[A]	ARG
1	B	337[B]	ARG
1	B	358	LYS
1	B	374	ASN
1	B	404	PRO
1	B	423	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	153	ASN
1	A	204	ASN
1	A	231	HIS

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Mol	Chain	Res	Type
1	A	235	GLN
1	A	329	ASN
1	A	354	GLN
1	A	364	ASN
1	A	374	ASN
1	A	392	ASN
1	A	421	GLN
1	B	153	ASN
1	B	190	GLN
1	B	204	ASN
1	B	231	HIS
1	B	329	ASN
1	B	364	ASN
1	B	374	ASN
1	B	421	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 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\#\|Z\|>2$
3	GOL	A	502[A]	-	5,5,5	1.04	1 (20%)	5,5,5	2.49	1 (20%)
3	GOL	A	502[B]	-	5,5,5	0.62	0	5,5,5	1.64	2 (40%)
4	FES	A	503	1	0,4,4	0.00	-	0,4,4	0.00	-
5	CHD	A	504	-	29,32,32	1.11	2 (6%)	48,51,51	2.21	26 (54%)
5	CHD	A	505	-	29,32,32	1.03	1 (3%)	48,51,51	2.90	25 (52%)
5	CHD	A	506	-	29,32,32	0.68	0	48,51,51	1.31	7 (14%)
4	FES	B	502	1	0,4,4	0.00	-	0,4,4	0.00	-
5	CHD	B	503	-	29,32,32	0.85	0	48,51,51	2.06	10 (20%)
5	CHD	B	504	-	29,32,32	0.68	0	48,51,51	1.94	13 (27%)
5	CHD	B	505	-	29,32,32	1.08	1 (3%)	48,51,51	2.93	24 (50%)

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
3	GOL	A	502[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	A	502[B]	-	-	0/4/4/4	0/0/0/0
4	FES	A	503	1	-	0/0/4/4	0/1/1/1
5	CHD	A	504	-	-	0/7/74/74	0/4/4/4
5	CHD	A	505	-	-	0/7/74/74	0/4/4/4
5	CHD	A	506	-	-	0/7/74/74	0/4/4/4
4	FES	B	502	1	-	0/0/4/4	0/1/1/1
5	CHD	B	503	-	-	0/7/74/74	0/4/4/4
5	CHD	B	504	-	-	0/7/74/74	0/4/4/4
5	CHD	B	505	-	-	0/7/74/74	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502[A]	GOL	O1-C1	2.12	1.51	1.42
5	A	504	CHD	C1-C2	2.18	1.58	1.53
5	A	504	CHD	O12-C12	2.32	1.47	1.43
5	B	505	CHD	O12-C12	2.39	1.47	1.43
5	A	505	CHD	C6-C7	2.41	1.56	1.52

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	505	CHD	C9-C8-C7	-9.08	101.19	111.92
5	B	505	CHD	C23-C22-C20	-7.20	106.26	114.75
5	B	505	CHD	C5-C6-C7	-6.64	107.03	114.44
5	B	505	CHD	C9-C8-C7	-6.32	104.45	111.92
5	A	505	CHD	C11-C9-C10	-5.99	107.56	113.79
5	B	503	CHD	O3-C3-C4	-5.74	98.45	109.86
5	B	503	CHD	C6-C5-C4	-5.53	104.87	111.05
5	A	505	CHD	C19-C10-C9	-5.32	103.20	111.18
5	B	504	CHD	C23-C22-C20	-5.27	108.54	114.75
5	A	505	CHD	C17-C13-C12	-4.51	113.68	117.68
5	B	504	CHD	C1-C10-C9	-4.47	104.24	111.45
5	B	505	CHD	C14-C8-C9	-3.79	104.41	109.62
5	A	504	CHD	C6-C7-C8	-3.63	107.61	111.47
5	A	504	CHD	C23-C22-C20	-3.57	110.54	114.75
5	A	504	CHD	C17-C13-C12	-3.21	114.83	117.68
5	A	505	CHD	C6-C5-C4	-3.11	107.57	111.05
5	B	505	CHD	C1-C10-C9	-3.11	106.43	111.45
5	B	505	CHD	C15-C14-C8	-3.06	113.88	118.32
5	B	504	CHD	C22-C23-C24	-3.01	100.73	113.02
5	B	503	CHD	C17-C13-C14	-3.01	97.01	100.05
5	A	504	CHD	C11-C9-C10	-2.99	110.68	113.79
