



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:21 AM GMT

PDB ID : 2QD5
Title : Structure of wild type human ferrochelatase in complex with a lead-porphyrin compound
Authors : Meldock, A.E.; Dailey, T.A.; Ross, T.A.; Dailey, H.A.; Lanzilotta, W.N.
Deposited on : 2007-06-20
Resolution : 2.30 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 (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

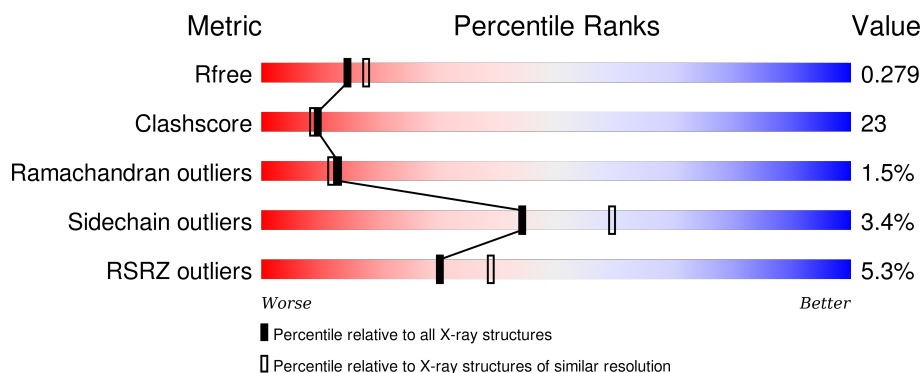
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	359	<div> <div>6%</div> <div>60%</div> <div>36%</div> <div>.</div> </div>
1	B	359	<div> <div>5%</div> <div>67%</div> <div>29%</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
4	CHD	A	701	-	-	-	X
4	CHD	B	1103	-	-	-	X
6	OXY	B	1001	-	-	-	X
7	GOL	A	601	-	-	-	X
8	ACY	A	801	-	-	-	X
8	ACY	A	803	-	-	X	X
8	ACY	B	1106	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6253 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.

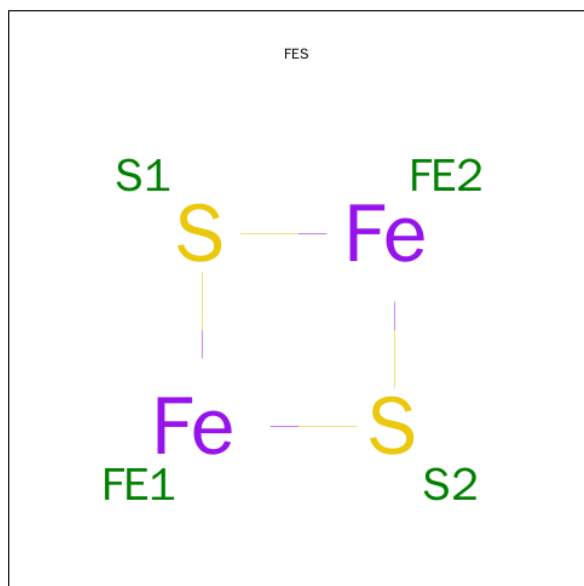
- Molecule 1 is a protein called Ferrochelatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	4	0
			2925	1861	508	537	19			
1	B	359	Total	C	N	O	S	0	3	0
			2917	1856	506	536	19			

- Molecule 2 is LEAD (II) ION (three-letter code: PB) (formula: Pb).

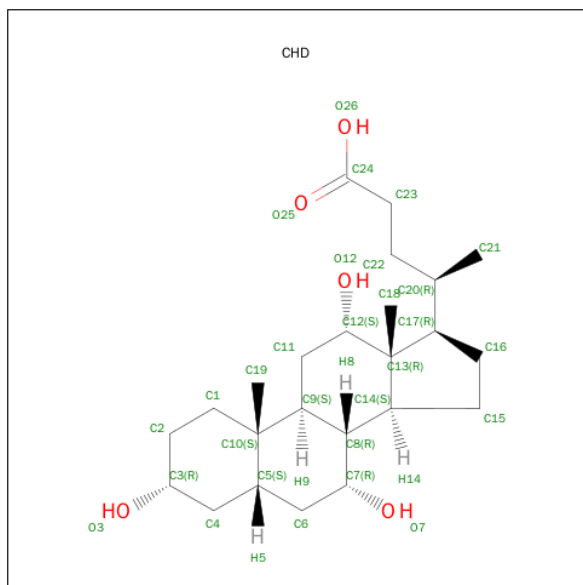
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Pb	0	1
			2	2		
2	A	1	Total	Pb	0	1
			2	2		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



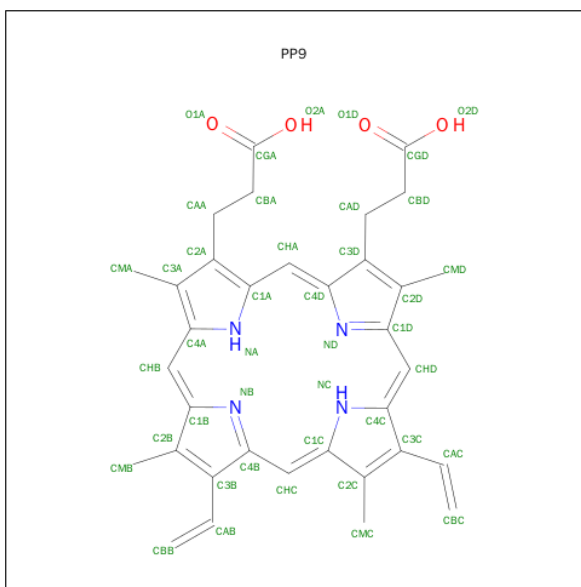
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



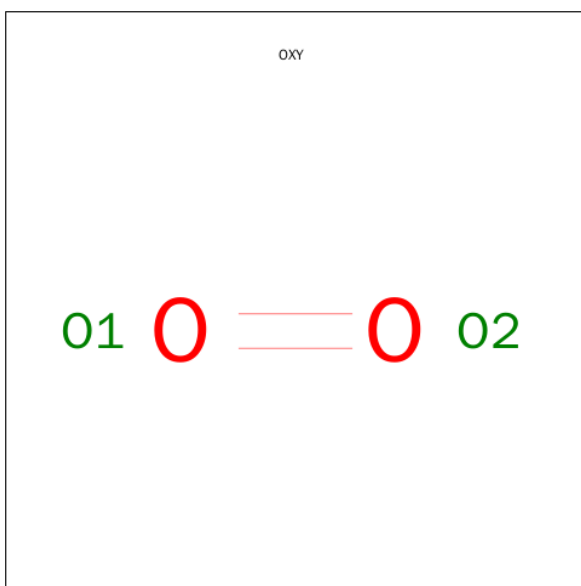
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			29	24	5		
4	A	1	Total	C	O	0	0
			29	24	5		
4	B	1	Total	C	O	0	0
			29	24	5		
4	B	1	Total	C	O	0	0
			29	24	5		

- Molecule 5 is PROTOPORPHYRIN IX (three-letter code: PP9) (formula: $C_{34}H_{34}N_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			42	34	4	4		
5	B	1	Total	C	N	O	0	0
			42	34	4	4		

