



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:53 PM GMT

PDB ID : 3PQ2
Title : Structure of I274C variant of E. coli KatE[] - Images 1-6
Authors : Loewen, P.C.; Jha, V.; Louis, S.; Chelikani, P.; Carpena, X.; Fita, I.
Deposited on : 2010-11-25
Resolution : 1.79 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

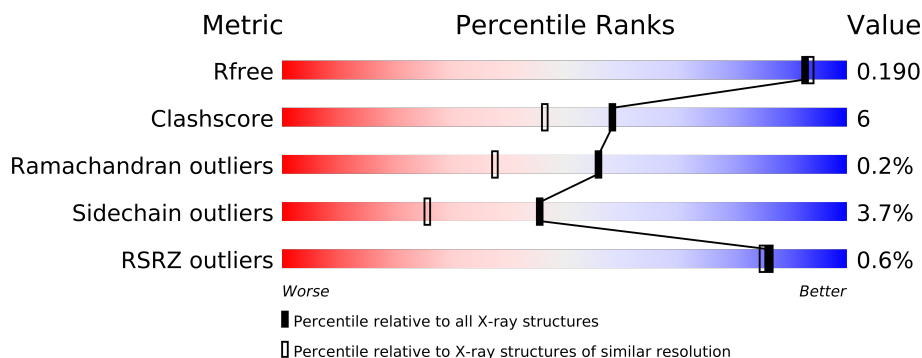
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.79 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}	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	753	
1	B	753	
1	C	753	
1	D	753	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	H2S	A	754	-	X
4	H2S	B	754	-	X
4	H2S	C	754	-	X
4	H2S	D	754	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26834 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

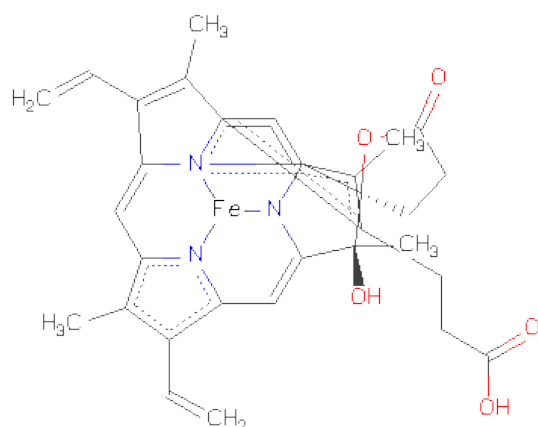
- Molecule 1 is a protein called Catalase HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	5	0
			5755	3652	1009	1083	11			
1	B	726	Total	C	N	O	S	0	5	0
			5757	3654	1009	1083	11			
1	C	726	Total	C	N	O	S	0	3	0
			5753	3652	1010	1080	11			
1	D	726	Total	C	N	O	S	0	8	0
			5768	3662	1010	1085	11			

There are 12 discrepancies between the modelled and reference sequences:

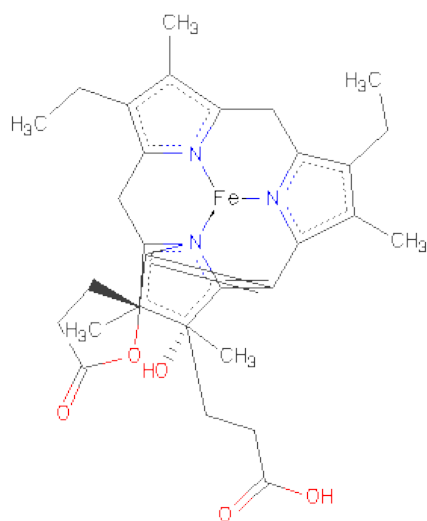
Chain	Residue	Modelled	Actual	Comment	Reference
A	274	CYS	ILE	ENGINEERED MUTATION	UNP P21179
A	438	ALA	CYS	ENGINEERED MUTATION	UNP P21179
A	669	ALA	CYS	ENGINEERED MUTATION	UNP P21179
B	274	CYS	ILE	ENGINEERED MUTATION	UNP P21179
B	438	ALA	CYS	ENGINEERED MUTATION	UNP P21179
B	669	ALA	CYS	ENGINEERED MUTATION	UNP P21179
C	274	CYS	ILE	ENGINEERED MUTATION	UNP P21179
C	438	ALA	CYS	ENGINEERED MUTATION	UNP P21179
C	669	ALA	CYS	ENGINEERED MUTATION	UNP P21179
D	274	CYS	ILE	ENGINEERED MUTATION	UNP P21179
D	438	ALA	CYS	ENGINEERED MUTATION	UNP P21179
D	669	ALA	CYS	ENGINEERED MUTATION	UNP P21179

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	B	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	C	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	D	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		

- Molecule 3 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE 17R, 18S (three-letter code: HDE) (formula: $C_{34}H_{38}FeN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 44	C 34	Fe 1	N 4	O 5	0	1
3	B	1	Total 44	C 34	Fe 1	N 4	O 5	0	1
3	C	1	Total 44	C 34	Fe 1	N 4	O 5	0	1
3	D	1	Total 44	C 34	Fe 1	N 4	O 5	0	1

- Molecule 4 is HYDROSULFURIC ACID (three-letter code: H₂S) (formula: H₂S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	S 1	0	0
4	B	1	Total 1	S 1	0	0
4	C	1	Total 1	S 1	0	0
4	D	1	Total 1	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	887	Total 887	O 887	0	0
5	B	801	Total 801	O 801	0	0

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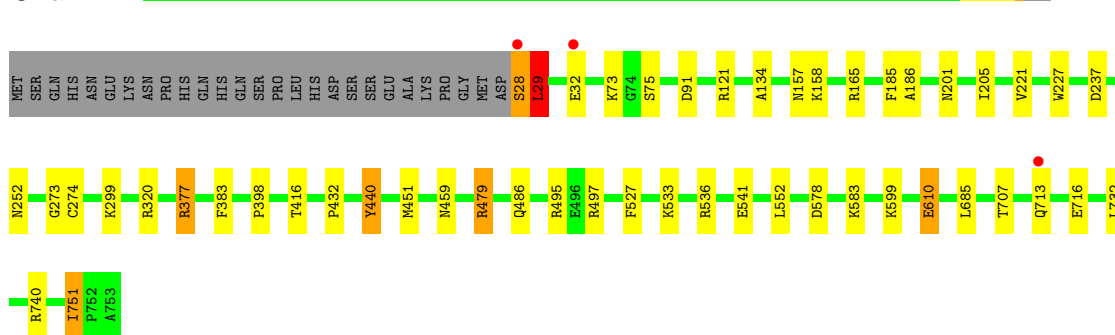
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	845	Total 845	O 845	0	0
5	D	912	Total 912	O 912	0	0

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.

