



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:24 PM GMT

PDB ID : 3TTX
Title : Structure of the F413K variant of E. coli KatE
Authors : Loewen, P.C.; Jha, V.
Deposited on : 2011-09-15
Resolution : 1.74 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

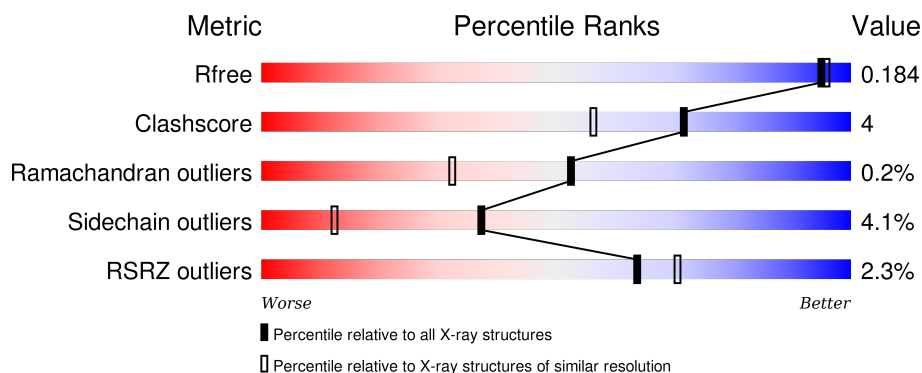
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	2417 (1.76-1.72)
Clashscore	102246	2570 (1.76-1.72)
Ramachandran outliers	100387	2544 (1.76-1.72)
Sidechain outliers	100360	2544 (1.76-1.72)
RSRZ outliers	91569	2420 (1.76-1.72)

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	753	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 86% 9% • • </div> </div>
1	B	753	<div> <div style="width: 4%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 4% </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 85% 9% • • </div> </div>
1	C	753	<div> <div style="width: 3%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 3% </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 82% 11% • • </div> </div>
1	D	753	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 85% 10% • • </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26010 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.

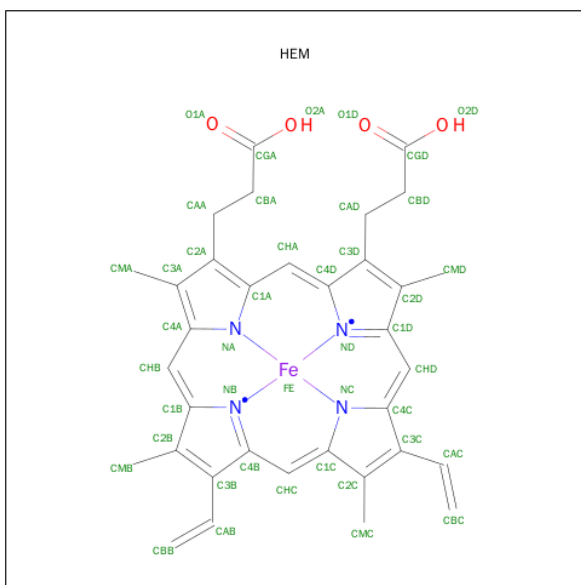
- Molecule 1 is a protein called Catalase HPIL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	1	0
			5745	3644	1007	1082	12			
1	B	726	Total	C	N	O	S	0	1	0
			5746	3645	1007	1082	12			
1	C	726	Total	C	N	O	S	0	1	0
			5745	3644	1007	1082	12			
1	D	726	Total	C	N	O	S	0	1	0
			5746	3645	1007	1082	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	413	LYS	PHE	ENGINEERED MUTATION	UNP P21179
B	413	LYS	PHE	ENGINEERED MUTATION	UNP P21179
C	413	LYS	PHE	ENGINEERED MUTATION	UNP P21179
D	413	LYS	PHE	ENGINEERED MUTATION	UNP P21179

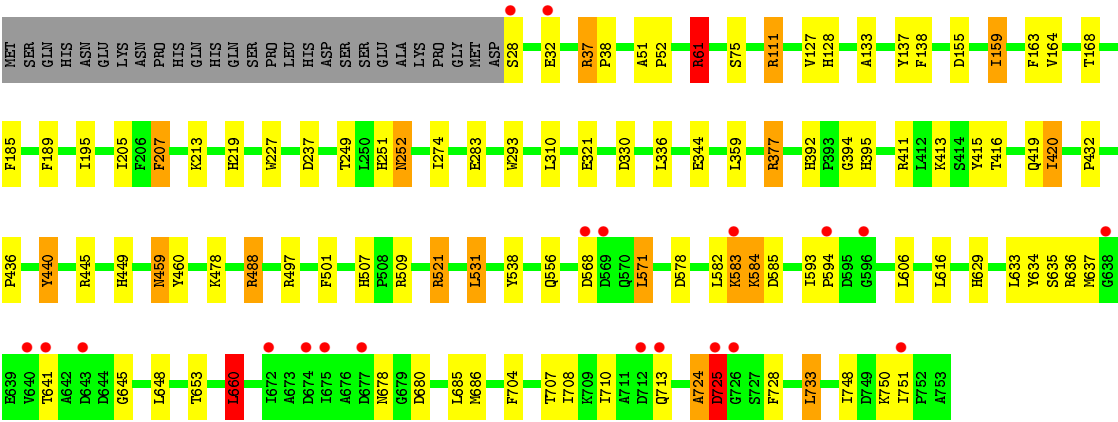
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