5	B	505	CHD	C14-C8-C7	-2.96	107.64	111.74
5	A	504	CHD	C17-C13-C14	-2.93	97.10	100.05
5	B	505	CHD	C18-C13-C17	-2.91	106.63	111.22
5	A	505	CHD	C13-C17-C20	-2.87	116.00	119.50
5	A	504	CHD	C9-C10-C5	-2.75	104.61	108.67
5	A	505	CHD	C15-C14-C13	-2.73	100.88	103.60
5	A	504	CHD	C21-C20-C22	-2.71	105.82	110.35
5	B	504	CHD	C11-C9-C10	-2.68	111.00	113.79
5	A	504	CHD	C11-C12-C13	-2.67	108.49	111.20
5	B	504	CHD	C13-C17-C20	-2.65	116.28	119.50
5	A	504	CHD	C16-C17-C13	-2.63	100.98	103.60
5	A	504	CHD	C15-C14-C8	-2.61	114.53	118.32
5	B	504	CHD	C6-C5-C4	-2.43	108.33	111.05
5	A	504	CHD	C16-C15-C14	-2.40	100.30	105.12
5	A	506	CHD	C6-C5-C4	-2.20	108.59	111.05
5	A	504	CHD	O3-C3-C4	-2.16	105.57	109.86
5	B	504	CHD	C17-C13-C12	-2.13	115.79	117.68
5	B	505	CHD	C21-C20-C22	-2.06	106.92	110.35
5	A	505	CHD	C1-C10-C9	-2.04	108.16	111.45
5	A	505	CHD	O3-C3-C4	-2.03	105.82	109.86
5	A	504	CHD	C13-C14-C8	-2.03	112.13	114.75
5	B	504	CHD	C5-C4-C3	-2.03	109.89	112.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	504	CHD	C19-C10-C1	-2.03	104.80	108.20
5	A	504	CHD	O7-C7-C6	-2.00	105.15	110.06
5	A	504	CHD	O12-C12-C13	2.02	114.39	111.11
5	A	506	CHD	C15-C14-C8	2.05	121.29	118.32
5	A	505	CHD	C19-C10-C1	2.06	111.67	108.20
5	B	505	CHD	C18-C13-C12	2.08	111.12	109.09
5	B	503	CHD	C6-C5-C10	2.08	114.95	112.66
5	A	505	CHD	C9-C11-C12	2.11	117.03	114.36
5	A	506	CHD	C14-C13-C12	2.15	109.32	107.39
5	B	503	CHD	C9-C11-C12	2.17	117.10	114.36
5	B	505	CHD	O3-C3-C4	2.17	114.18	109.86
5	B	505	CHD	C17-C13-C12	2.23	119.65	117.68
5	A	504	CHD	C1-C10-C9	2.25	115.08	111.45
5	A	506	CHD	C6-C7-C8	2.27	113.88	111.47
5	A	505	CHD	C22-C20-C17	2.27	115.02	110.24
5	A	505	CHD	C17-C13-C14	2.29	102.37	100.05
5	A	504	CHD	C1-C10-C5	2.31	111.60	107.81
5	A	504	CHD	C18-C13-C12	2.32	111.35	109.09
5	B	504	CHD	C16-C17-C20	2.36	116.27	112.05
3	A	502[B]	GOL	O2-C2-C3	2.42	119.76	108.65
5	A	505	CHD	C1-C10-C5	2.48	111.88	107.81
5	A	506	CHD	C10-C9-C8	2.53	114.66	111.88
3	A	502[B]	GOL	O2-C2-C1	2.64	120.75	108.65
5	B	505	CHD	C13-C14-C8	2.69	118.21	114.75
5	A	506	CHD	C16-C17-C13	2.76	106.34	103.60
5	A	505	CHD	C15-C14-C8	2.80	122.38	118.32
5	B	504	CHD	C1-C10-C5	2.82	112.44	107.81
5	A	504	CHD	C22-C23-C24	2.83	124.56	113.02
5	A	504	CHD	C15-C14-C13	2.87	106.46	103.60
5	A	504	CHD	C13-C17-C20	2.93	123.06	119.50
5	A	504	CHD	C9-C8-C7	2.96	115.42	111.92
5	A	505	CHD	C11-C9-C8	3.01	115.00	110.73
5	B	503	CHD	C21-C20-C17	3.01	117.97	112.96
5	A	505	CHD	C4-C5-C10	3.01	115.98	112.66
5	B	503	CHD	C1-C10-C5	3.04	112.81	107.81
5	A	505	CHD	O12-C12-C13	3.08	116.11	111.11
5	B	504	CHD	C11-C9-C8	3.11	115.14	110.73
5	B	505	CHD	C6-C7-C8	3.11	114.77	111.47
5	B	504	CHD	C21-C20-C17	3.24	118.35	112.96