- Molecule 6 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



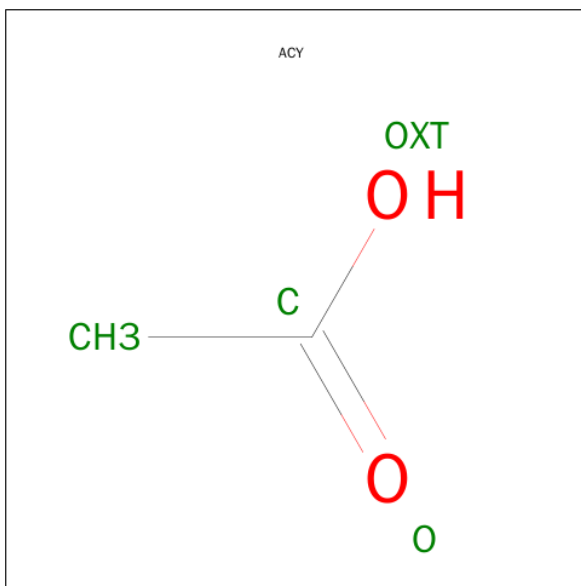
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	O	0	0
			2	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		

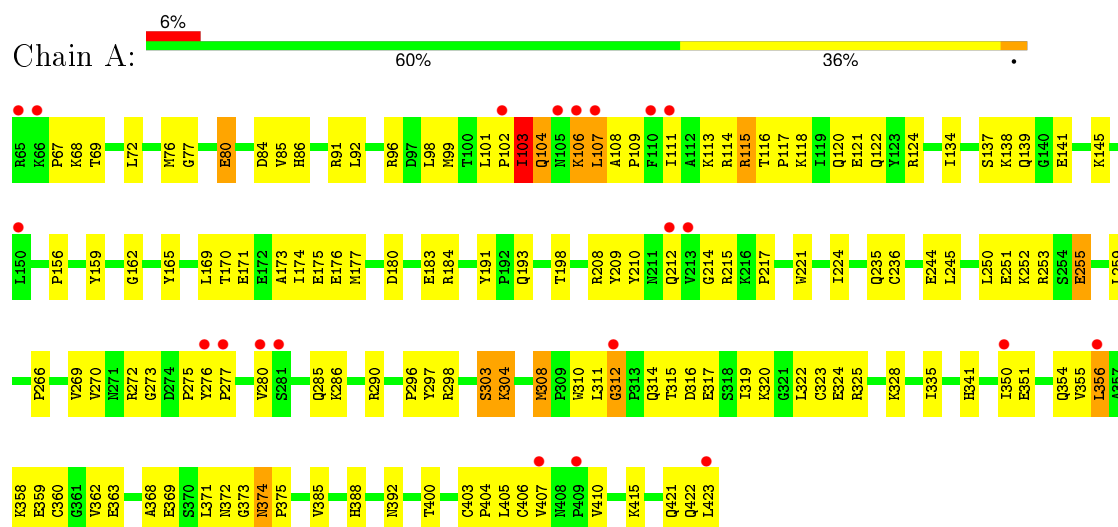
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	94	Total 94	O 94	0	0
9	B	85	Total 85	O 85	0	0

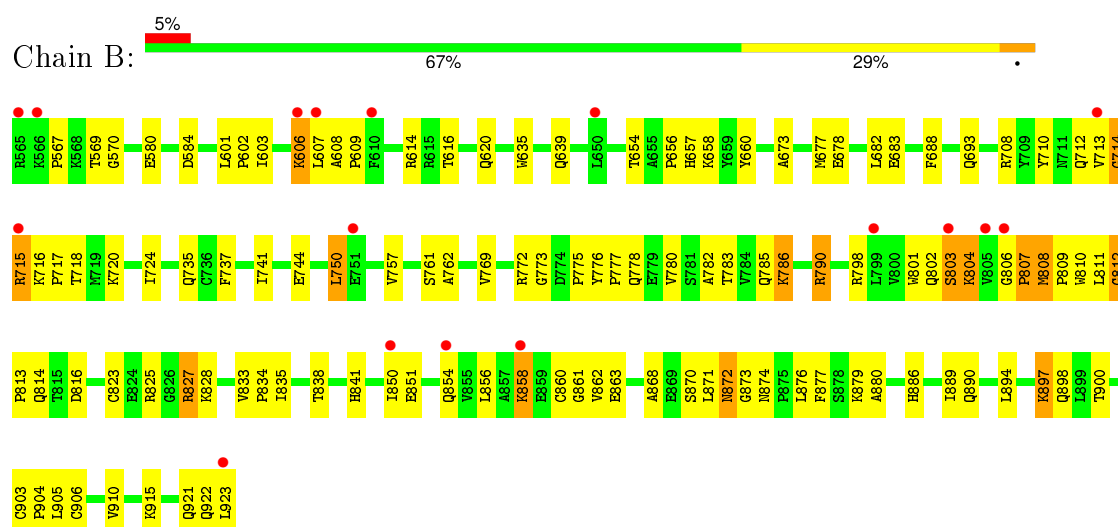
3 Residue-property plots

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



• Molecule 1: Ferrochelatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.22Å 92.81Å 109.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.26 – 2.30 47.25 – 2.19	Depositor EDS
% Data completeness (in resolution range)	95.0 (47.26-2.30) 94.0 (47.25-2.19)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.280 0.241 , 0.279	Depositor DCC
R_{free} test set	1949 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	3 of 83648 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6253	wwPDB-VP
Average B, all atoms (Å ²)	54.0	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 51.84 % 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 5.2967e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, CHD, OXY, PB, FES, PP9, ACY

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	0/2995	0.61	2/4056 (0.0%)
1	B	0.37	0/2987	0.60	1/4046 (0.0%)
All	All	0.37	0/5982	0.61	3/8102 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	ILE	N-CA-C	-5.32	96.64	111.00
1	A	103	ILE	N-CA-C	-5.23	96.89	111.00
1	B	724	ILE	N-CA-C	-5.03	97.41	111.00

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	2925	0	2928	156	0
1	B	2917	0	2918	129	0
2	A	2	0	0	1	0
2	B	2	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	58	0	78	7	0
4	B	58	0	78	3	0
5	A	42	0	31	1	0
5	B	42	0	30	4	0
6	B	2	0	0	0	0
7	A	6	0	8	2	0
8	A	8	0	6	5	0
8	B	4	0	3	4	0
9	A	94	0	0	9	0
9	B	85	0	0	2	0
All	All	6253	0	6080	274	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 23.