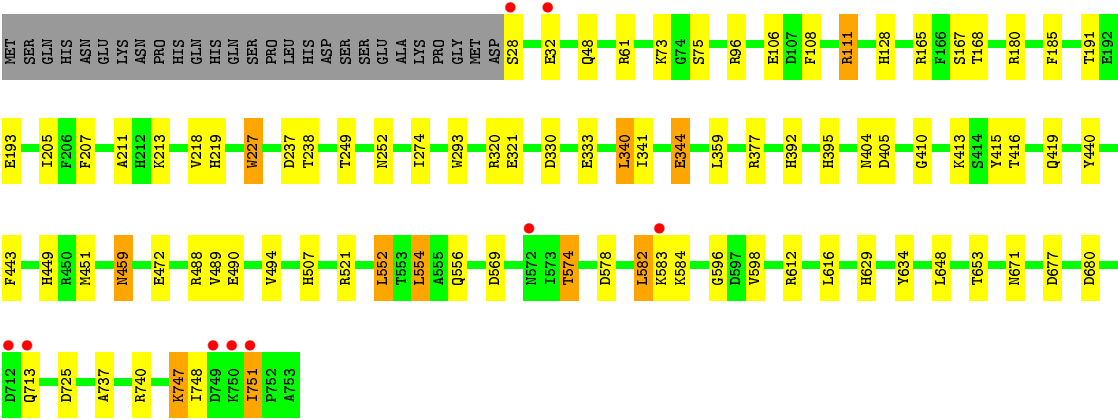
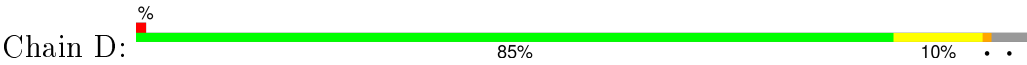
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	771	Total O 771 771	0	0
3	B	650	Total O 650 650	0	0
3	C	690	Total O 690 690	0	0
3	D	745	Total O 745 745	0	0



● Molecule 1: Catalase HP11



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.50Å 132.96Å 122.03Å 90.00° 109.69° 90.00°	Depositor
Resolution (Å)	35.18 – 1.74 35.18 – 1.74	Depositor EDS
% Data completeness (in resolution range)	97.0 (35.18-1.74) 97.1 (35.18-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.146 , 0.185 0.146 , 0.184	Depositor DCC
R_{free} test set	14075 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	12.3	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.6	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 278239 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	26010	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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, 0.375 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: HEM, OCS

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	1.27	19/5895 (0.3%)	1.03	15/8012 (0.2%)
1	B	1.22	9/5895 (0.2%)	1.04	16/8012 (0.2%)
1	C	1.23	13/5895 (0.2%)	1.03	17/8012 (0.2%)
1	D	1.25	12/5895 (0.2%)	1.04	19/8012 (0.2%)
All	All	1.24	53/23580 (0.2%)	1.04	67/32048 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	189	PHE	CE2-CZ	7.83	1.52	1.37
1	B	321	GLU	CB-CG	7.71	1.66	1.52
1	D	333	GLU	CD-OE2	-7.57	1.17	1.25
1	A	321	GLU	CD-OE1	7.52	1.33	1.25
1	C	321	GLU	CD-OE1	7.48	1.33	1.25
1	A	383	PHE	CE1-CZ	7.40	1.51	1.37
1	A	440	TYR	CE1-CZ	7.35	1.48	1.38
1	A	684	TYR	CD2-CE2	6.93	1.49	1.39
1	B	283	GLU	CG-CD	6.89	1.62	1.51
1	B	568	ASP	CB-CG	6.85	1.66	1.51
1	A	41	GLU	CG-CD	6.71	1.62	1.51
1	B	497	ARG	CZ-NH2	6.51	1.41	1.33
1	D	320	ARG	CZ-NH1	6.12	1.41	1.33
1	A	334	TYR	CD1-CE1	6.11	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	344	GLU	CD-OE1	6.10	1.32	1.25
1	C	419	GLN	CB-CG	6.01	1.68	1.52
1	C	207	PHE	CE1-CZ	6.00	1.48	1.37
1	A	489	VAL	CB-CG1	5.97	1.65	1.52
1	D	167	SER	CB-OG	5.87	1.49	1.42
1	A	440	TYR	CD1-CE1	5.77	1.48	1.39
1	D	494	VAL	CB-CG1	5.76	1.65	1.52
1	D	443	PHE	CG-CD2	5.72	1.47	1.38
1	A	411	ARG	CZ-NH1	5.71	1.40	1.33
1	C	497	ARG	CZ-NH2	5.70	1.40	1.33
1	B	163	PHE	CE1-CZ	5.68	1.48	1.37
1	C	127	VAL	CB-CG2	5.61	1.64	1.52
1	D	293	TRP	CE3-CZ3	5.57	1.48	1.38
1	C	501	PHE	CE1-CZ	5.55	1.48	1.37
1	B	331	PHE	CE2-CZ	5.55	1.47	1.37
1	D	489	VAL	CB-CG1	5.51	1.64	1.52
1	A	338	PHE	CE1-CZ	5.50	1.47	1.37
1	A	242	TYR	CD1-CE1	5.47	1.47	1.39
1	A	213	LYS	CD-CE	5.46	1.64	1.51
1	D	108	PHE	CE2-CZ	5.46	1.47	1.37
1	A	603	VAL	CB-CG1	-5.45	1.41	1.52
1	C	538	TYR	CD2-CE2	5.40	1.47	1.39
1	A	239	PHE	CE1-CZ	5.38	1.47	1.37
1	D	193	GLU	CG-CD	5.35	1.59	1.51
1	D	472	GLU	CD-OE2	5.32	1.31	1.25
1	A	190	TYR	CE1-CZ	5.32	1.45	1.38
1	B	521	ARG	CG-CD	5.31	1.65	1.51
1	A	289	VAL	CB-CG1	5.31	1.64	1.52
1	A	111	ARG	CG-CD	5.30	1.65	1.51
1	C	111	ARG	CG-CD	5.18	1.64	1.51
1	B	402	PHE	CD2-CE2	5.17	1.49	1.39
1	C	138	PHE	CE2-CZ	5.15	1.47	1.37
1	C	440	TYR	CE1-CZ	5.14	1.45	1.38
1	D	218	VAL	CB-CG2	5.09	1.63	1.52
1	C	163	PHE	CD1-CE1	5.08	1.49	1.39
1	A	303	VAL	CB-CG1	5.06	1.63	1.52
1	A	428	PHE	CE2-CZ	5.06	1.47	1.37
1	B	227	TRP	CZ3-CH2	5.05	1.48	1.40
1	D	106	GLU	CD-OE2	5.02	1.31	1.25