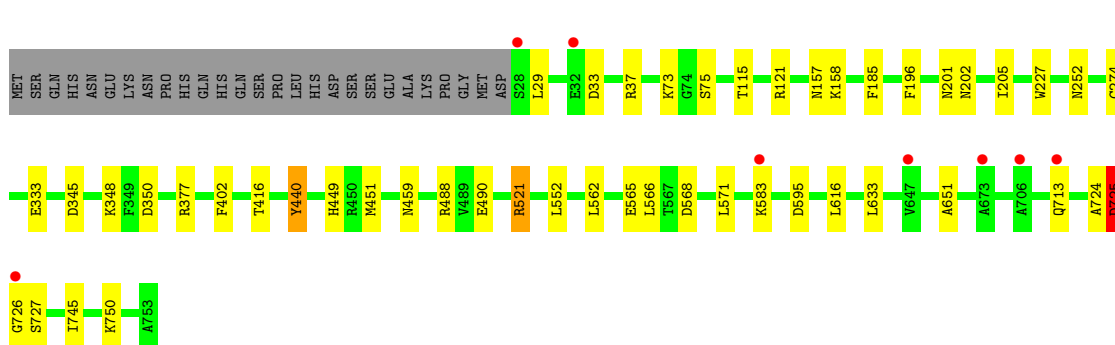
• Molecule 1: Catalase HP1I

Chain A:



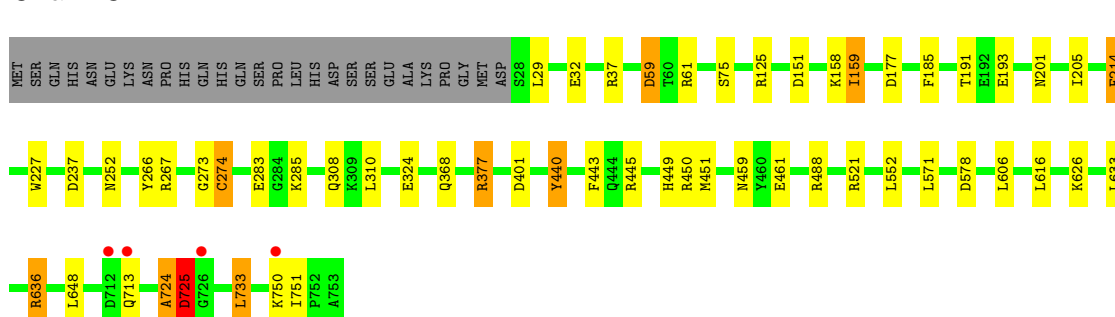
• Molecule 1: Catalase HP1I

Chain B:



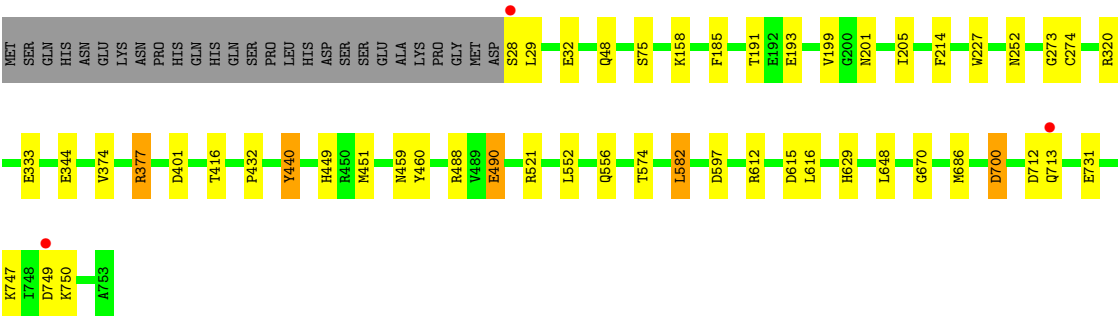
• Molecule 1: Catalase HP1I

Chain C:



● Molecule 1: Catalase HP1I

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.51Å 133.03Å 122.65Å 90.00° 109.39° 90.00°	Depositor
Resolution (Å)	31.27 – 1.79 31.27 – 1.79	Depositor EDS
% Data completeness (in resolution range)	92.2 (31.27-1.79) 92.2 (31.27-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.142 , 0.189 0.142 , 0.190	Depositor DCC
R_{free} test set	12150 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	11.1	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.6	EDS
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 242917 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26834	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HDE, HDD, H2S

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	1.18	6/5932 (0.1%)	0.96	12/8064 (0.1%)
1	B	1.14	6/5931 (0.1%)	0.95	5/8062 (0.1%)
1	C	1.13	6/5919 (0.1%)	0.96	13/8047 (0.2%)
1	D	1.22	6/5955 (0.1%)	0.97	9/8095 (0.1%)
All	All	1.17	24/23737 (0.1%)	0.96	39/32268 (0.1%)

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 (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	440	TYR	CE1-CZ	7.34	1.48	1.38
1	A	440	TYR	CE1-CZ	6.96	1.47	1.38
1	D	333	GLU	CD-OE2	-6.74	1.18	1.25
1	D	460	TYR	CD1-CE1	5.72	1.48	1.39
1	B	196	PHE	CE1-CZ	5.67	1.48	1.37
1	A	186	ALA	CA-CB	5.67	1.64	1.52
1	D	199	VAL	CB-CG1	5.51	1.64	1.52
1	C	266	TYR	CD2-CE2	5.48	1.47	1.39
1	C	443	PHE	CE2-CZ	5.45	1.47	1.37
1	C	59	ASP	CB-CG	5.43	1.63	1.51
1	A	134	ALA	CA-CB	5.37	1.63	1.52
1	D	193	GLU	CB-CG	5.30	1.62	1.52
1	B	333	GLU	CD-OE1	-5.29	1.19	1.25
1	A	527	PHE	CE2-CZ	5.29	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	28	SER	CB-OG	5.26	1.49	1.42
1	A	383	PHE	CD2-CE2	5.24	1.49	1.39
1	C	125	ARG	CG-CD	5.21	1.65	1.51
1	A	221	VAL	CB-CG2	5.16	1.63	1.52
1	B	37	ARG	CZ-NH2	5.12	1.39	1.33
1	C	193	GLU	CB-CG	5.11	1.61	1.52
1	D	374	VAL	CB-CG2	5.10	1.63	1.52
1	B	440	TYR	CD1-CE1	5.10	1.47	1.39
1	B	402	PHE	CE2-CZ	5.07	1.47	1.37
1	C	214	PHE	CE1-CZ	5.03	1.47	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	636	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	C	636	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	C	59	ASP	CB-CG-OD1	7.36	124.92	118.30
1	A	536	ARG	NE-CZ-NH2	7.13	123.86	120.30
1	A	121	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	536	ARG	NE-CZ-NH1	-6.75	116.92	120.30
1	C	310	LEU	CB-CG-CD1	6.56	122.16	111.00
1	C	445	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	A	740	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	521	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	479	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	C	159	ILE	CB-CG1-CD1	-6.01	97.08	113.90
1	A	165	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	121	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	D	582	LEU	CB-CG-CD1	5.79	120.84	111.00
1	D	521	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	495	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	C	733	LEU	CA-CB-CG	5.72	128.46	115.30
1	D	401	ASP	CB-CG-OD2	5.64	123.38	118.30
1	D	320	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	685	LEU	CB-CG-CD1	-5.59	101.49	111.00
1	B	33	ASP	CB-CG-OD1	5.50	123.25	118.30
1	D	615	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	450	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	320	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	377	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	D	612	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	C	37	ARG	NE-CZ-NH2	-5.26	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	686	MET	CG-SD-CE	5.24	108.59	100.20
1	B	377	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	B	350	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	29	LEU	CA-CB-CG	5.19	127.23	115.30
1	C	445	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	177	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	C	401	ASP	CB-CG-OD2	5.14	122.93	118.30
1	C	377	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	A	497	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	D	377	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	D	612	ARG	NE-CZ-NH1	-5.02	117.79	120.30