All (274) 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)
5:B:1105:PP9:O1D	5:B:1105:PP9:CGD	1.64	1.46
5:B:1105:PP9:C2C	5:B:1105:PP9:C1C	1.74	1.38
1:A:311:LEU:HD12	1:A:312:GLY:H	1.16	1.04
1:B:811:LEU:HD12	1:B:812:GLY:H	1.23	1.01
1:A:285:GLN:HG2	1:B:778:GLN:HE22	1.31	0.95
1:A:285:GLN:HG3	1:B:782:ALA:HB2	1.50	0.93
1:A:297:TYR:H	1:B:898:GLN:HE22	1.17	0.91
1:A:115:ARG:HH12	4:A:701:CHD:H222	1.36	0.90
1:B:750:LEU:H	1:B:750:LEU:HD12	1.37	0.89
1:A:308[A]:MET:SD	4:A:701:CHD:H21	2.12	0.89
2:A:1101[A]:PB:PB	8:A:803:ACY:OXT	1.34	0.88
1:A:250:LEU:HD12	1:A:250:LEU:H	1.40	0.85
1:A:107:LEU:HD23	1:A:108:ALA:N	1.91	0.85
1:A:67:PRO:HA	1:A:156:PRO:HG2	1.58	0.84
1:A:303:SER:CB	8:A:803:ACY:H2	2.08	0.83
1:A:303:SER:HB2	8:A:803:ACY:H2	1.59	0.83
1:A:272:ARG:HD2	9:A:1130:HOH:O	1.77	0.82
1:A:311:LEU:HD12	1:A:312:GLY:N	1.94	0.81
1:B:757:VAL:HG21	1:B:827:ARG:HG2	1.60	0.81
1:B:708:ARG:NH2	1:B:910:VAL:HG21	1.96	0.80
1:B:790:ARG:HH11	1:B:790:ARG:HG2	1.44	0.80
1:B:814:GLN:HE21	1:B:816:ASP:HB2	1.45	0.80
1:B:601:LEU:HD21	4:B:1103:CHD:H151	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:SER:O	1:A:141:GLU:HG3	1.83	0.79
1:A:350:ILE:O	1:A:354:GLN:HG3	1.84	0.78
1:B:811:LEU:CD1	1:B:812:GLY:H	1.97	0.78
1:B:806:GLY:HA3	9:B:1108:HOH:O	1.83	0.77
1:A:314:GLN:HB3	1:A:317:GLU:HG2	1.67	0.76
4:A:701:CHD:H151	4:A:702:CHD:H151	1.66	0.76
1:A:244:GLU:HG3	1:A:368:ALA:HA	1.68	0.74
1:A:311:LEU:CD1	1:A:312:GLY:H	1.99	0.74
1:A:103:ILE:O	1:A:107:LEU:HD22	1.88	0.74
1:B:744:GLU:HG3	1:B:868:ALA:HA	1.68	0.73
1:A:171:GLU:O	1:A:175:GLU:HG3	1.88	0.73
1:A:356:LEU:HD12	1:A:362:VAL:HG21	1.69	0.72
1:B:903:CYS:HB2	1:B:906:CYS:HB2	1.71	0.72
1:A:103:ILE:HD13	1:A:103:ILE:H	1.55	0.71
1:A:208:ARG:NH2	1:A:410:VAL:HG21	2.04	0.71
1:A:235:GLN:HG3	1:A:290:ARG:NH2	2.06	0.70
1:A:68:LYS:HD2	1:A:183:GLU:HB2	1.73	0.70
1:B:639:GLN:HE21	1:B:873:GLY:HA2	1.56	0.70
1:A:285:GLN:HG3	1:B:782:ALA:CB	2.22	0.70
1:B:757:VAL:CG2	1:B:827:ARG:HG2	2.22	0.70
1:A:208:ARG:HH22	1:A:410:VAL:HG21	1.56	0.70
1:B:750:LEU:CD1	1:B:750:LEU:H	2.05	0.69
1:B:735:GLN:HG3	1:B:790:ARG:NH2	2.07	0.69
1:A:351:GLU:H	1:A:351:GLU:CD	1.95	0.69
1:B:811:LEU:HD12	1:B:812:GLY:N	2.04	0.69
1:B:856:LEU:HG	1:B:862:VAL:HG21	1.75	0.69
1:B:897:LYS:HB2	1:B:897:LYS:NZ	2.07	0.69
1:A:374:ASN:HD22	1:A:375:PRO:CD	2.05	0.69
1:A:107:LEU:HD23	1:A:108:ALA:H	1.59	0.68
1:B:735:GLN:HG3	1:B:790:ARG:HH22	1.59	0.67
1:B:823:CYS:SG	1:B:862:VAL:HG22	2.34	0.67
1:B:608:ALA:HB3	1:B:609:PRO:HD3	1.77	0.67
1:B:673:ALA:O	1:B:677:MET:HG3	1.95	0.66
1:B:850:ILE:O	1:B:854:GLN:HG3	1.95	0.66
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.76	0.66
1:A:139:GLN:HE21	1:A:373:GLY:HA2	1.61	0.66
5:B:1105:PP9:C2C	5:B:1105:PP9:CHC	2.67	0.64
1:B:683:GLU:O	1:B:720:LYS:HG2	1.97	0.64
1:B:804:LYS:HZ3	1:B:814:GLN:HB2	1.62	0.64
1:A:374:ASN:HD22	1:A:375:PRO:HD2	1.62	0.64
1:A:85:VAL:HG21	1:A:120:GLN:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLN:NE2	1:A:373:GLY:HA2	2.13	0.63
1:A:314:GLN:HE21	1:A:316:ASP:HB2	1.63	0.63
1:B:710:TYR:HA	1:B:713:VAL:HG12	1.81	0.63
1:A:208:ARG:NH1	1:A:410:VAL:HG11	2.14	0.63
1:B:713:VAL:O	1:B:715:ARG:HG2	1.98	0.63
1:B:603:ILE:HG13	1:B:603:ILE:O	1.98	0.62
1:A:374:ASN:HD22	1:A:375:PRO:N	1.96	0.62
1:B:803:SER:C	1:B:804:LYS:HG3	2.19	0.62
1:A:86:HIS:NE2	1:A:113:LYS:HG2	2.14	0.62
1:B:841:HIS:HB2	5:B:1105:PP9:O2D	1.98	0.62
1:B:804:LYS:HD2	1:B:814:GLN:HG3	1.81	0.61
1:B:811:LEU:CG	1:B:812:GLY:N	2.63	0.61
1:A:277:PRO:HB3	7:A:601:GOL:H2	1.82	0.61
1:A:298:ARG:NH1	1:B:773:GLY:O	2.33	0.61
1:B:735:GLN:HA	1:B:790:ARG:NH1	2.15	0.61
1:A:311:LEU:CD1	1:A:312:GLY:N	2.61	0.61
1:A:320:LYS:HG3	1:A:356:LEU:HD21	1.84	0.60
1:A:303:SER:HB3	8:A:803:ACY:H2	1.81	0.60
1:B:639:GLN:NE2	1:B:873:GLY:HA2	2.16	0.60
1:B:811:LEU:O	1:B:812:GLY:O	2.19	0.60
1:B:808[A]:MET:HB2	1:B:809:PRO:HD2	1.82	0.60
1:A:80:GLU:HG3	1:A:84:ASP:OD2	2.02	0.60
1:A:115:ARG:HA	9:A:1120:HOH:O	2.01	0.60
1:B:858:LYS:HE2	1:B:858:LYS:HA	1.83	0.60
1:A:403:CYS:HB2	1:A:406:CYS:HB2	1.83	0.59
1:A:276:TYR:HB3	1:A:277:PRO:HD3	1.85	0.59
1:B:790:ARG:NH1	1:B:790:ARG:HG2	2.14	0.58
1:B:874:ASN:ND2	1:B:876:LEU:HB3	2.19	0.58
1:A:145:LYS:HB3	9:A:1142:HOH:O	2.02	0.58