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ARG	NE-CZ-NH2	-13.18	113.71	120.30
1	B	111	ARG	NE-CZ-NH1	-11.18	114.71	120.30
1	C	111	ARG	NE-CZ-NH1	-10.96	114.82	120.30
1	B	521	ARG	NE-CZ-NH2	10.90	125.75	120.30
1	D	320	ARG	NE-CZ-NH2	-8.93	115.84	120.30
1	D	61	ARG	NE-CZ-NH2	7.87	124.24	120.30
1	D	554	LEU	CB-CG-CD2	7.64	123.98	111.00
1	A	111	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	C	37	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	B	130	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	B	350	ASP	CB-CG-OD1	-7.09	111.92	118.30
1	B	96	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	D	111	ARG	NE-CZ-NH1	-7.07	116.77	120.30
1	B	70	ASP	CB-CG-OD1	7.03	124.63	118.30
1	B	111	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	A	377	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	D	340	LEU	CB-CG-CD1	6.71	122.40	111.00
1	D	165	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	C	420	ILE	CG1-CB-CG2	-6.46	97.18	111.40
1	B	377	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	C	660	LEU	CB-CG-CD1	6.43	121.93	111.00
1	D	680	ASP	CB-CG-OD2	6.42	124.08	118.30
1	C	509	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	D	377	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	C	37	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	521	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	B	130	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	B	72	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	C	377	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	A	552	LEU	CB-CG-CD1	6.23	121.59	111.00
1	B	121	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	A	542	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	C	61	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	C	155	ASP	CB-CG-OD1	-6.03	112.88	118.30
1	A	740	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	445	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	D	340	LEU	CB-CG-CD2	5.86	120.96	111.00
1	C	571	LEU	CA-CB-CG	5.85	128.76	115.30
1	A	710	ILE	N-CA-C	5.80	126.66	111.00
1	B	419	GLN	CB-CA-C	5.71	121.82	110.40
1	C	213	LYS	CD-CE-NZ	-5.68	98.64	111.70
1	D	582	LEU	CB-CG-CD1	5.55	120.43	111.00
1	A	350	ASP	CB-CG-OD1	-5.54	113.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	ARG	CG-CD-NE	-5.51	100.23	111.80
1	A	420	ILE	CG1-CB-CG2	-5.50	99.31	111.40
1	B	615	ASP	CB-CG-OD2	5.46	123.21	118.30
1	D	569	ASP	CB-CG-OD1	5.45	123.21	118.30
1	D	96	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	733	LEU	CB-CG-CD1	5.42	120.21	111.00
1	C	531	LEU	CB-CG-CD1	5.41	120.20	111.00
1	A	419	GLN	CB-CA-C	5.40	121.19	110.40
1	D	180	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	D	344	GLU	CA-CB-CG	5.35	125.17	113.40
1	B	267	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	598	VAL	CG1-CB-CG2	5.27	119.33	110.90
1	B	521	ARG	CD-NE-CZ	5.26	130.96	123.60
1	D	740	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	260	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	725	ASP	N-CA-C	5.20	125.03	111.00
1	D	61	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	121	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	419	GLN	CB-CA-C	5.17	120.75	110.40
1	C	585	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	213	LYS	CD-CE-NZ	-5.15	99.85	111.70
1	D	419	GLN	CB-CA-C	5.13	120.66	110.40
1	D	725	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	241	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	724	ALA	Peptide
1	C	725	ASP	Peptide

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	5745	0	5579	40	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5746	0	5584	51	1
1	C	5745	0	5580	61	0
1	D	5746	0	5584	50	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
2	C	43	0	30	4	0
2	D	43	0	30	1	0
3	A	771	0	0	14	0
3	B	650	0	0	12	0
3	C	690	0	0	18	1
3	D	745	0	0	13	1
All	All	26010	0	22447	196	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 4.