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5755	0	0	29	0
1	B	5757	0	0	22	0
1	C	5753	0	0	25	0
1	D	5768	0	0	24	0
2	A	44	0	0	5	0
2	B	44	0	0	4	0
2	C	44	0	0	5	0
2	D	44	0	0	5	0
3	A	44	0	36	7	0
3	B	44	0	36	10	0
3	C	44	0	36	11	0
3	D	44	0	36	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	4	0
4	B	1	0	0	5	0
4	C	1	0	0	5	0
4	D	1	0	0	5	0
5	A	887	0	0	15	1
5	B	801	0	0	6	0
5	C	845	0	0	18	0
5	D	912	0	0	22	1
All	All	26834	0	144	145	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (145) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:760[A]:HDD:CBB	4:B:754:H2S:S	2.18	1.32
3:B:761[B]:HDE:CBC	3:B:761[B]:HDE:HMC	1.57	1.28
1:C:274:CYS:CB	4:C:754:H2S:S	2.21	1.28
1:C:449[B]:HIS:CE1	5:C:3610:HOH:O	1.68	1.27
1:D:449[B]:HIS:CE1	5:D:3616:HOH:O	1.63	1.27
2:D:760[A]:HDD:CBB	4:D:754:H2S:S	2.23	1.25
1:A:274:CYS:CB	4:A:754:H2S:S	2.23	1.25
2:C:760[A]:HDD:CBB	4:C:754:H2S:S	2.28	1.21
1:D:274:CYS:CB	4:D:754:H2S:S	2.29	1.21
1:D:451:MET:SD	5:D:3617:HOH:O	1.95	1.20
1:B:274:CYS:CB	4:B:754:H2S:S	2.30	1.20
3:D:761[B]:HDE:HMC	3:D:761[B]:HDE:HBCB	1.16	1.14
3:B:761[B]:HDE:HBCA	3:B:761[B]:HDE:CMC	1.70	1.11
3:C:761[B]:HDE:HBCB	3:C:761[B]:HDE:HMC	1.13	1.08
3:A:761[B]:HDE:HBCB	3:A:761[B]:HDE:HMC	1.34	1.06
1:B:451:MET:SD	5:B:3614:HOH:O	2.14	1.05
3:D:761[B]:HDE:HMC	3:D:761[B]:HDE:CBC	1.91	1.01
3:C:761[B]:HDE:CBC	3:C:761[B]:HDE:HMC	1.91	0.99
1:C:451:MET:SD	5:C:3612:HOH:O	2.25	0.95
1:A:28:SER:O	1:A:28:SER:OG	1.76	0.93
1:A:274:CYS:SG	2:A:760[A]:HDD:CMB	2.58	0.90
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:CBB	2.01	0.90
1:D:416[A]:THR:CG2	5:D:3576:HOH:O	2.21	0.89
1:A:451:MET:SD	5:A:3609:HOH:O	2.31	0.89
3:B:761[B]:HDE:HBCA	3:B:761[B]:HDE:HMC	0.89	0.88
3:A:761[B]:HDE:CBC	3:A:761[B]:HDE:HMC	2.03	0.87
2:A:760[A]:HDD:CBB	4:A:754:H2S:S	2.63	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:CBB	2.05	0.86
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:HBBB	1.58	0.84
1:B:29:LEU:N	5:B:2571:HOH:O	2.11	0.84
3:B:761[B]:HDE:CMC	3:B:761[B]:HDE:CBC	2.33	0.84
1:D:488:ARG:NE	5:D:2698:HOH:O	2.10	0.84
1:C:440:TYR:CD1	5:C:3454:HOH:O	2.32	0.82
1:D:274:CYS:SG	2:D:760[A]:HDD:CMB	2.68	0.82
1:C:274:CYS:SG	2:C:760[A]:HDD:CMB	2.66	0.81
3:B:761[B]:HDE:HMB	3:B:761[B]:HDE:HBBB	1.62	0.81
1:A:610:GLU:CG	5:A:3555:HOH:O	2.29	0.81
1:A:541:GLU:OE2	5:A:2550:HOH:O	1.97	0.80
1:C:578:ASP:CB	5:C:2919:HOH:O	2.29	0.80
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:HBBA	1.65	0.78
3:A:761[B]:HDE:HBBB	3:A:761[B]:HDE:HMB	1.64	0.78
3:C:761[B]:HDE:CMC	3:C:761[B]:HDE:HBCB	1.94	0.77
1:A:716:GLU:CG	5:A:3090:HOH:O	2.32	0.77
1:B:274:CYS:SG	2:B:760[A]:HDD:CMB	2.74	0.75
1:C:449[B]:HIS:NE2	5:C:3610:HOH:O	1.89	0.73
3:D:761[B]:HDE:CMC	3:D:761[B]:HDE:HBCB	1.95	0.73
3:D:761[B]:HDE:HMC	4:D:754:H2S:S	2.29	0.72
1:C:368:GLN:NE2	5:C:1787:HOH:O	2.23	0.72
3:C:761[B]:HDE:CBC	3:C:761[B]:HDE:CMC	2.60	0.72
3:B:761[B]:HDE:CBB	3:B:761[B]:HDE:HMB	2.20	0.71
1:D:490:GLU:OE1	5:D:2308:HOH:O	2.09	0.70
1:C:29:LEU:N	5:C:2891:HOH:O	2.24	0.70
3:B:761[B]:HDE:HBCB	3:B:761[B]:HDE:HMC	1.68	0.69
1:A:610:GLU:OE1	5:A:2394:HOH:O	2.12	0.68
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:HBBA	1.73	0.67
1:D:440:TYR:CZ	5:D:3517:HOH:O	2.48	0.67
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:HBBB	1.76	0.67
1:C:59:ASP:OD2	5:C:2529:HOH:O	2.13	0.67
1:C:324:GLU:OE1	5:C:2088:HOH:O	2.14	0.66
1:D:731:GLU:OE2	5:D:3028:HOH:O	2.15	0.65
3:D:761[B]:HDE:CMC	3:D:761[B]:HDE:CBC	2.59	0.64
1:D:29:LEU:N	5:D:2467:HOH:O	2.30	0.64
3:B:761[B]:HDE:CMC	3:B:761[B]:HDE:HBCB	2.26	0.64
1:C:267:ARG:CG	5:C:2916:HOH:O	2.46	0.64