1:B:900:THR:O	1:B:915:LYS:HE2	2.04	0.58
1:B:811:LEU:HG	1:B:812:GLY:N	2.17	0.58
1:A:69:THR:HG23	1:A:184:ARG:HD2	1.86	0.58
1:A:103:ILE:O	1:A:107:LEU:CD2	2.53	0.57
1:B:886:HIS:O	1:B:890:GLN:HG2	2.05	0.57
1:A:244:GLU:CG	1:A:368:ALA:HA	2.34	0.57
1:A:170:THR:O	1:A:174:ILE:HG13	2.04	0.57
1:B:811:LEU:CD1	1:B:812:GLY:N	2.65	0.57
1:B:804:LYS:H	8:B:1106:ACY:H1	1.69	0.57
1:A:115:ARG:HH11	1:A:115:ARG:HG2	1.69	0.56
1:A:356:LEU:O	1:A:362:VAL:HG23	2.04	0.56
1:A:285:GLN:HG2	1:B:778:GLN:NE2	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:CG	1:A:312:GLY:N	2.68	0.56
1:B:922:GLN:HG2	1:B:923:LEU:HD22	1.87	0.56
1:B:823:CYS:HB3	1:B:860:CYS:HB3	1.88	0.56
1:B:851[A]:GLU:H	1:B:851[A]:GLU:CD	2.08	0.55
1:A:255:GLU:O	1:A:255:GLU:HG2	2.07	0.55
1:A:191:TYR:CZ	1:A:198:THR:HB	2.41	0.55
1:A:116:THR:N	1:A:117:PRO:CD	2.69	0.55
1:B:803:SER:HB3	8:B:1106:ACY:OXT	2.06	0.55
1:A:311:LEU:O	1:A:312:GLY:O	2.24	0.55
1:B:580[B]:GLU:HG3	1:B:584:ASP:OD2	2.07	0.55
1:A:296:PRO:HD3	1:B:897:LYS:HD2	1.89	0.55
1:A:275:PRO:HD3	1:B:798:ARG:HH12	1.70	0.55
1:A:85:VAL:HG12	1:A:116:THR:HG23	1.89	0.55
1:A:323:CYS:SG	1:A:362:VAL:HG22	2.46	0.55
1:B:776:TYR:HB3	1:B:777:PRO:HD3	1.88	0.54
1:B:828:LYS:HB3	1:B:863:GLU:H	1.73	0.54
1:A:308[A]:MET:HE3	1:A:310:TRP:NE1	2.22	0.54
1:B:606:LYS:HB3	1:B:606:LYS:NZ	2.21	0.54
1:A:245:LEU:HB3	1:A:253:ARG:NH1	2.22	0.54
1:B:804:LYS:CD	1:B:814:GLN:HG3	2.37	0.54
1:B:750:LEU:N	1:B:750:LEU:HD12	2.16	0.54
1:A:99:MET:HB2	4:A:701:CHD:C19	2.37	0.54
1:B:922:GLN:HG2	1:B:923:LEU:CD2	2.37	0.54
1:A:173:ALA:O	1:A:177:MET:HG3	2.07	0.53
1:A:297:TYR:N	1:B:898:GLN:HE22	1.95	0.53
1:A:96:ARG:HA	1:A:99:MET:O	2.07	0.53
1:A:308[A]:MET:CE	1:A:310:TRP:HE1	2.22	0.53
1:A:212:GLN:OE1	1:A:212:GLN:HA	2.08	0.53
1:A:358:LYS:O	1:A:358:LYS:HD3	2.09	0.53
1:A:98:LEU:HD13	8:A:801:ACY:H3	1.91	0.53
1:B:922:GLN:O	1:B:923:LEU:HB2	2.09	0.53
1:B:874:ASN:HD22	1:B:876:LEU:HB3	1.73	0.53
1:B:616:THR:O	1:B:620:GLN:HG3	2.09	0.52
1:A:253:ARG:HD2	9:A:1115:HOH:O	2.09	0.52
1:B:783:THR:HG22	1:B:835:ILE:HD11	1.91	0.52
1:A:328:LYS:HB3	1:A:363:GLU:HG2	1.91	0.52
1:A:400:THR:O	1:A:415:LYS:HE2	2.09	0.52
1:A:250:LEU:CD1	1:A:250:LEU:H	2.16	0.51
1:A:266:PRO:HB3	1:A:308[A]:MET:HE3	1.91	0.51
1:A:114:ARG:HH12	4:A:702:CHD:H42	1.75	0.51
1:A:350:ILE:HG13	1:A:351:GLU:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:PRO:HA	1:B:656:PRO:HG2	1.91	0.51
1:A:422:GLN:O	1:A:423:LEU:HB2	2.10	0.51
1:B:744:GLU:CG	1:B:868:ALA:HA	2.39	0.51
1:B:897:LYS:HB2	1:B:897:LYS:HZ3	1.75	0.50
1:B:602:PRO:O	1:B:607:LEU:HD12	2.12	0.50
1:A:114:ARG:NH1	4:A:702:CHD:H42	2.26	0.50
1:B:735:GLN:HG3	1:B:790:ARG:CZ	2.42	0.50
1:A:374:ASN:ND2	1:A:375:PRO:HD2	2.26	0.49
1:B:804:LYS:NZ	1:B:814:GLN:HB2	2.27	0.49
1:B:870:SER:HB2	1:B:872:ASN:ND2	2.27	0.49
1:A:116:THR:O	1:A:120:GLN:HG3	2.13	0.49
1:A:273:GLY:HA3	1:A:404:PRO:HD2	1.94	0.49
1:A:422:GLN:HG2	1:A:423:LEU:HD22	1.95	0.49
1:A:221:TRP:O	1:A:421:GLN:HG3	2.12	0.49
1:A:285:GLN:CG	1:B:778:GLN:HE22	2.13	0.48
1:A:208:ARG:HH12	1:A:410:VAL:HG11	1.78	0.48
1:A:308[A]:MET:HE2	1:A:310:TRP:HE1	1.78	0.48
1:B:762:ALA:O	1:B:801:TRP:HA	2.13	0.48
1:A:304:LYS:HE2	1:A:310:TRP:HB2	1.95	0.48
1:B:856:LEU:HG	1:B:862:VAL:CG2	2.44	0.48
1:B:737:PHE:O	1:B:741:ILE:HG13	2.13	0.48
1:B:894:LEU:HD22	1:B:921:GLN:HB2	1.96	0.48
1:A:106:LYS:O	1:A:109:PRO:HD2	2.13	0.48
1:B:801:TRP:N	1:B:801:TRP:CD1	2.81	0.48
1:A:103:ILE:HG12	1:A:103:ILE:O	2.13	0.47
1:B:790:ARG:NH1	1:B:790:ARG:CG	2.77	0.47
1:B:803:SER:CB	8:B:1106:ACY:OXT	2.62	0.47
1:B:772:ARG:HA	1:B:905:LEU:HB2	1.96	0.47
1:A:355:VAL:HG13	1:A:359:GLU:OE2	2.13	0.47
1:A:236:CYS:HB3	1:A:371:LEU:HD22	1.96	0.47
1:A:298:ARG:HH12	1:B:775:PRO:HD3	1.78	0.47
1:A:175:GLU:HG2	1:A:209:TYR:OH	2.14	0.47
1:A:252:LYS:HA	1:A:255:GLU:OE2	2.15	0.47
1:A:335:ILE:O	1:A:335:ILE:HG13	2.15	0.47
1:A:72:LEU:HD11	1:A:162:GLY:HA3	1.97	0.47
1:A:275:PRO:HD3	1:B:798:ARG:NH1	2.29	0.46
1:A:351:GLU:HA	1:A:354:GLN:CD	2.35	0.46
1:A:212:GLN:C	1:A:214:GLY:N	2.67	0.46
1:A:176:GLU:HG2	1:A:180:ASP:OD2	2.16	0.46
1:B:735:GLN:HG3	1:B:790:ARG:NH1	2.31	0.46
1:A:341:HIS:HB2	5:A:901:PP9:O2D	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:MET:HG3	1:A:77:GLY:O	2.15	0.46