All (196) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:HIS:ND1	1:D:415:TYR:CB	1.69	1.52
1:B:392:HIS:ND1	1:B:415:TYR:CB	1.71	1.49
1:C:392:HIS:ND1	1:C:415:TYR:CB	1.84	1.40
1:D:449[B]:HIS:CE1	3:D:3262:HOH:O	1.71	1.32
1:D:392:HIS:CE1	1:D:415:TYR:HB2	1.64	1.29
1:C:449[A]:HIS:CE1	3:C:3266:HOH:O	1.65	1.26
1:B:392:HIS:CE1	1:B:415:TYR:HB2	1.71	1.24
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.91	1.23
1:A:713:GLN:HG2	3:A:2153:HOH:O	1.40	1.19
1:B:392:HIS:ND1	1:B:415:TYR:HB2	0.80	1.12
1:D:392:HIS:ND1	1:D:415:TYR:HB2	0.80	1.11
1:D:451:MET:SD	3:D:3264:HOH:O	2.07	1.10
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.88	1.07
1:A:710:ILE:HG12	1:A:715:GLU:OE1	1.55	1.05
1:B:267:ARG:HG3	3:B:3310:HOH:O	1.64	0.97
1:A:111:ARG:HB2	3:A:3292:HOH:O	1.68	0.92
1:D:521:ARG:HD3	3:D:3252:HOH:O	1.78	0.82
1:A:28:SER:OG	1:A:28:SER:O	1.98	0.80
1:C:416:THR:HG21	3:C:3270:HOH:O	1.81	0.79
1:B:521:ARG:HD3	3:B:3047:HOH:O	1.81	0.79
3:B:2705:HOH:O	1:D:73:LYS:CD	2.30	0.79
3:B:2705:HOH:O	1:D:73:LYS:HE3	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2705:HOH:O	1:D:73:LYS:CE	2.34	0.74
1:D:552:LEU:O	1:D:552:LEU:HD23	1.87	0.74
3:B:2705:HOH:O	1:D:73:LYS:HD3	1.89	0.72
1:C:704:PHE:O	1:C:707:THR:HG22	1.90	0.72
1:D:629:HIS:HD2	3:D:1554:HOH:O	1.74	0.71
1:D:321:GLU:HG3	3:D:2151:HOH:O	1.92	0.70
1:C:283:GLU:OE1	3:C:2292:HOH:O	2.09	0.69
1:B:533:LYS:HE2	3:B:3100:HOH:O	1.94	0.68
1:D:392:HIS:ND1	1:D:415:TYR:HB3	1.99	0.68
1:A:479:ARG:NH2	3:A:2607:HOH:O	2.08	0.67
1:C:416:THR:CG2	3:C:3270:HOH:O	2.40	0.66
1:B:583:LYS:NZ	1:B:583:LYS:H	1.95	0.65
1:D:677:ASP:HB2	3:D:3247:HOH:O	1.95	0.65
1:A:29:LEU:HB2	3:C:2405:HOH:O	1.98	0.63
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.63	0.63
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.80	0.63
1:B:281:ASN:OD1	1:B:283:GLU:HG3	1.99	0.63
1:C:488:ARG:HD2	3:C:2379:HOH:O	1.98	0.62
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.82	0.62
1:A:751:ILE:O	1:A:751:ILE:HD12	1.97	0.62
1:A:111:ARG:HD3	3:A:3287:HOH:O	1.99	0.62
1:B:111:ARG:HB2	3:B:3290:HOH:O	1.99	0.61
1:B:449[A]:HIS:CG	1:D:449[A]:HIS:CG	2.44	0.61
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.83	0.60
1:B:392:HIS:ND1	1:B:415:TYR:HB3	2.04	0.60
1:A:395:HIS:HE1	3:A:3308:HOH:O	1.84	0.60
1:D:416:THR:HG21	3:D:3280:HOH:O	2.00	0.60
1:D:552:LEU:CD2	1:D:556:GLN:NE2	2.65	0.59
1:B:583:LYS:O	1:B:584:LYS:HB3	2.02	0.59
1:C:449[A]:HIS:ND1	3:C:3267:HOH:O	0.76	0.59
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.64	0.59
1:A:29:LEU:HD22	3:C:2405:HOH:O	2.02	0.58
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	1.87	0.57
1:B:612:ARG:NH1	1:B:612:ARG:HB2	2.20	0.57
1:B:359:LEU:H	1:B:507:HIS:HD2	1.52	0.57
1:C:583:LYS:O	1:C:584:LYS:HB3	2.04	0.57
1:D:111:ARG:HD3	3:D:3305:HOH:O	2.05	0.57
1:C:556:GLN:NE2	3:C:2533:HOH:O	2.37	0.56
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.87	0.56
1:A:416:THR:HG21	3:A:3307:HOH:O	2.05	0.56
2:B:760:HEM:CMC	2:B:760:HEM:HBC2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:ASN:OD1	1:B:680:ASP:HB2	2.06	0.55
1:B:416:THR:HG21	3:B:3285:HOH:O	2.05	0.55
1:A:533:LYS:NZ	3:A:2232:HOH:O	2.38	0.55
1:C:678:ASN:OD1	1:C:680:ASP:HB2	2.06	0.55
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	1.87	0.55
1:A:36:HIS:HE1	3:A:1872:HOH:O	1.89	0.55
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.89	0.55
1:B:629:HIS:HD2	3:B:1055:HOH:O	1.88	0.55
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.89	0.55
1:C:488:ARG:CD	3:C:2379:HOH:O	2.52	0.54
1:B:612:ARG:HG3	1:B:612:ARG:O	2.06	0.54
1:B:634:TYR:O	1:B:653:THR:HA	2.07	0.54
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.23	0.54
1:B:395:HIS:HE1	3:B:3300:HOH:O	1.91	0.54
2:C:760:HEM:CMB	2:C:760:HEM:HBB2	2.38	0.54
1:C:578:ASP:HB2	1:C:582:LEU:O	2.07	0.53
1:B:38:PRO:HG2	1:B:51:ALA:HB2	1.91	0.53
1:D:747:LYS:HD2	1:D:747:LYS:H	1.74	0.53
1:D:341:ILE:HG13	3:D:3022:HOH:O	2.09	0.52
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.39	0.52
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.92	0.52
1:A:111:ARG:NH2	3:A:3292:HOH:O	2.43	0.52
1:C:359:LEU:H	1:C:507:HIS:HD2	1.58	0.52
1:B:448:MET:HG3	1:B:449[A]:HIS:CD2	2.45	0.51
1:B:725:ASP:OD2	1:B:727:SER:HB3	2.11	0.51
1:A:111:ARG:CD	3:A:3287:HOH:O	2.58	0.51
1:B:449[B]:HIS:CD2	1:D:449[B]:HIS:CD2	2.99	0.50
1:C:724:ALA:O	1:C:725:ASP:HB2	2.11	0.50
1:C:629:HIS:HD2	3:C:1129:HOH:O	1.95	0.50
1:C:748:ILE:O	1:C:751:ILE:HG22	2.12	0.50
1:B:686:MET:HB3	1:B:751:ILE:HD11	1.93	0.50
1:D:449[B]:HIS:NE2	3:D:3262:HOH:O	2.03	0.50
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.43	0.49
1:B:37:ARG:HD3	3:B:2886:HOH:O	2.12	0.49
2:B:760:HEM:HMB1	2:B:760:HEM:HBB2	1.94	0.49