3:D:761[B]:HDE:HBCB	4:D:754:H2S:S	2.39	0.63
3:C:761[B]:HDE:HMC	4:C:754:H2S:S	2.38	0.63
1:A:201:ASN:CG	2:A:760[A]:HDD:CMB	2.67	0.62
1:A:751:ILE:O	1:A:751:ILE:CD1	2.48	0.62
1:A:377:ARG:NH1	5:A:991:HOH:O	2.33	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:761[B]:HDE:CBB	3:A:761[B]:HDE:HMB	2.30	0.61
1:B:201:ASN:CG	2:B:760[A]:HDD:CMB	2.70	0.60
1:A:274:CYS:CA	4:A:754:H2S:S	2.90	0.59
1:A:201:ASN:ND2	2:A:760[A]:HDD:CMB	2.67	0.58
1:D:377:ARG:NH1	5:D:1500:HOH:O	2.36	0.58
1:B:73:LYS:CE	5:D:3517:HOH:O	2.51	0.58
1:C:274:CYS:CB	2:C:760[A]:HDD:CBB	2.82	0.57
1:D:597:ASP:OD2	5:D:2709:HOH:O	2.17	0.57
3:B:761[B]:HDE:HMC	4:B:754:H2S:S	2.44	0.57
1:D:201:ASN:CG	2:D:760[A]:HDD:CMB	2.74	0.56
1:D:670:GLY:O	1:D:700:ASP:OD2	2.23	0.56
1:A:29:LEU:CD2	5:C:2405:HOH:O	2.53	0.56
3:A:761[B]:HDE:CBC	3:A:761[B]:HDE:CMC	2.77	0.56
1:A:610:GLU:CD	5:A:3555:HOH:O	2.43	0.56
1:B:416:THR:CG2	5:D:2464:HOH:O	2.54	0.56
1:B:724:ALA:O	1:B:725:ASP:O	2.25	0.54
3:D:761[B]:HDE:CMB	3:D:761[B]:HDE:CBB	2.74	0.54
1:A:416[A]:THR:CG2	5:C:3313:HOH:O	2.57	0.53
1:B:274:CYS:CB	2:B:760[A]:HDD:CBB	2.88	0.52
3:D:761[B]:HDE:CMB	3:D:761[B]:HDE:HBBB	2.34	0.52
1:B:73:LYS:CD	5:D:3517:HOH:O	2.57	0.52
1:A:610:GLU:OE2	5:A:3555:HOH:O	2.19	0.52
3:A:761[B]:HDE:CMC	3:A:761[B]:HDE:HBCB	2.20	0.51
1:A:479:ARG:NH2	5:A:2607:HOH:O	2.43	0.51
1:D:416[A]:THR:CG2	5:D:3334:HOH:O	2.59	0.51
1:D:449[A]:HIS:CE1	5:D:1789:HOH:O	2.64	0.51
1:C:274:CYS:CA	4:C:754:H2S:S	2.96	0.50
2:A:760[A]:HDD:CAB	4:A:754:H2S:S	2.99	0.50
1:D:158:LYS:NZ	5:D:2950:HOH:O	2.45	0.49
1:A:599:LYS:NZ	5:A:2049:HOH:O	2.44	0.49
1:D:416[B]:THR:CG2	5:D:1415:HOH:O	2.60	0.49
1:A:273:GLY:C	1:A:274:CYS:SG	2.91	0.48
1:D:274:CYS:CB	2:D:760[A]:HDD:CBB	2.91	0.48
3:B:761[B]:HDE:CBC	4:B:754:H2S:S	3.02	0.48
1:C:151:ASP:OD1	5:C:3101:HOH:O	2.20	0.48
1:C:725:ASP:O	5:C:2403:HOH:O	2.19	0.48
3:C:761[B]:HDE:HBCB	4:C:754:H2S:S	2.54	0.48
1:A:533:LYS:NZ	5:A:2232:HOH:O	2.47	0.47
1:B:115:THR:CG2	5:D:3420:HOH:O	2.62	0.47
1:B:449[B]:HIS:CE1	5:D:1789:HOH:O	2.68	0.47
1:D:629:HIS:CD2	5:D:1554:HOH:O	2.67	0.47
1:B:488:ARG:NE	1:B:490:GLU:OE2	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:556:GLN:NE2	5:D:2773:HOH:O	2.48	0.46
1:C:214:PHE:CD1	2:C:760[A]:HDD:CAC	2.99	0.46
1:C:273:GLY:C	1:C:274:CYS:SG	2.94	0.46
1:B:725:ASP:OD2	1:B:727:SER:N	2.48	0.46
1:C:713:GLN:CB	5:C:3004:HOH:O	2.63	0.46
1:B:521:ARG:NH2	1:B:745:ILE:CD1	2.78	0.46
1:B:725:ASP:OD2	1:B:726:GLY:N	2.48	0.46
1:D:273:GLY:C	1:D:274:CYS:SG	2.95	0.46
3:C:761[B]:HDE:CMB	3:C:761[B]:HDE:HBBA	2.41	0.45
1:A:578:ASP:OD1	1:A:583:LYS:NZ	2.50	0.45
3:C:761[B]:HDE:HAAA	3:C:761[B]:HDE:HMAA	1.81	0.44
1:B:202:ASN:ND2	5:B:3407:HOH:O	2.50	0.44
1:B:449[B]:HIS:CD2	5:B:3613:HOH:O	2.71	0.44
3:D:761[B]:HDE:CMB	3:D:761[B]:HDE:HBBA	2.41	0.43
1:B:651:ALA:O	5:B:1845:HOH:O	2.21	0.43
1:C:158:LYS:NZ	5:C:3556:HOH:O	2.52	0.42
1:C:201:ASN:CG	2:C:760[A]:HDD:CMB	2.88	0.42
3:D:761[B]:HDE:CBC	4:D:754:H2S:S	3.06	0.42
1:A:157:ASN:ND2	5:A:3445:HOH:O	2.53	0.42
1:B:345:ASP:OD1	1:B:348:LYS:NZ	2.53	0.42
1:C:308:GLN:NE2	5:C:3278:HOH:O	2.53	0.41
1:D:214:PHE:CD1	2:D:760[A]:HDD:CAC	3.03	0.41
1:B:274:CYS:CA	4:B:754:H2S:S	3.05	0.41
1:C:449[A]:HIS:CD2	5:C:3611:HOH:O	2.72	0.41
3:D:761[B]:HDE:HMAA	3:D:761[B]:HDE:HAAA	1.87	0.41
1:A:201:ASN:CG	3:A:761[B]:HDE:HAC	2.40	0.41
1:D:712:ASP:N	5:D:3483:HOH:O	2.52	0.41
1:A:299:LYS:NZ	5:A:1927:HOH:O	2.54	0.41
1:A:486:GLN:OE1	5:A:2605:HOH:O	2.22	0.41
1:A:91:ASP:OD1	1:C:461:GLU:OE1	2.38	0.41
1:C:724:ALA:O	1:C:725:ASP:CB	2.69	0.40
1:B:726:GLY:O	5:B:2261:HOH:O	2.22	0.40
1:A:416[B]:THR:CG2	5:A:900:HOH:O	2.69	0.40