1:B:838:THR:HG22	1:B:871:LEU:HD12	1.96	0.46
1:A:374:ASN:C	1:A:374:ASN:HD22	2.17	0.46
1:A:99:MET:HB2	4:A:701:CHD:H191	1.96	0.46
1:A:191:TYR:CE1	1:A:198:THR:HB	2.51	0.46
1:B:769:VAL:O	1:B:772:ARG:HG2	2.16	0.46
1:A:311:LEU:HG	1:A:312:GLY:N	2.29	0.46
1:B:677:MET:HB3	1:B:682:LEU:HD12	1.97	0.46
1:A:210:TYR:CE2	1:A:217:PRO:HA	2.52	0.46
1:B:827:ARG:HG3	9:B:1157:HOH:O	2.16	0.45
1:A:103:ILE:N	1:A:103:ILE:HD13	2.26	0.45
1:A:92:LEU:HD23	1:A:92:LEU:C	2.36	0.45
1:A:270:VAL:HG12	1:B:812:GLY:HA2	1.98	0.45
1:B:570:GLY:HA3	1:B:682:LEU:HD13	1.98	0.45
1:B:635:TRP:HA	1:B:635:TRP:CE3	2.51	0.45
1:B:897:LYS:HZ2	1:B:897:LYS:HB2	1.79	0.45
1:B:858:LYS:CE	1:B:858:LYS:HA	2.45	0.45
1:B:708:ARG:CZ	1:B:910:VAL:HG21	2.46	0.45
1:A:134:ILE:O	1:A:138[B]:LYS:HG2	2.17	0.45
1:B:654:THR:OG1	1:B:657:HIS:NE2	2.48	0.45
1:A:369[B]:GLU:HG2	9:A:1113:HOH:O	2.15	0.45
1:B:876:LEU:HD12	1:B:879:LYS:HD3	1.98	0.45
1:B:828:LYS:HD3	1:B:861:GLY:O	2.16	0.45
1:A:303:SER:C	1:A:304:LYS:HG3	2.37	0.45
1:B:804:LYS:HZ2	1:B:814:GLN:HA	1.81	0.44
1:A:115:ARG:NH1	1:A:115:ARG:HG2	2.32	0.44
1:A:107:LEU:O	1:A:111:ILE:HG13	2.17	0.44
1:B:715:ARG:H	1:B:715:ARG:HG2	1.62	0.44
1:B:810:TRP:CZ3	8:B:1106:ACY:H3	2.53	0.44
1:A:101:LEU:H	1:A:104:GLN:NE2	2.16	0.44
1:B:851[A]:GLU:N	1:B:851[A]:GLU:CD	2.71	0.43
1:B:761:SER:OG	1:B:802:GLN:HB3	2.18	0.43
1:B:877:PHE:O	1:B:880:ALA:HB3	2.18	0.43
1:A:286:LYS:HZ1	1:B:786:LYS:HE2	1.84	0.43
1:B:569:THR:OG1	1:B:654:THR:HB	2.18	0.43
1:A:322:LEU:HG	1:B:904:PRO:HB3	1.99	0.43
1:A:266:PRO:HG2	1:A:269:VAL:HG23	2.00	0.43
1:A:106:LYS:HA	1:A:106:LYS:NZ	2.33	0.43
1:A:107:LEU:HD23	1:A:107:LEU:C	2.38	0.43
1:B:693:GLN:HG2	1:B:780:VAL:HA	2.01	0.43
1:A:91:ARG:HD2	1:A:165:TYR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:833:VAL:HA	1:B:834:PRO:HD3	1.93	0.43
1:A:320:LYS:HA	1:A:356:LEU:HD11	2.01	0.43
1:B:602:PRO:O	1:B:603:ILE:C	2.57	0.43
1:B:658:LYS:HD3	1:B:660:TYR:OH	2.19	0.43
1:A:272:ARG:HA	1:A:405:LEU:HB2	2.01	0.43
1:B:678:GLU:OE2	1:B:718:THR:HG23	2.19	0.43
1:A:103:ILE:CD1	1:A:107:LEU:HD13	2.49	0.42
1:A:141:GLU:O	1:A:145:LYS:HG2	2.18	0.42
1:A:323:CYS:HB3	1:A:360:CYS:HB3	2.02	0.42
1:A:117:PRO:HD2	9:A:1120:HOH:O	2.18	0.42
1:A:320:LYS:HE2	1:A:324:GLU:OE2	2.20	0.42
1:B:858:LYS:HE2	1:B:858:LYS:CA	2.48	0.42
1:B:654:THR:HG21	1:B:889:ILE:HG21	2.01	0.42
1:A:208:ARG:CZ	1:A:410:VAL:HG21	2.49	0.42
1:A:259:LEU:HD23	1:A:298:ARG:HB2	2.00	0.42
1:A:103:ILE:H	1:A:103:ILE:CD1	2.28	0.42
1:A:104:GLN:HE21	1:A:104:GLN:HB2	1.55	0.42
1:A:270:VAL:O	1:B:813:PRO:HD3	2.20	0.42
1:B:825:ARG:HH11	1:B:825:ARG:HG3	1.84	0.42
1:A:80:GLU:H	1:A:80:GLU:HG2	1.44	0.41
1:B:712:GLN:C	1:B:714:GLY:H	2.24	0.41
1:A:210:TYR:HE2	1:A:217:PRO:HA	1.85	0.41
1:B:712:GLN:HA	1:B:712:GLN:OE1	2.20	0.41
1:B:614:ARG:HH11	1:B:614:ARG:HG2	1.85	0.41
1:A:121:GLU:CD	1:A:124:ARG:HH21	2.24	0.41
1:A:385:VAL:O	1:A:388:HIS:HB3	2.20	0.41
1:A:106:LYS:C	1:A:109:PRO:HD2	2.41	0.41
1:B:808[A]:MET:CB	1:B:809:PRO:HD2	2.51	0.41
1:A:139:GLN:HG3	9:A:1177:HOH:O	2.21	0.41
1:B:823:CYS:HB3	1:B:860:CYS:CB	2.51	0.41
7:A:601:GOL:H31	1:B:777:PRO:HB2	2.03	0.41
1:A:118:LYS:O	1:A:122:GLN:HG2	2.21	0.41
1:B:808[A]:MET:CE	4:B:1103:CHD:H21	2.51	0.41
1:A:91:ARG:NH2	1:A:169:LEU:HD11	2.36	0.41
1:A:215:ARG:HA	1:A:215:ARG:HD3	1.82	0.40
1:A:171:GLU:N	1:A:171:GLU:OE1	2.24	0.40
1:B:808[A]:MET:SD	4:B:1103:CHD:H112	2.61	0.40
1:A:325:ARG:HG3	1:A:325:ARG:HH11	1.87	0.40
9:A:1128:HOH:O	1:B:785:GLN:HG2	2.22	0.40
9:A:1128:HOH:O	1:B:785:GLN:CG	2.68	0.40
1:A:407:VAL:O	1:A:407:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:TYR:C	1:A:159:TYR:CD1	2.95	0.40
1:A:251:GLU:H	1:A:251:GLU:CD	2.24	0.40
1:A:315:THR:O	1:A:319:ILE:HG13	2.21	0.40
1:B:716:LYS:HB2	1:B:717:PRO:HD2	2.02	0.40
1:A:193:GLN:HG2	1:A:280:VAL:HA	2.04	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	361/359 (101%)	332 (92%)	24 (7%)	5 (1%)	14	13
1	B	360/359 (100%)	336 (93%)	18 (5%)	6 (2%)	11	10
All	All	721/718 (100%)	668 (93%)	42 (6%)	11 (2%)	13	12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	PRO
1	A	312	GLY
1	A	372	ASN
1	B	812	GLY
1	B	872	ASN
1	A	304	LYS
1	B	804	LYS
1	A	303	SER
1	B	803	SER
1	B	807	PRO
1	B	714	GLY