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.95	0.49
1:D:552:LEU:HD22	1:D:556:GLN:NE2	2.27	0.49
2:B:760:HEM:CMB	2:B:760:HEM:HBB2	2.43	0.49
1:B:556:GLN:HG2	1:B:566:LEU:HD23	1.94	0.49
2:C:760:HEM:HMB1	2:C:760:HEM:HBB2	1.94	0.48
1:D:634:TYR:O	1:D:653:THR:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ARG:HD3	3:C:3296:HOH:O	2.13	0.48
1:C:686:MET:HB3	1:C:751:ILE:HD11	1.94	0.48
1:D:578:ASP:CG	1:D:583:LYS:HG2	2.33	0.48
1:D:552:LEU:C	1:D:552:LEU:HD23	2.33	0.48
1:A:469:TRP:CE3	1:A:471:ARG:HG3	2.48	0.48
1:B:392:HIS:CG	1:B:415:TYR:CB	2.83	0.48
1:A:111:ARG:CZ	3:A:3292:HOH:O	2.62	0.48
1:D:671:ASN:ND2	3:D:2248:HOH:O	2.41	0.47
2:B:760:HEM:HMC1	2:B:760:HEM:HBC2	1.95	0.47
1:D:574:THR:HG23	3:D:1614:HOH:O	2.14	0.47
1:B:583:LYS:HZ3	1:B:583:LYS:H	1.63	0.46
1:C:395:HIS:HE1	3:C:3269:HOH:O	1.99	0.46
1:D:395:HIS:HE1	3:D:3303:HOH:O	1.98	0.46
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.51	0.46
1:D:488:ARG:NH1	1:D:490:GLU:OE1	2.46	0.46
1:B:207:PHE:O	1:B:249:THR:HA	2.16	0.46
1:D:128:HIS:HA	1:D:168:THR:O	2.15	0.46
1:A:449[A]:HIS:CD2	1:C:449[A]:HIS:CD2	3.03	0.46
1:C:111:ARG:CD	3:C:3296:HOH:O	2.64	0.46
1:C:195:ILE:HD11	1:C:436:PRO:HA	1.98	0.46
1:A:36:HIS:CD2	1:A:36:HIS:H	2.35	0.45
1:B:562:LEU:HA	1:C:637:MET:HB2	1.99	0.45
1:C:359:LEU:H	1:C:507:HIS:CD2	2.35	0.45
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.52	0.45
1:B:392:HIS:CD2	1:B:394:GLY:H	2.34	0.44
1:D:552:LEU:HD21	1:D:556:GLN:NE2	2.32	0.44
1:C:634:TYR:O	1:C:653:THR:HA	2.17	0.44
3:A:3250:HOH:O	1:C:111:ARG:HD3	2.16	0.44
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.99	0.44
1:C:51:ALA:HB1	1:C:52:PRO:HD2	2.00	0.44
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.52	0.44
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.21	0.44
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.99	0.44
1:C:28:SER:N	3:C:2523:HOH:O	2.50	0.44
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:CG	2.54	0.44
1:B:612:ARG:HH11	1:B:612:ARG:HB2	1.82	0.44
1:B:359:LEU:H	1:B:507:HIS:CD2	2.35	0.44
1:B:344:GLU:H	1:B:344:GLU:CD	2.21	0.44
1:C:459:ASN:HD22	1:C:459:ASN:H	1.66	0.44
1:D:359:LEU:H	1:D:507:HIS:HD2	1.66	0.44
1:C:411:ARG:HG2	2:C:760:HEM:C2C	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:MET:O	1:A:449[B]:HIS:HB2	2.18	0.43
1:A:252:ASN:HA	1:A:252:ASN:HD22	1.70	0.43
1:C:310:LEU:HD13	1:C:660:LEU:HB3	1.99	0.43
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.99	0.43
1:C:252:ASN:HD22	1:C:252:ASN:HA	1.65	0.43
1:B:725:ASP:OD2	1:B:727:SER:N	2.49	0.43
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.33	0.43
1:A:319:ARG:HD3	1:D:227:TRP:O	2.18	0.43
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.54	0.43
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.00	0.43
1:B:97:ALA:O	1:B:101:GLY:HA3	2.18	0.43
1:C:207:PHE:O	1:C:249:THR:HA	2.18	0.43
1:B:583:LYS:HZ2	1:B:583:LYS:H	1.63	0.43
1:A:416:THR:HB	3:A:3250:HOH:O	2.18	0.43
1:C:724:ALA:O	1:C:725:ASP:CB	2.67	0.43
1:D:552:LEU:C	1:D:552:LEU:CD2	2.86	0.43
1:C:634:TYR:CG	1:C:635:SER:N	2.87	0.43
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.34	0.42
1:D:748:ILE:HA	1:D:751:ILE:HG23	2.01	0.42
1:A:92:GLN:HA	1:D:213:LYS:HD3	2.00	0.42
1:C:460:TYR:CE2	1:D:238:THR:HB	2.54	0.42
1:A:411:ARG:HG2	2:A:760:HEM:C2C	2.54	0.42
1:B:558:VAL:HG12	1:B:562:LEU:HD22	2.01	0.42
1:A:460:TYR:CE2	1:B:238:THR:HB	2.54	0.42
1:C:392:HIS:CD2	1:C:394:GLY:H	2.37	0.42
1:C:449[A]:HIS:CE1	3:C:3267:HOH:O	1.64	0.42
1:B:38:PRO:HA	1:B:48:GLN:OE1	2.20	0.42
1:C:583:LYS:HE2	1:C:583:LYS:HB2	1.76	0.42
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.55	0.42
1:C:521:ARG:HB2	1:C:521:ARG:HH11	1.85	0.42
1:C:593:ILE:HA	1:C:594:PRO:HD2	1.92	0.41
1:D:48:GLN:HB3	1:D:48:GLN:HE21	1.74	0.41
1:D:552:LEU:HD21	1:D:556:GLN:CD	2.41	0.41
1:B:732:LEU:HD13	1:B:732:LEU:C	2.41	0.41
1:C:293:TRP:CZ3	1:C:336:LEU:HB2	2.56	0.41
1:D:207:PHE:O	1:D:249:THR:HA	2.20	0.41
1:A:128:HIS:HA	1:A:168:THR:O	2.21	0.41
1:C:725:ASP:HA	1:C:728:PHE:HB3	2.03	0.41
1:D:596:GLY:HA3	1:D:737:ALA:O	2.21	0.41
3:A:938:HOH:O	1:C:52:PRO:HG3	2.20	0.41
1:C:748:ILE:O	1:C:751:ILE:CG2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:PRO:HG2	1:C:51:ALA:HB2	2.03	0.40
1:B:369:ARG:HE	1:B:369:ARG:HB2	1.23	0.40
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.56	0.40
1:D:404:ASN:O	1:D:405:ASP:C	2.59	0.40
1:A:104:LEU:HB3	3:C:775:HOH:O	2.21	0.40
1:C:128:HIS:HA	1:C:168:THR:O	2.20	0.40
1:C:61:ARG:HG3	3:C:2648:HOH:O	2.20	0.40
1:B:521:ARG:HD2	1:B:745:ILE:HG21	2.03	0.40
1:C:641:THR:CG2	1:C:645:GLY:HA2	2.51	0.40
1:C:133:ALA:HA	1:C:164:VAL:O	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)
1:A:59:ASP:OD1	1:B:369:ARG:NH1[2_545]	2.10	0.10
3:C:2040:HOH:O	3:D:2980:HOH:O[2_545]	2.13	0.07