All (1) 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	Distance(Å)	Clash(Å)
5:A:3241:HOH:O	5:D:2457:HOH:O[2_646]	2.18	0.02

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	729/753 (97%)	709 (97%)	19 (3%)	1 (0%)	59	41
1	B	729/753 (97%)	709 (97%)	18 (2%)	2 (0%)	50	31
1	C	727/753 (96%)	705 (97%)	20 (3%)	2 (0%)	50	31
1	D	732/753 (97%)	712 (97%)	19 (3%)	1 (0%)	59	41
All	All	2917/3012 (97%)	2835 (97%)	76 (3%)	6 (0%)	56	38

All (6) Ramachandran outliers are listed below:

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

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	614/634 (97%)	595 (97%)	19 (3%)	52	33
1	B	614/634 (97%)	593 (97%)	21 (3%)	49	29
1	C	612/634 (96%)	582 (95%)	30 (5%)	35	15
1	D	617/634 (97%)	595 (96%)	22 (4%)	47	27
All	All	2457/2536 (97%)	2365 (96%)	92 (4%)	45	26

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	29	LEU
1	A	32	GLU
1	A	73	LYS
1	A	185	PHE
1	A	205	ILE
1	A	227	TRP
1	A	237	ASP
1	A	252	ASN
1	A	398	PRO
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	610	GLU
1	A	707	THR
1	A	713	GLN
1	A	732	LEU
1	A	751	ILE
1	B	157	ASN
1	B	158	LYS
1	B	185	PHE
1	B	205	ILE
1	B	227	TRP
1	B	252	ASN
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	616	LEU
1	B	633	LEU
1	B	713	GLN
1	B	725	ASP
1	B	750	LYS
1	C	32	GLU
1	C	61	ARG
1	C	159	ILE

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Mol	Chain	Res	Type
1	C	185	PHE
1	C	191	THR
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	274	CYS
1	C	283	GLU
1	C	285	LYS
1	C	377	ARG
1	C	440	TYR
1	C	459	ASN
1	C	488[A]	ARG
1	C	488[B]	ARG
1	C	521	ARG
1	C	552	LEU
1	C	571	LEU
1	C	606	LEU
1	C	616	LEU
1	C	626	LYS
1	C	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS
1	C	751	ILE
1	D	32	GLU
1	D	48	GLN
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	252	ASN
1	D	344	GLU
1	D	432	PRO
1	D	440	TYR
1	D	459	ASN
1	D	490	GLU
1	D	552	LEU
1	D	574	THR
1	D	582	LEU

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Mol	Chain	Res	Type
1	D	616	LEU
1	D	648	LEU
1	D	700	ASP
1	D	713	GLN
1	D	747	LYS
1	D	749	ASP
1	D	750	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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, 4 are modelled with single atom - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HDD	A	760[A]	1,5	52,52,52	2.53	16 (30%)	70,89,89	2.16	23 (32%)
3	HDE	A	761[B]	1,5	52,52,52	2.99	22 (42%)	75,89,89	2.56	32 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HDD	B	760[A]	1,5	52,52,52	2.33	17 (32%)	70,89,89	2.10	17 (24%)
3	HDE	B	761[B]	1,5	52,52,52	3.04	21 (40%)	75,89,89	2.73	32 (42%)
2	HDD	C	760[A]	1,5	52,52,52	2.32	19 (36%)	70,89,89	2.35	30 (42%)
3	HDE	C	761[B]	1,5	52,52,52	2.84	19 (36%)	75,89,89	2.61	35 (46%)
2	HDD	D	760[A]	1,5	52,52,52	2.64	21 (40%)	70,89,89	2.34	30 (42%)
3	HDE	D	761[B]	1,5	52,52,52	2.94	21 (40%)	75,89,89	2.71	38 (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	HDD	A	760[A]	1,5	-	0/5/89/89	0/1/9/9
3	HDE	A	761[B]	1,5	-	2/9/89/89	0/1/9/9
2	HDD	B	760[A]	1,5	-	0/5/89/89	0/1/9/9
3	HDE	B	761[B]	1,5	-	1/9/89/89	0/1/9/9
2	HDD	C	760[A]	1,5	-	0/5/89/89	0/1/9/9
3	HDE	C	761[B]	1,5	-	1/9/89/89	0/1/9/9
2	HDD	D	760[A]	1,5	-	0/5/89/89	0/1/9/9
3	HDE	D	761[B]	1,5	-	1/9/89/89	0/1/9/9