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	328/324 (101%)	316 (96%)	12 (4%)	41	55
1	B	327/324 (101%)	315 (96%)	12 (4%)	41	55
All	All	655/648 (101%)	631 (96%)	24 (4%)	44	55

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	103	ILE
1	A	104	GLN
1	A	106	LYS
1	A	107	LEU
1	A	115	ARG
1	A	255	GLU
1	A	308[A]	MET
1	A	308[B]	MET
1	A	356	LEU
1	A	374	ASN
1	A	392	ASN
1	B	606	LYS
1	B	688	PHE
1	B	715	ARG
1	B	750	LEU
1	B	786	LYS
1	B	790	ARG
1	B	807	PRO
1	B	808[A]	MET
1	B	808[B]	MET
1	B	827	ARG
1	B	858	LYS
1	B	897	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	153	ASN
1	A	211	ASN
1	A	285	GLN
1	A	302	GLN
1	A	314	GLN
1	A	354	GLN
1	A	374	ASN
1	B	653	ASN
1	B	711	ASN
1	B	735	GLN
1	B	778	GLN
1	B	814	GLN
1	B	874	ASN
1	B	898	GLN
1	B	921	GLN
1	B	922	GLN

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 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	FES	A	501	-	0,4,4	0.00	-	0,4,4	0.00	-
7	GOL	A	601	-	5,5,5	0.07	0	5,5,5	0.11	0
4	CHD	A	701	-	29,32,32	1.89	10 (34%)	48,51,51	1.82	13 (27%)
4	CHD	A	702	-	29,32,32	1.94	12 (41%)	48,51,51	1.75	14 (29%)
8	ACY	A	801	-	1,3,3	1.69	0	0,3,3	0.00	-
8	ACY	A	803	-	1,3,3	1.70	0	0,3,3	0.00	-
5	PP9	A	901	-	33,46,46	6.32	14 (42%)	35,68,68	2.73	15 (42%)
6	OXY	B	1001	-	1,1,1	1.36	0	0,0,0	0.00	-
4	CHD	B	1103	-	29,32,32	1.95	12 (41%)	48,51,51	1.85	14 (29%)
4	CHD	B	1104	-	29,32,32	1.97	12 (41%)	48,51,51	1.77	13 (27%)
5	PP9	B	1105	-	33,46,46	5.95	18 (54%)	35,68,68	2.81	15 (42%)
8	ACY	B	1106	-	1,3,3	1.66	0	0,3,3	0.00	-
3	FES	B	502	-	0,4,4	0.00	-	0,4,4	0.00	-

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	FES	A	501	-	-	0/0/4/4	0/1/1/1
7	GOL	A	601	-	-	0/4/4/4	0/0/0/0
4	CHD	A	701	-	-	0/7/74/74	0/4/4/4
4	CHD	A	702	-	-	0/7/74/74	0/4/4/4
8	ACY	A	801	-	-	0/0/0/0	0/0/0/0
8	ACY	A	803	-	-	0/0/0/0	0/0/0/0
5	PP9	A	901	-	-	0/20/62/62	0/0/5/5
6	OXY	B	1001	-	-	0/0/0/0	0/0/0/0
4	CHD	B	1103	-	-	0/7/74/74	0/4/4/4
4	CHD	B	1104	-	-	0/7/74/74	0/4/4/4
5	PP9	B	1105	-	-	0/20/62/62	0/0/5/5
8	ACY	B	1106	-	-	0/0/0/0	0/0/0/0
3	FES	B	502	-	-	0/0/4/4	0/1/1/1