5	B	505	CHD	C4-C5-C10	3.29	116.28	112.66
5	B	505	CHD	C6-C5-C10	3.29	116.28	112.66
5	A	505	CHD	C5-C6-C7	3.40	118.23	114.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	503	CHD	C15-C14-C13	3.42	107.00	103.60
5	A	506	CHD	C15-C14-C13	3.48	107.06	103.60
5	A	504	CHD	C6-C5-C4	3.53	114.99	111.05
5	A	505	CHD	C6-C7-C8	3.69	115.39	111.47
5	A	505	CHD	C5-C4-C3	3.76	118.51	112.91
5	B	505	CHD	C14-C13-C12	3.76	110.76	107.39
5	A	505	CHD	C9-C10-C5	3.89	114.43	108.67
5	B	505	CHD	C11-C9-C10	3.89	117.83	113.79
5	B	505	CHD	C9-C10-C5	3.94	114.50	108.67
5	B	505	CHD	C1-C10-C5	3.96	114.31	107.81
5	B	505	CHD	O12-C12-C13	3.96	117.54	111.11
5	A	504	CHD	C5-C6-C7	3.99	118.89	114.44
5	A	504	CHD	C14-C13-C12	4.08	111.05	107.39
5	B	505	CHD	C11-C9-C8	4.12	116.58	110.73
5	B	504	CHD	C14-C13-C12	4.12	111.08	107.39
5	A	505	CHD	C14-C8-C7	4.12	117.46	111.74
5	B	503	CHD	C11-C9-C8	4.39	116.97	110.73
5	A	505	CHD	C23-C22-C20	4.50	120.06	114.75
5	B	505	CHD	C9-C11-C12	4.74	120.35	114.36
3	A	502[A]	GOL	C3-C2-C1	5.04	130.89	111.12
5	B	505	CHD	C15-C14-C13	5.04	108.61	103.60
5	A	505	CHD	C14-C13-C12	5.06	111.92	107.39
5	B	503	CHD	C14-C13-C12	5.26	112.10	107.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502[A]	GOL	1	0
3	A	502[B]	GOL	1	0
5	A	504	CHD	8	0
5	A	505	CHD	4	0
5	B	504	CHD	1	0
5	B	505	CHD	11	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, 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	359/359 (100%)	-0.10	9 (2%)	61	56	9, 20, 39, 67	0
1	B	359/359 (100%)	-0.15	9 (2%)	61	56	10, 20, 46, 59	0
All	All	718/718 (100%)	-0.13	18 (2%)	61	56	9, 20, 42, 67	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	ARG	13.9
1	B	76[A]	MET	3.9
1	A	66	LYS	3.2
1	A	103	ILE	3.0
1	B	358	LYS	2.9
1	A	214	GLY	2.9
1	B	103	ILE	2.7
1	A	356	LEU	2.7
1	B	100	THR	2.7
1	A	358	LYS	2.7
1	B	97[A]	ASP	2.4
1	B	359	GLU	2.3
1	B	214	GLY	2.3
1	A	360	CYS	2.2
1	B	414	THR	2.2
1	A	215	ARG	2.1
1	B	212	GLN	2.1
1	A	213	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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
3	GOL	A	502[A]	6/6	0.96	0.20	3.24	11,13,19,23	6
5	CHD	A	505	29/29	0.85	0.19	2.92	27,41,63,66	0
3	GOL	A	502[B]	6/6	0.96	0.20	2.76	13,19,21,21	6
5	CHD	A	506	29/29	0.86	0.26	2.16	51,54,75,76	0
5	CHD	B	504	29/29	0.88	0.27	1.88	42,49,74,76	0
5	CHD	A	504	29/29	0.86	0.16	1.25	25,28,58,59	0
5	CHD	B	505	29/29	0.78	0.20	0.89	41,53,62,65	0
5	CHD	B	503	29/29	0.85	0.15	0.79	37,44,59,65	0
2	CL	B	501	1/1	0.99	0.09	0.19	24,24,24,24	0
2	CL	A	501	1/1	0.99	0.08	-0.35	22,22,22,22	0
4	FES	A	503	4/4	0.99	0.08	-0.64	16,16,17,18	0
4	FES	B	502	4/4	0.99	0.07	-0.79	17,17,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.