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	761[B]	HDE	CHC-C4B	-9.67	1.42	1.51
3	B	761[B]	HDE	CHC-C4B	-9.16	1.43	1.51
3	C	761[B]	HDE	C4C-C3C	7.65	1.48	1.37
3	B	761[B]	HDE	C4C-C3C	7.60	1.48	1.37
3	A	761[B]	HDE	C4C-C3C	7.47	1.47	1.37
2	D	760[A]	HDD	FE-ND	7.21	2.25	1.97
3	A	761[B]	HDE	CHC-C1C	-7.18	1.44	1.51
2	C	760[A]	HDD	FE-ND	6.96	2.24	1.97
3	D	761[B]	HDE	C4C-C3C	6.89	1.47	1.37
3	C	761[B]	HDE	CHC-C4B	-6.84	1.45	1.51
2	A	760[A]	HDD	C3C-CAC	6.54	1.55	1.49
3	B	761[B]	HDE	C1C-NC	6.43	1.43	1.35
3	B	761[B]	HDE	CHD-C4C	-6.30	1.45	1.51
3	A	761[B]	HDE	C1C-NC	6.27	1.43	1.35
2	D	760[A]	HDD	C3C-CAC	6.23	1.55	1.49
3	D	761[B]	HDE	CHD-C4C	-6.17	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	761[B]	HDE	C4C-NC	6.15	1.43	1.35
3	C	761[B]	HDE	C1C-NC	6.13	1.43	1.35
3	D	761[B]	HDE	CHD-C1D	-6.02	1.45	1.51
3	A	761[B]	HDE	CHD-C1D	-5.97	1.45	1.51
3	D	761[B]	HDE	CHC-C1C	-5.93	1.46	1.51
3	A	761[B]	HDE	CHC-C4B	-5.84	1.46	1.51
2	A	760[A]	HDD	O1D-C3D	-5.71	1.37	1.46
3	B	761[B]	HDE	C4C-NC	5.66	1.42	1.35
3	B	761[B]	HDE	CHD-C1D	-5.59	1.46	1.51
3	C	761[B]	HDE	C4C-NC	5.57	1.42	1.35
3	C	761[B]	HDE	CHC-C1C	-5.32	1.46	1.51
2	A	760[A]	HDD	C4B-C3B	5.29	1.48	1.41
3	D	761[B]	HDE	C4C-NC	5.28	1.42	1.35
3	C	761[B]	HDE	C4B-NB	5.07	1.41	1.35
3	C	761[B]	HDE	CHD-C1D	-5.02	1.46	1.51
3	C	761[B]	HDE	O1A-CGA	4.91	1.44	1.35
3	A	761[B]	HDE	O1A-CGA	4.91	1.44	1.35
2	B	760[A]	HDD	C4B-C3B	4.86	1.47	1.41
3	A	761[B]	HDE	CHD-C4C	-4.86	1.47	1.51
3	A	761[B]	HDE	C4B-NB	4.77	1.41	1.35
2	C	760[A]	HDD	C4A-C3A	4.75	1.46	1.40
3	B	761[B]	HDE	CHC-C1C	-4.71	1.47	1.51
3	C	761[B]	HDE	CHD-C4C	-4.69	1.47	1.51
2	A	760[A]	HDD	C3C-C4C	4.68	1.47	1.40
2	B	760[A]	HDD	C3C-CAC	4.65	1.53	1.49
2	D	760[A]	HDD	O1D-C3D	-4.64	1.38	1.46
2	D	760[A]	HDD	FE-NB	4.57	2.12	1.92
2	B	760[A]	HDD	C3C-C2C	-4.55	1.33	1.41
3	B	761[B]	HDE	C4B-NB	4.54	1.41	1.35
2	B	760[A]	HDD	C1C-C2C	4.52	1.45	1.40
2	D	760[A]	HDD	C4A-C3A	4.41	1.45	1.40
2	D	760[A]	HDD	C3B-C2B	-4.40	1.33	1.41
2	A	760[A]	HDD	C3B-C2B	-4.37	1.33	1.41
2	B	760[A]	HDD	C4A-C3A	4.32	1.45	1.40
3	B	761[B]	HDE	O1A-CGA	4.27	1.43	1.35
2	B	760[A]	HDD	FE-NC	4.23	2.10	1.92
2	A	760[A]	HDD	C1C-C2C	4.21	1.45	1.40
2	A	760[A]	HDD	C4A-C3A	4.18	1.45	1.40
3	B	761[B]	HDE	FE-ND	4.17	2.10	1.92
3	D	761[B]	HDE	FE-ND	4.17	2.10	1.92
2	D	760[A]	HDD	C3C-C4C	4.13	1.46	1.40
2	A	760[A]	HDD	C2D-C1D	-4.12	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760[A]	HDD	C3C-C2C	-4.10	1.34	1.41
2	D	760[A]	HDD	C3C-C2C	-4.08	1.34	1.41
3	B	761[B]	HDE	C1A-NA	3.96	1.44	1.38
2	A	760[A]	HDD	FE-NB	3.94	2.09	1.92
2	D	760[A]	HDD	C1C-C2C	3.89	1.45	1.40
2	C	760[A]	HDD	C4B-C3B	3.87	1.46	1.41
2	B	760[A]	HDD	C2D-C1D	-3.87	1.45	1.52
2	C	760[A]	HDD	C3C-C2C	-3.85	1.34	1.41
3	C	761[B]	HDE	FE-ND	3.83	2.08	1.92
3	A	761[B]	HDE	FE-ND	3.83	2.08	1.92
2	C	760[A]	HDD	C3C-C4C	3.82	1.46	1.40
3	D	761[B]	HDE	C4A-NA	3.82	1.44	1.38
3	D	761[B]	HDE	C4B-NB	3.80	1.40	1.35
2	B	760[A]	HDD	O1D-C3D	-3.79	1.40	1.46
3	A	761[B]	HDE	C4A-NA	3.78	1.44	1.38
2	A	760[A]	HDD	FE-ND	3.77	2.12	1.97
3	D	761[B]	HDE	O1A-CGA	3.76	1.42	1.35
3	B	761[B]	HDE	C3B-C2B	3.74	1.48	1.37
2	B	760[A]	HDD	C3C-C4C	3.71	1.46	1.40
3	C	761[B]	HDE	C3B-C2B	3.68	1.48	1.37
3	A	761[B]	HDE	C3B-C2B	3.67	1.48	1.37
2	B	760[A]	HDD	FE-ND	3.66	2.11	1.97
2	C	760[A]	HDD	C3B-C2B	-3.65	1.34	1.41
3	D	761[B]	HDE	C3B-C2B	3.62	1.48	1.37
2	D	760[A]	HDD	C3B-CAB	3.61	1.55	1.48
2	B	760[A]	HDD	C3B-C2B	-3.58	1.35	1.41
3	A	761[B]	HDE	C3C-C2C	3.57	1.48	1.37
3	D	761[B]	HDE	C1C-NC	3.45	1.39	1.35
2	D	760[A]	HDD	CHD-C1D	3.44	1.42	1.36
3	A	761[B]	HDE	C3D-C2D	3.40	1.47	1.37
3	D	761[B]	HDE	C1A-NA	3.35	1.43	1.38
2	C	760[A]	HDD	C1C-C2C	3.34	1.44	1.40
3	C	761[B]	HDE	C3D-C2D	3.34	1.47	1.37
3	B	761[B]	HDE	C4D-CHA	3.33	1.49	1.39
2	C	760[A]	HDD	C3C-CAC	3.33	1.52	1.49
2	C	760[A]	HDD	O1D-C3D	-3.33	1.41	1.46
3	D	761[B]	HDE	C3C-C2C	3.32	1.47	1.37
3	C	761[B]	HDE	C3C-C2C	3.28	1.47	1.37
2	C	760[A]	HDD	CMD-C2D	3.27	1.58	1.53
2	D	760[A]	HDD	C3D-C4D	-3.24	1.46	1.51
3	C	761[B]	HDE	C4D-C3D	3.23	1.49	1.43
2	C	760[A]	HDD	FE-NB	3.23	2.06	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	761[B]	HDE	C1A-NA	3.22	1.43	1.38
2	C	760[A]	HDD	C3B-CAB	3.17	1.54	1.48
2	A	760[A]	HDD	C3D-C4D	-3.15	1.46	1.51
2	D	760[A]	HDD	FE-NA	3.11	2.05	1.92
2	D	760[A]	HDD	C4B-C3B	3.11	1.45	1.41
3	D	761[B]	HDE	C3D-C2D	3.10	1.46	1.37
2	D	760[A]	HDD	C2D-C1D	-3.04	1.46	1.52
2	D	760[A]	HDD	CMD-C2D	3.03	1.57	1.53
3	B	761[B]	HDE	C3C-C2C	3.03	1.46	1.37
2	C	760[A]	HDD	CHA-C4D	3.02	1.41	1.36
3	A	761[B]	HDE	C4D-C3D	2.98	1.48	1.43
3	D	761[B]	HDE	C4D-C3D	2.97	1.48	1.43
2	B	760[A]	HDD	C3B-CAB	2.97	1.53	1.48
2	A	760[A]	HDD	C3B-CAB	2.95	1.53	1.48
2	C	760[A]	HDD	C2D-C1D	-2.93	1.47	1.52
2	D	760[A]	HDD	CHA-C4D	2.92	1.41	1.36
3	B	761[B]	HDE	C4D-C3D	2.90	1.48	1.43
2	A	760[A]	HDD	CMC-C2C	2.90	1.57	1.51
3	A	761[B]	HDE	C1A-NA	2.88	1.42	1.38
3	D	761[B]	HDE	C4D-CHA	2.87	1.47	1.39
3	C	761[B]	HDE	C4D-CHA	2.85	1.47	1.39
3	A	761[B]	HDE	C1B-CHB	2.84	1.47	1.39
3	B	761[B]	HDE	C4A-NA	2.81	1.42	1.38
2	C	760[A]	HDD	CHD-C1D	2.78	1.41	1.36
2	D	760[A]	HDD	FE-NC	2.76	2.04	1.92
3	C	761[B]	HDE	C1B-CHB	2.72	1.47	1.39
2	C	760[A]	HDD	FE-NC	2.70	2.04	1.92
2	B	760[A]	HDD	CMD-C2D	2.67	1.57	1.53
3	A	761[B]	HDE	C4D-CHA	2.64	1.47	1.39
2	B	760[A]	HDD	C4D-ND	2.62	1.42	1.38
3	C	761[B]	HDE	C4A-NA	2.61	1.42	1.38
3	B	761[B]	HDE	C3D-C2D	2.60	1.45	1.37
3	B	761[B]	HDE	CHB-C4A	-2.55	1.32	1.36
2	C	760[A]	HDD	C1A-NA	2.52	1.41	1.36
3	A	761[B]	HDE	C1B-NB	2.49	1.41	1.36
2	D	760[A]	HDD	OND-C2D	2.47	1.47	1.42
3	D	761[B]	HDE	C1B-CHB	2.46	1.46	1.39
3	A	761[B]	HDE	FE-NC	2.42	2.02	1.92
3	A	761[B]	HDE	C1C-C2C	2.34	1.42	1.38
3	B	761[B]	HDE	FE-NC	2.30	2.02	1.92
2	A	760[A]	HDD	CHD-C1D	2.26	1.40	1.36
3	C	761[B]	HDE	FE-NC	2.19	2.01	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	760[A]	HDD	C1A-C2A	2.17	1.47	1.43
2	B	760[A]	HDD	CMA-C3A	2.16	1.56	1.51
3	A	761[B]	HDE	C1B-C2B	2.14	1.42	1.40
3	B	761[B]	HDE	C1B-CHB	2.13	1.45	1.39
2	A	760[A]	HDD	FE-NC	2.12	2.01	1.92
2	C	760[A]	HDD	CMC-C2C	2.12	1.56	1.51
3	B	761[B]	HDE	O1A-C2A	-2.11	1.43	1.46
2	D	760[A]	HDD	CAA-C2A	2.08	1.55	1.52
2	D	760[A]	HDD	O2D-CGD	2.07	1.28	1.22
2	B	760[A]	HDD	FE-NB	2.07	2.01	1.92
3	D	761[B]	HDE	FE-NC	2.05	2.01	1.92
3	D	761[B]	HDE	C1B-NB	2.03	1.40	1.36
3	D	761[B]	HDE	FE-NB	2.03	2.01	1.92
2	B	760[A]	HDD	C1B-NB	2.01	1.39	1.37