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	724/753 (96%)	703 (97%)	19 (3%)	2 (0%)	46	26
1	B	724/753 (96%)	703 (97%)	19 (3%)	2 (0%)	46	26
1	C	724/753 (96%)	701 (97%)	21 (3%)	2 (0%)	46	26
1	D	724/753 (96%)	708 (98%)	15 (2%)	1 (0%)	56	36
All	All	2896/3012 (96%)	2815 (97%)	74 (3%)	7 (0%)	52	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	711	ALA
1	B	725	ASP
1	A	75	SER
1	C	75	SER
1	B	75	SER
1	C	725	ASP
1	D	75	SER

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	611/635 (96%)	596 (98%)	15 (2%)	55	29
1	B	611/635 (96%)	585 (96%)	26 (4%)	35	11
1	C	611/635 (96%)	577 (94%)	34 (6%)	26	6
1	D	611/635 (96%)	587 (96%)	24 (4%)	39	13
All	All	2444/2540 (96%)	2345 (96%)	99 (4%)	37	12

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	73	LYS
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	252	ASN
1	A	369	ARG
1	A	420	ILE
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	732	LEU
1	A	750	LYS

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Mol	Chain	Res	Type
1	B	142	LYS
1	B	185	PHE
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN
1	B	283	GLU
1	B	369	ARG
1	B	370	VAL
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	595	ASP
1	B	612	ARG
1	B	621	LYS
1	B	633	LEU
1	B	703	LYS
1	B	713	GLN
1	B	751	ILE
1	C	32	GLU
1	C	37	ARG
1	C	61	ARG
1	C	159	ILE
1	C	185	PHE
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	377	ARG
1	C	413	LYS
1	C	420	ILE
1	C	432	PRO
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS

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Mol	Chain	Res	Type
1	C	488	ARG
1	C	521	ARG
1	C	531	LEU
1	C	568	ASP
1	C	571	LEU
1	C	583	LYS
1	C	584	LYS
1	C	606	LEU
1	C	616	LEU
1	C	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	713	GLN
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS
1	D	28	SER
1	D	32	GLU
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	340	LEU
1	D	344	GLU
1	D	413	LYS
1	D	440	TYR
1	D	459	ASN
1	D	552	LEU
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	584	LYS
1	D	612	ARG
1	D	616	LEU
1	D	648	LEU
1	D	713	GLN
1	D	747	LYS
1	D	751	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	556	GLN
1	A	713	GLN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	252	ASN
1	C	368	GLN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	459	ASN
1	D	507	HIS
1	D	546	GLN
1	D	556	GLN
1	D	629	HIS
1	D	671	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	OCS	A	669	1	7,8,9	0.85	0	7,11,13	0.90	0
1	OCS	B	669	1	7,8,9	0.79	0	7,11,13	3.05	2 (28%)
1	OCS	C	669	1	7,8,9	1.73	1 (14%)	7,11,13	1.75	2 (28%)
1	OCS	D	669	1	7,8,9	1.45	1 (14%)	7,11,13	2.52	2 (28%)

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
1	OCS	A	669	1	-	1/4/7/9	0/0/0/0
1	OCS	B	669	1	-	1/4/7/9	0/0/0/0
1	OCS	C	669	1	-	1/4/7/9	0/0/0/0
1	OCS	D	669	1	-	1/4/7/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	669	OCS	CB-SG	2.81	1.82	1.77
1	C	669	OCS	CB-SG	3.61	1.83	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	669	OCS	OD3-SG-CB	-3.65	103.87	106.94
1	D	669	OCS	OD3-SG-CB	-3.31	104.15	106.94
1	C	669	OCS	OD1-SG-CB	-2.30	105.00	106.94
1	C	669	OCS	OD3-SG-CB	3.03	109.50	106.94
1	D	669	OCS	OD1-SG-CB	5.52	111.59	106.94
1	B	669	OCS	OD1-SG-CB	6.89	112.75	106.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	669	OCS	SG-CB-CA-N
1	B	669	OCS	SG-CB-CA-N
1	A	669	OCS	SG-CB-CA-N
1	D	669	OCS	SG-CB-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	HEM	A	760	1,3	30,50,50	2.36	6 (20%)	24,82,82	3.23	15 (62%)
2	HEM	B	760	1,3	30,50,50	2.17	9 (30%)	24,82,82	3.24	16 (66%)
2	HEM	C	760	1,3	30,50,50	2.85	11 (36%)	24,82,82	3.41	13 (54%)
2	HEM	D	760	1,3	30,50,50	2.36	6 (20%)	24,82,82	3.30	12 (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
2	HEM	A	760	1,3	-	0/10/54/54	0/0/8/8
2	HEM	B	760	1,3	-	0/10/54/54	0/0/8/8
2	HEM	C	760	1,3	-	0/10/54/54	0/0/8/8
2	HEM	D	760	1,3	-	0/10/54/54	0/0/8/8