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	PP9	C1D-ND	-14.24	1.07	1.38
5	B	1105	PP9	C1D-ND	-11.78	1.12	1.38
5	B	1105	PP9	C4A-NA	-6.71	1.16	1.39
5	B	1105	PP9	C3C-CAC	-5.12	1.36	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	PP9	C3C-CAC	-4.80	1.37	1.47
5	A	901	PP9	C4A-NA	-4.06	1.25	1.39
5	B	1105	PP9	C4B-NB	-3.84	1.30	1.38
5	B	1105	PP9	C4C-CHD	-3.26	1.28	1.40
5	B	1105	PP9	C1B-NB	-2.72	1.30	1.37
5	B	1105	PP9	C1C-CHC	-2.48	1.31	1.40
5	A	901	PP9	C4D-C3D	-2.34	1.41	1.45
5	A	901	PP9	C4C-CHD	-2.29	1.31	1.40
4	A	701	CHD	C13-C12	2.05	1.57	1.54
4	A	702	CHD	O7-C7	2.05	1.48	1.43
4	B	1103	CHD	O7-C7	2.09	1.48	1.43
4	B	1104	CHD	C4-C3	2.09	1.55	1.51
4	B	1103	CHD	C4-C3	2.15	1.55	1.51
4	B	1104	CHD	C20-C17	2.15	1.58	1.54
4	A	702	CHD	C20-C17	2.16	1.58	1.54
4	B	1103	CHD	C19-C10	2.17	1.58	1.54
4	A	702	CHD	C19-C10	2.17	1.58	1.54
5	B	1105	PP9	CMD-C2D	2.18	1.55	1.50
4	B	1104	CHD	C19-C10	2.19	1.58	1.54
4	B	1103	CHD	C20-C17	2.21	1.58	1.54
4	A	701	CHD	C8-C7	2.27	1.57	1.53
4	A	701	CHD	O7-C7	2.28	1.48	1.43
4	B	1103	CHD	C8-C7	2.30	1.57	1.53
4	A	702	CHD	C13-C12	2.35	1.58	1.54
4	B	1104	CHD	C8-C14	2.45	1.58	1.53
4	A	701	CHD	C8-C14	2.46	1.58	1.53
4	B	1104	CHD	C10-C9	2.51	1.61	1.56
4	A	702	CHD	C8-C14	2.52	1.58	1.53
4	A	701	CHD	C18-C13	2.54	1.58	1.54
5	B	1105	PP9	C1A-NA	2.55	1.47	1.39
4	A	702	CHD	C18-C13	2.56	1.58	1.54
4	A	701	CHD	O12-C12	2.61	1.48	1.43
4	B	1103	CHD	C18-C13	2.65	1.58	1.54
4	A	702	CHD	C10-C9	2.66	1.61	1.56
4	B	1103	CHD	O12-C12	2.68	1.48	1.43
4	B	1103	CHD	C6-C5	2.68	1.58	1.53
5	A	901	PP9	C3B-C4B	2.68	1.49	1.43
4	B	1104	CHD	C8-C7	2.69	1.57	1.53
4	B	1103	CHD	C8-C14	2.70	1.59	1.53
4	B	1104	CHD	C18-C13	2.70	1.58	1.54
4	A	702	CHD	O12-C12	2.71	1.48	1.43
4	A	702	CHD	C8-C7	2.76	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1104	CHD	C13-C12	2.77	1.58	1.54
4	B	1104	CHD	C6-C5	2.81	1.58	1.53
4	B	1104	CHD	O12-C12	2.87	1.48	1.43
4	A	701	CHD	C6-C5	2.93	1.58	1.53
4	A	702	CHD	C6-C5	3.01	1.59	1.53
4	A	701	CHD	C16-C17	3.02	1.61	1.54
4	A	702	CHD	C16-C17	3.06	1.61	1.54
4	B	1103	CHD	C10-C9	3.10	1.62	1.56
5	B	1105	PP9	C3B-C4B	3.12	1.50	1.43
4	B	1103	CHD	C16-C17	3.18	1.61	1.54
4	B	1104	CHD	C16-C17	3.31	1.62	1.54
5	A	901	PP9	C3C-C2C	3.35	1.44	1.40
4	A	701	CHD	C10-C9	3.45	1.62	1.56
4	B	1103	CHD	C11-C9	3.72	1.59	1.53
5	A	901	PP9	CBD-CAD	3.75	1.72	1.52
4	A	702	CHD	C11-C9	3.81	1.60	1.53
4	A	701	CHD	C11-C9	3.82	1.60	1.53
4	B	1104	CHD	C11-C9	3.83	1.60	1.53
5	B	1105	PP9	C3D-C2D	4.25	1.45	1.36
5	B	1105	PP9	C3C-C2C	4.30	1.46	1.40
5	B	1105	PP9	C1D-C2D	4.94	1.56	1.45
5	A	901	PP9	C2A-C3A	5.14	1.52	1.37
5	B	1105	PP9	C2A-C3A	5.49	1.53	1.37
5	A	901	PP9	CHC-C4B	7.05	1.41	1.35
5	A	901	PP9	C1D-C2D	7.52	1.62	1.45
5	A	901	PP9	C3B-C2B	8.67	1.55	1.36
5	B	1105	PP9	CHC-C4B	8.85	1.42	1.35
5	B	1105	PP9	C3B-C2B	9.74	1.57	1.36
5	B	1105	PP9	CHD-C1D	16.04	1.49	1.35
5	A	901	PP9	CHD-C1D	18.65	1.51	1.35
5	B	1105	PP9	C3C-C4C	18.93	1.67	1.40
5	A	901	PP9	C3C-C4C	21.20	1.70	1.40