All (237) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	761[B]	HDE	C2C-C1C-NC	6.80	117.53	110.11
2	A	760[A]	HDD	O1D-CGD-CBD	-6.75	102.20	110.21
3	A	761[B]	HDE	C2D-C1D-ND	6.66	117.37	110.11
3	B	761[B]	HDE	C2B-C1B-NB	6.64	114.42	109.41
2	C	760[A]	HDD	C3C-CAC-CBC	-6.60	112.28	125.95
2	B	760[A]	HDD	O1D-CGD-O2D	6.51	127.23	120.81
3	B	761[B]	HDE	C2D-C1D-ND	6.33	117.01	110.11
3	B	761[B]	HDE	C2C-C1C-NC	6.25	116.93	110.11
2	C	760[A]	HDD	O1D-CGD-O2D	6.03	126.76	120.81
3	D	761[B]	HDE	C2D-C1D-ND	6.01	116.66	110.11
3	A	761[B]	HDE	C2C-C1C-NC	5.93	116.57	110.11
3	C	761[B]	HDE	C2C-C1C-NC	5.90	116.55	110.11
3	B	761[B]	HDE	CAA-C2A-C3A	-5.87	110.48	116.32
3	C	761[B]	HDE	C2D-C1D-ND	5.85	116.48	110.11
3	D	761[B]	HDE	C2B-C1B-NB	5.82	113.80	109.41
2	A	760[A]	HDD	O1D-C3D-CAD	-5.66	101.46	105.29
3	D	761[B]	HDE	C4C-CHD-C1D	5.52	123.82	112.60
2	B	760[A]	HDD	C3B-CAB-CBB	-5.51	114.54	125.95
3	C	761[B]	HDE	CMA-C3A-C4A	-5.48	103.76	113.22
3	B	761[B]	HDE	C4C-CHD-C1D	5.48	123.73	112.60
2	D	760[A]	HDD	O1D-CGD-O2D	5.41	126.15	120.81
2	D	760[A]	HDD	C3B-CAB-CBB	-5.27	115.03	125.95
3	C	761[B]	HDE	C4D-C3D-C2D	-5.27	101.46	106.92
2	B	760[A]	HDD	C3C-CAC-CBC	-5.20	115.19	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	760[A]	HDD	C4D-ND-C1D	5.16	111.43	107.94
3	B	761[B]	HDE	C3A-C4A-NA	5.14	114.68	105.53
3	B	761[B]	HDE	C4A-NA-C1A	-5.11	104.48	107.94
2	A	760[A]	HDD	C3B-CAB-CBB	-5.10	115.40	125.95
3	D	761[B]	HDE	C4A-NA-C1A	-5.08	104.50	107.94
3	A	761[B]	HDE	CHD-C1D-C2D	-5.04	119.53	129.63
2	D	760[A]	HDD	O1D-CGD-CBD	-4.94	104.35	110.21
3	C	761[B]	HDE	C1B-CHB-C4A	-4.80	120.07	130.06
3	A	761[B]	HDE	C4C-NC-C1C	-4.73	102.60	107.92
2	C	760[A]	HDD	OND-C2D-CMD	-4.72	101.39	109.57
3	A	761[B]	HDE	C2A-C1A-NA	4.69	113.72	105.75
3	C	761[B]	HDE	C4C-CHD-C1D	4.67	122.09	112.60
3	D	761[B]	HDE	C3A-C4A-NA	4.65	113.81	105.53
3	A	761[B]	HDE	CAA-C2A-C1A	-4.63	108.51	116.02
3	C	761[B]	HDE	C2B-C1B-NB	4.60	112.89	109.41
3	D	761[B]	HDE	C3B-C4B-NB	4.57	114.90	110.07
3	A	761[B]	HDE	C4D-C3D-C2D	-4.53	102.23	106.92
2	B	760[A]	HDD	O1D-CGD-CBD	-4.52	104.85	110.21
3	A	761[B]	HDE	C4A-NA-C1A	-4.48	104.91	107.94
3	C	761[B]	HDE	C4A-NA-C1A	-4.44	104.93	107.94
3	C	761[B]	HDE	CHD-C1D-C2D	-4.43	120.75	129.63
3	C	761[B]	HDE	C3A-C4A-NA	4.43	113.42	105.53
2	D	760[A]	HDD	C3A-C4A-NA	-4.39	106.09	109.41
3	B	761[B]	HDE	CHD-C1D-C2D	-4.38	120.86	129.63
3	D	761[B]	HDE	C4D-C3D-C2D	-4.37	102.40	106.92
3	B	761[B]	HDE	C3B-C4B-NB	4.35	114.67	110.07
3	D	761[B]	HDE	C1B-CHB-C4A	-4.33	121.04	130.06
3	A	761[B]	HDE	C3A-C4A-NA	4.30	113.19	105.53
2	C	760[A]	HDD	C1B-CHB-C4A	-4.26	121.86	127.47
3	A	761[B]	HDE	C4C-CHD-C1D	4.25	121.23	112.60
3	C	761[B]	HDE	C2A-C1A-NA	4.22	112.92	105.75
3	C	761[B]	HDE	C3B-C4B-NB	4.11	114.41	110.07
3	D	761[B]	HDE	CAD-CBD-CGD	-4.08	100.36	113.47
2	D	760[A]	HDD	C4B-C3B-C2B	4.03	109.69	106.87
3	B	761[B]	HDE	C4C-NC-C1C	-4.00	103.43	107.92
2	D	760[A]	HDD	O1D-C3D-CAD	-3.98	102.59	105.29
2	C	760[A]	HDD	C4D-ND-C1D	3.97	110.62	107.94
3	D	761[B]	HDE	C2A-C1A-NA	3.97	112.49	105.75
2	C	760[A]	HDD	C3B-CAB-CBB	-3.96	117.75	125.95
3	A	761[B]	HDE	C4B-CHC-C1C	3.94	120.61	112.60
2	A	760[A]	HDD	C3C-CAC-CBC	-3.93	117.81	125.95
2	B	760[A]	HDD	CMB-C2B-C3B	3.89	131.10	124.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	761[B]	HDE	C1B-CHB-C4A	-3.86	122.03	130.06
2	A	760[A]	HDD	C3D-C4D-ND	3.83	112.27	105.75
3	C	761[B]	HDE	C4C-NC-C1C	-3.82	103.63	107.92
3	D	761[B]	HDE	CBC-CAC-C3C	-3.82	99.12	111.99
2	A	760[A]	HDD	CAD-C3D-C2D	3.81	120.12	116.32
3	D	761[B]	HDE	CAA-C2A-C3A	-3.81	112.53	116.32
3	B	761[B]	HDE	C1B-C2B-C3B	-3.77	104.38	107.00