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	760	HEM	C3B-C4B	-11.10	1.41	1.51
2	D	760	HEM	C3B-C4B	-8.31	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	C3D-C4D	-7.42	1.42	1.51
2	A	760	HEM	C3B-C4B	-7.24	1.45	1.51
2	B	760	HEM	C3B-C4B	-5.91	1.46	1.51
2	C	760	HEM	C3D-C4D	-5.49	1.44	1.51
2	D	760	HEM	C3D-C4D	-5.21	1.44	1.51
2	B	760	HEM	C2C-C1C	-4.09	1.44	1.52
2	D	760	HEM	C2C-C1C	-3.93	1.45	1.52
2	C	760	HEM	C2C-C1C	-3.45	1.46	1.52
2	B	760	HEM	C3D-C4D	-3.22	1.47	1.51
2	A	760	HEM	C2C-C1C	-3.01	1.46	1.52
2	B	760	HEM	C2D-C1D	-2.84	1.42	1.51
2	A	760	HEM	C2D-C1D	-2.81	1.42	1.51
2	D	760	HEM	C2D-C1D	-2.47	1.43	1.51
2	B	760	HEM	C2B-C1B	-2.18	1.44	1.51
2	C	760	HEM	CMC-C2C	2.01	1.57	1.53
2	C	760	HEM	CMA-C3A	2.07	1.55	1.51
2	A	760	HEM	C1C-NC	2.12	1.38	1.36
2	C	760	HEM	FE-NC	2.18	2.04	1.95
2	B	760	HEM	FE-ND	2.18	2.09	1.97
2	D	760	HEM	FE-NC	2.38	2.05	1.95
2	C	760	HEM	C3B-CAB	2.53	1.56	1.51
2	C	760	HEM	C4C-NC	2.63	1.39	1.36
2	C	760	HEM	FE-ND	2.73	2.12	1.97
2	B	760	HEM	CMA-C3A	2.77	1.57	1.51
2	B	760	HEM	FE-NB	2.88	2.12	1.97
2	D	760	HEM	C4C-NC	2.97	1.39	1.36
2	C	760	HEM	CAA-C2A	3.09	1.57	1.52
2	A	760	HEM	CMC-C2C	3.40	1.61	1.53
2	C	760	HEM	C1C-NC	3.94	1.40	1.36
2	B	760	HEM	FE-NC	5.14	2.16	1.95