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	PP9	C1D-C2D-C3D	-5.20	100.27	106.50
5	B	1105	PP9	C3B-C2B-C1B	-4.95	97.72	106.87
5	B	1105	PP9	C1D-C2D-C3D	-4.77	100.79	106.50
5	B	1105	PP9	CHC-C4B-NB	-4.40	120.80	128.67
5	A	901	PP9	CHC-C4B-NB	-4.28	121.01	128.67
4	B	1104	CHD	C18-C13-C12	-4.09	105.10	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	CHD	O12-C12-C13	-4.02	104.59	111.11
4	A	701	CHD	C19-C10-C1	-3.83	101.75	108.20
4	B	1103	CHD	O12-C12-C13	-3.83	104.90	111.11
4	B	1103	CHD	C19-C10-C1	-3.76	101.88	108.20
4	B	1103	CHD	C18-C13-C12	-3.73	105.45	109.09
4	A	702	CHD	C18-C13-C12	-3.73	105.45	109.09
5	A	901	PP9	C3B-C2B-C1B	-3.57	100.26	106.87
4	B	1104	CHD	C19-C10-C1	-3.50	102.31	108.20
4	A	701	CHD	C18-C13-C12	-3.46	105.71	109.09
4	A	702	CHD	C19-C10-C1	-3.34	102.59	108.20
4	A	702	CHD	O12-C12-C13	-3.33	105.71	111.11
5	B	1105	PP9	CHD-C1D-ND	-3.31	122.75	128.67
4	B	1104	CHD	O12-C12-C13	-3.18	105.96	111.11
4	B	1103	CHD	C9-C8-C7	-3.04	108.33	111.92
4	B	1103	CHD	C6-C5-C10	-2.87	109.49	112.66
5	A	901	PP9	CHB-C1B-NB	-2.83	119.52	124.91
4	A	701	CHD	C6-C5-C10	-2.69	109.69	112.66
4	A	701	CHD	C9-C8-C7	-2.68	108.75	111.92
4	A	702	CHD	C9-C11-C12	-2.60	111.08	114.36
4	B	1103	CHD	C16-C17-C13	-2.60	101.02	103.60
4	A	702	CHD	C16-C17-C13	-2.59	101.03	103.60
4	B	1104	CHD	C6-C5-C10	-2.53	109.86	112.66
4	A	702	CHD	C6-C5-C10	-2.53	109.87	112.66
4	B	1104	CHD	C11-C9-C10	-2.52	111.17	113.79
4	A	701	CHD	C9-C11-C12	-2.52	111.18	114.36
4	A	702	CHD	C9-C8-C7	-2.49	108.97	111.92
4	B	1104	CHD	C9-C11-C12	-2.47	111.24	114.36
4	B	1104	CHD	C9-C8-C7	-2.38	109.10	111.92
4	A	702	CHD	C11-C9-C10	-2.35	111.35	113.79
4	B	1103	CHD	C9-C11-C12	-2.35	111.40	114.36
4	B	1103	CHD	C11-C9-C10	-2.32	111.38	113.79
4	B	1104	CHD	C16-C17-C13	-2.29	101.32	103.60
5	B	1105	PP9	C4D-C3D-C2D	-2.27	104.28	106.81
4	A	701	CHD	C5-C4-C3	-2.12	109.77	112.91
4	B	1103	CHD	C5-C4-C3	-2.07	109.84	112.91
4	A	702	CHD	C19-C10-C9	2.02	114.21	111.18
4	A	701	CHD	C19-C10-C9	2.04	114.24	111.18
4	A	702	CHD	C1-C10-C5	2.06	111.19	107.81
5	B	1105	PP9	CAB-C3B-C4B	2.10	132.78	124.01
4	B	1104	CHD	C1-C10-C5	2.14	111.33	107.81
4	A	701	CHD	C1-C10-C5	2.21	111.44	107.81
5	A	901	PP9	C2C-C1C-NC	2.26	113.99	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1103	CHD	C1-C10-C5	2.27	111.53	107.81
5	A	901	PP9	CAD-C3D-C4D	2.31	129.18	125.06
5	A	901	PP9	CMD-C2D-C3D	2.35	132.77	125.94
4	B	1104	CHD	C6-C5-C4	2.51	113.85	111.05
4	B	1104	CHD	C11-C12-C13	2.51	113.75	111.20
4	A	702	CHD	C6-C5-C4	2.60	113.95	111.05
4	B	1103	CHD	C11-C12-C13	2.62	113.86	111.20
5	A	901	PP9	CMB-C2B-C1B	2.68	129.42	125.06
4	A	702	CHD	C11-C12-C13	2.70	113.94	111.20
5	A	901	PP9	CMC-C2C-C3C	2.71	130.40	125.09
4	A	701	CHD	C6-C5-C4	2.82	114.19	111.05
4	A	701	CHD	C11-C12-C13	2.90	114.14	111.20
5	B	1105	PP9	CMD-C2D-C1D	3.00	129.94	125.06
5	A	901	PP9	C2B-C1B-NB	3.08	117.57	110.55
5	A	901	PP9	CMA-C3A-C2A	3.09	131.69	125.24
4	A	702	CHD	C17-C13-C12	3.13	120.45	117.68
4	A	701	CHD	C17-C13-C12	3.15	120.48	117.68
5	B	1105	PP9	CMA-C3A-C2A	3.20	131.93	125.24
4	A	701	CHD	C17-C13-C14	3.23	103.32	100.05
5	B	1105	PP9	CAD-C3D-C4D	3.24	130.85	125.06
4	B	1103	CHD	C17-C13-C14	3.25	103.33	100.05
4	A	702	CHD	C17-C13-C14	3.32	103.41	100.05
4	B	1104	CHD	C17-C13-C12	3.33	120.63	117.68
4	B	1103	CHD	C17-C13-C12	3.34	120.64	117.68
5	B	1105	PP9	C2B-C1B-NB	3.37	118.23	110.55
4	B	1104	CHD	C17-C13-C14	3.39	103.48	100.05
5	B	1105	PP9	CMB-C2B-C1B	3.55	130.84	125.06
5	B	1105	PP9	CMC-C2C-C3C	3.59	132.10	125.09
4	B	1103	CHD	C6-C5-C4	3.61	115.07	111.05
5	A	901	PP9	CAA-C2A-C1A	4.03	131.38	127.01
5	A	901	PP9	C1D-ND-C4D	4.39	115.18	106.51
5	A	901	PP9	CAD-CBD-CGD	4.43	120.86	112.75
5	B	1105	PP9	C1D-ND-C4D	4.77	115.94	106.51
5	B	1105	PP9	CAD-CBD-CGD	5.82	123.42	112.75
5	B	1105	PP9	C3C-CAC-CBC	5.90	138.40	126.32
5	A	901	PP9	C3C-CAC-CBC	8.36	143.43	126.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	601	GOL	2	0
4	A	701	CHD	5	0
4	A	702	CHD	3	0
8	A	801	ACY	1	0
8	A	803	ACY	4	0
5	A	901	PP9	1	0
4	B	1103	CHD	3	0
5	B	1105	PP9	4	0
8	B	1106	ACY	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	359/359 (100%)	0.50	21 (5%) 26 35	27, 56, 82, 92	0
1	B	359/359 (100%)	0.41	17 (4%) 35 44	24, 51, 75, 86	0
All	All	718/718 (100%)	0.45	38 (5%) 30 39	24, 54, 79, 92	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	423	LEU	6.6
1	B	923	LEU	6.0
1	B	565	ARG	5.3
1	B	850	ILE	4.6
1	A	110	PHE	4.3
1	A	107	LEU	4.1
1	A	65	ARG	3.9
1	B	803	SER	3.7
1	A	350	ILE	3.5
1	A	409	PRO	3.4
1	A	102	PRO	3.4
1	A	356	LEU	3.2
1	B	715	ARG	3.0
1	A	212	GLN	2.6
1	B	713	VAL	2.6
1	A	106	LYS	2.6
1	A	66	LYS	2.6
1	B	566	LYS	2.5
1	A	213	VAL	2.5
1	B	854	GLN	2.4
1	B	858	LYS	2.4
1	B	610	PHE	2.4
1	A	150	LEU	2.4
1	B	607	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	606	LYS	2.2
1	A	280	VAL	2.2
1	A	407	VAL	2.2
1	A	277	PRO	2.2
1	B	805	VAL	2.2
1	B	650	LEU	2.2
1	A	281	SER	2.1
1	A	105	ASN	2.0
1	A	312	GLY	2.0
1	B	806	GLY	2.0
1	A	276	TYR	2.0
1	B	751	GLU	2.0
1	A	111	ILE	2.0
1	B	799	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
4	CHD	A	701	29/29	0.79	0.28	4.03	96,97,97,98	0
6	OXY	B	1001	2/2	0.75	0.26	3.92	62,62,62,63	0
8	ACY	A	803	4/4	0.84	0.27	2.81	64,64,64,65	4
7	GOL	A	601	6/6	0.88	0.29	2.65	48,49,50,50	0
8	ACY	A	801	4/4	0.89	0.25	2.60	55,55,55,55	4
4	CHD	B	1103	29/29	0.69	0.28	2.44	80,80,84,84	0
4	CHD	B	1104	29/29	0.83	0.34	1.40	98,98,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	ACY	B	1106	4/4	0.83	0.27	0.93	42,42,43,44	4
5	PP9	A	901	42/42	0.89	0.18	0.76	43,49,51,53	0
5	PP9	B	1105	42/42	0.92	0.18	0.40	38,42,46,47	0
4	CHD	A	702	29/29	0.83	0.30	0.34	96,96,97,97	0
3	FES	A	501	4/4	0.90	0.08	-2.38	55,56,56,56	0
3	FES	B	502	4/4	0.95	0.06	-2.41	53,54,54,55	0
2	PB	B	1102[A]	1/1	0.91	0.14	-	43,43,43,43	1
2	PB	A	1101[B]	1/1	0.83	0.15	-	49,49,49,49	1
2	PB	A	1101[A]	1/1	0.83	0.15	-	51,51,51,51	1
2	PB	B	1102[B]	1/1	0.91	0.14	-	43,43,43,43	1

6.5 Other polymers

There are no such residues in this entry.