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	760	HEM	CBD-CAD-C3D	-9.48	85.97	113.55
2	D	760	HEM	CBD-CAD-C3D	-9.38	86.26	113.55
2	A	760	HEM	CBD-CAD-C3D	-8.53	88.72	113.55
2	B	760	HEM	CBD-CAD-C3D	-7.65	91.30	113.55
2	C	760	HEM	C3B-CAB-CBB	-5.83	115.51	124.46
2	A	760	HEM	C3C-CAC-CBC	-5.15	116.56	124.46
2	B	760	HEM	CAA-CBA-CGA	-5.04	103.51	112.75
2	D	760	HEM	C3B-CAB-CBB	-4.41	117.69	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	HEM	C3C-CAC-CBC	-4.29	117.87	124.46
2	D	760	HEM	CAA-CBA-CGA	-4.13	105.18	112.75
2	B	760	HEM	C3B-C4B-NB	-4.00	103.99	111.63
2	C	760	HEM	CAA-CBA-CGA	-3.77	105.83	112.75
2	D	760	HEM	CMA-C3A-C4A	-3.48	122.61	128.36
2	D	760	HEM	CAA-C2A-C1A	-3.42	123.30	127.01
2	A	760	HEM	CMA-C3A-C4A	-3.42	122.71	128.36
2	D	760	HEM	CAD-CBD-CGD	-3.28	99.62	113.02
2	C	760	HEM	C3C-CAC-CBC	-3.20	119.55	124.46
2	A	760	HEM	C3B-C4B-NB	-3.04	105.81	111.63
2	C	760	HEM	CAD-CBD-CGD	-2.78	101.66	113.02
2	A	760	HEM	CAA-CBA-CGA	-2.70	107.79	112.75
2	D	760	HEM	C3C-CAC-CBC	-2.54	120.55	124.46
2	A	760	HEM	C4B-CHC-C1C	-2.41	121.80	125.82
2	B	760	HEM	C3B-CAB-CBB	-2.36	120.83	124.46
2	A	760	HEM	C1D-CHD-C4C	-2.24	122.07	125.82
2	B	760	HEM	CAA-C2A-C1A	-2.23	124.59	127.01
2	C	760	HEM	CMA-C3A-C4A	-2.21	124.71	128.36
2	A	760	HEM	CAD-CBD-CGD	-2.13	104.31	113.02
2	C	760	HEM	C3B-C4B-NB	-2.12	107.58	111.63
2	B	760	HEM	C2C-C1C-NC	-2.05	106.76	110.21
2	B	760	HEM	CAD-CBD-CGD	-2.04	104.70	113.02
2	C	760	HEM	C2D-C3D-C4D	2.04	104.96	101.50
2	B	760	HEM	CMD-C2D-C3D	2.22	124.18	114.35
2	D	760	HEM	C2D-C3D-C4D	2.33	105.45	101.50
2	B	760	HEM	CHC-C4B-NB	2.34	130.16	124.52
2	A	760	HEM	C2D-C3D-C4D	2.39	105.56	101.50
2	A	760	HEM	CMD-C2D-C3D	2.48	125.31	114.35
2	B	760	HEM	C2D-C3D-C4D	2.60	105.90	101.50
2	C	760	HEM	CMD-C2D-C3D	2.74	126.47	114.35
2	D	760	HEM	CMC-C2C-C3C	2.82	123.56	116.53
2	A	760	HEM	CAD-C3D-C2D	2.93	121.63	113.22
2	B	760	HEM	C2C-C1C-CHC	3.03	128.29	123.68
2	A	760	HEM	C3B-C4B-CHC	3.04	127.44	123.16
2	C	760	HEM	CMC-C2C-C3C	3.76	125.92	116.53
2	D	760	HEM	CAD-C3D-C2D	3.86	124.32	113.22
2	B	760	HEM	CAD-C3D-C2D	3.88	124.38	113.22
2	A	760	HEM	CMB-C2B-C3B	4.05	126.64	116.53
2	A	760	HEM	CMC-C2C-C3C	4.07	126.68	116.53
2	C	760	HEM	CAD-C3D-C2D	4.31	125.60	113.22
2	B	760	HEM	CMC-C2C-C3C	4.60	128.00	116.53
2	B	760	HEM	CMB-C2B-C3B	4.63	128.08	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	760	HEM	CAD-C3D-C4D	4.80	129.39	112.47
2	B	760	HEM	CAD-C3D-C4D	4.80	129.40	112.47
2	D	760	HEM	CAD-C3D-C4D	5.02	130.19	112.47
2	D	760	HEM	CMB-C2B-C3B	5.14	129.37	116.53
2	C	760	HEM	CMB-C2B-C3B	5.20	129.52	116.53
2	A	760	HEM	CAD-C3D-C4D	5.74	132.70	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	760	HEM	2	0
2	B	760	HEM	4	0
2	C	760	HEM	4	0
2	D	760	HEM	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	725/753 (96%)	-0.52	11 (1%) 76 82	4, 10, 27, 46	1 (0%)
1	B	725/753 (96%)	-0.34	27 (3%) 45 51	5, 12, 33, 48	1 (0%)
1	C	725/753 (96%)	-0.39	20 (2%) 56 62	5, 11, 32, 47	1 (0%)
1	D	725/753 (96%)	-0.55	9 (1%) 81 87	4, 10, 26, 46	1 (0%)
All	All	2900/3012 (96%)	-0.45	67 (2%) 64 70	4, 11, 31, 48	4 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	7.2
1	A	710	ILE	7.1
1	B	28	SER	4.5
1	D	28	SER	4.4
1	B	32	GLU	4.4
1	A	32	GLU	4.3
1	A	713	GLN	4.2
1	B	673	ALA	4.1
1	A	711	ALA	3.8
1	A	28	SER	3.7
1	C	726	GLY	3.7
1	B	713	GLN	3.6
1	C	594	PRO	3.5
1	B	711	ALA	3.3
1	D	749	ASP	3.3
1	C	751	ILE	3.3
1	C	675	ILE	3.2
1	C	596	GLY	3.2
1	B	647	VAL	3.1
1	B	712	ASP	3.0
1	B	677	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	612	ARG	2.9
1	B	572	ASN	2.8
1	A	712	ASP	2.8
1	C	568	ASP	2.7
1	D	750	LYS	2.7
1	B	583	LYS	2.6
1	A	29	LEU	2.6
1	B	727	SER	2.6
1	A	37	ARG	2.6
1	B	568	ASP	2.6
1	D	583	LYS	2.5
1	C	641	THR	2.5
1	C	677	ASP	2.5
1	A	726	GLY	2.5
1	C	713	GLN	2.5
1	C	725	ASP	2.4
1	C	672	ILE	2.4
1	D	713	GLN	2.4
1	B	641	THR	2.4
1	B	725	ASP	2.4
1	A	749	ASP	2.4
1	A	35	SER	2.4
1	B	34	GLY	2.4
1	B	610	GLU	2.3
1	B	645	GLY	2.3
1	B	646	THR	2.3
1	D	572	ASN	2.3
1	C	640	VAL	2.3
1	C	28	SER	2.2
1	B	565	GLU	2.2
1	B	611	VAL	2.2
1	D	751	ILE	2.2
1	C	32	GLU	2.2
1	D	712	ASP	2.1
1	C	643	ASP	2.1
1	D	32	GLU	2.1
1	B	37	ARG	2.1
1	B	722	ASP	2.1
1	C	569	ASP	2.1
1	C	674	ASP	2.1
1	C	638	GLY	2.1
1	C	712	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	583	LYS	2.0
1	B	594	PRO	2.0
1	B	569	ASP	2.0
1	B	571	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	OCS	B	669	9/10	0.95	0.14	-	27,29,36,37	0
1	OCS	A	669	9/10	0.94	0.09	-	15,18,27,29	0
1	OCS	D	669	9/10	0.96	0.10	-	19,20,25,28	0
1	OCS	C	669	9/10	0.92	0.16	-	26,29,36,36	0

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
2	HEM	B	760	43/43	0.98	0.07	0.16	4,7,13,21	0
2	HEM	C	760	43/43	0.98	0.07	0.01	3,7,13,21	0
2	HEM	A	760	43/43	0.98	0.08	-0.12	3,6,12,18	0
2	HEM	D	760	43/43	0.98	0.07	-0.25	2,6,12,17	0

6.5 Other polymers

There are no such residues in this entry.