2	B	760[A]	HDD	C4D-ND-C1D	3.75	110.48	107.94
2	A	760[A]	HDD	C1B-CHB-C4A	-3.75	122.53	127.47
2	C	760[A]	HDD	C3B-C4B-NB	-3.75	106.11	111.52
3	D	761[B]	HDE	CHD-C1D-C2D	-3.73	122.16	129.63
2	B	760[A]	HDD	C2C-C1C-NC	-3.70	106.62	109.41
3	C	761[B]	HDE	CHC-C1C-C2C	-3.69	122.24	129.63
3	B	761[B]	HDE	C1B-NB-C4B	-3.65	101.37	106.67
3	A	761[B]	HDE	CAD-CBD-CGD	-3.64	101.76	113.47
3	D	761[B]	HDE	CHC-C1C-C2C	-3.64	122.33	129.63
3	A	761[B]	HDE	CHD-C4C-NC	3.62	126.32	120.95
2	D	760[A]	HDD	CBD-CAD-C3D	-3.60	99.35	105.00
3	D	761[B]	HDE	C4D-CHA-C1A	-3.59	122.60	130.06
3	B	761[B]	HDE	CMC-C2C-C1C	3.58	131.68	127.13
2	D	760[A]	HDD	C3C-CAC-CBC	-3.56	118.58	125.95
3	B	761[B]	HDE	C4D-CHA-C1A	-3.54	122.69	130.06
3	B	761[B]	HDE	C2A-C1A-NA	3.53	111.76	105.75
3	B	761[B]	HDE	CHC-C1C-C2C	-3.53	122.55	129.63
3	D	761[B]	HDE	CMA-C3A-C4A	-3.53	107.13	113.22
3	C	761[B]	HDE	CAA-C2A-C3A	-3.52	112.83	116.32
3	B	761[B]	HDE	C1C-C2C-C3C	-3.48	101.40	106.07
3	A	761[B]	HDE	CAB-C3B-C4B	-3.47	123.53	127.14
3	C	761[B]	HDE	C4D-CHA-C1A	-3.46	122.87	130.06
3	D	761[B]	HDE	C1B-NB-C4B	-3.44	101.67	106.67
3	B	761[B]	HDE	CBC-CAC-C3C	-3.43	100.42	111.99
2	D	760[A]	HDD	C2C-C1C-NC	-3.43	106.82	109.41
2	B	760[A]	HDD	C4B-C3B-C2B	3.42	109.26	106.87
3	A	761[B]	HDE	CHC-C4B-C3B	-3.41	122.79	129.63
2	C	760[A]	HDD	CMA-C3A-C4A	-3.39	123.40	128.62
3	D	761[B]	HDE	C4C-NC-C1C	-3.39	104.12	107.92
2	C	760[A]	HDD	C2C-C1C-NC	-3.36	106.88	109.41
3	A	761[B]	HDE	CHD-C4C-C3C	-3.35	122.92	129.63
3	D	761[B]	HDE	C4B-CHC-C1C	3.35	119.40	112.60
3	D	761[B]	HDE	CHD-C4C-NC	3.33	125.88	120.95
3	A	761[B]	HDE	CHC-C1C-C2C	-3.32	122.98	129.63
3	A	761[B]	HDE	C1B-CHB-C4A	-3.30	123.19	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	761[B]	HDE	CBC-CAC-C3C	-3.29	100.88	111.99
2	A	760[A]	HDD	CAD-CBD-CGD	-3.28	98.87	104.56
3	C	761[B]	HDE	C4B-CHC-C1C	3.27	119.24	112.60
3	B	761[B]	HDE	C4D-C3D-C2D	-3.27	103.54	106.92
3	B	761[B]	HDE	C4B-CHC-C1C	3.23	119.16	112.60
2	B	760[A]	HDD	C1A-CHA-C4D	-3.23	123.34	130.06
3	D	761[B]	HDE	CMC-C2C-C3C	3.23	131.03	124.94
2	D	760[A]	HDD	OND-C2D-CMD	-3.21	104.00	109.57
2	C	760[A]	HDD	C4B-C3B-C2B	3.21	109.11	106.87
2	C	760[A]	HDD	O1D-CGD-CBD	-3.21	106.41	110.21
2	C	760[A]	HDD	CHD-C4C-NC	3.20	129.91	124.58
3	D	761[B]	HDE	C1B-C2B-C3B	-3.19	104.78	107.00
2	C	760[A]	HDD	CBD-CAD-C3D	-3.19	100.00	105.00
3	B	761[B]	HDE	CHC-C4B-C3B	-3.16	123.29	129.63
3	A	761[B]	HDE	C3D-C4D-ND	3.15	114.11	109.73
2	B	760[A]	HDD	OND-C2D-CMD	-3.15	104.11	109.57
2	A	760[A]	HDD	C3B-C4B-NB	-3.14	106.98	111.52
2	C	760[A]	HDD	CMC-C2C-C1C	-3.13	123.81	128.62
3	D	761[B]	HDE	C1C-C2C-C3C	-3.10	101.91	106.07
3	C	761[B]	HDE	C3D-C4D-ND	3.07	114.00	109.73
2	D	760[A]	HDD	C2A-C1A-NA	-3.07	105.48	109.73
3	B	761[B]	HDE	CHD-C4C-NC	3.05	125.46	120.95
3	C	761[B]	HDE	C1C-C2C-C3C	-3.01	102.03	106.07
2	C	760[A]	HDD	C3C-C4C-NC	-3.01	105.72	108.64
3	B	761[B]	HDE	C2B-C1B-CHB	-2.99	120.33	126.00
3	C	761[B]	HDE	CHD-C4C-NC	2.98	125.37	120.95
2	A	760[A]	HDD	CMC-C2C-C1C	-2.98	124.04	128.62
2	D	760[A]	HDD	C4A-NA-C1A	2.95	110.66	106.76
3	A	761[B]	HDE	C1B-C2B-C3B	-2.95	104.94	107.00
2	D	760[A]	HDD	O1D-C3D-C2D	2.94	115.00	109.46
3	C	761[B]	HDE	C2B-C1B-CHB	-2.94	120.43	126.00
3	A	761[B]	HDE	C1C-C2C-C3C	-2.92	102.15	106.07
2	B	760[A]	HDD	C3B-C4B-NB	-2.92	107.30	111.52
3	C	761[B]	HDE	CMC-C2C-C3C	2.92	130.45	124.94
2	A	760[A]	HDD	CBD-CAD-C3D	-2.92	100.43	105.00
2	D	760[A]	HDD	C4A-C3A-C2A	2.90	109.02	107.00
3	D	761[B]	HDE	CHC-C4B-C3B	-2.90	123.82	129.63
3	A	761[B]	HDE	C3B-C4B-NB	2.89	113.13	110.07
2	A	760[A]	HDD	CHA-C1A-NA	2.89	129.41	124.58
2	C	760[A]	HDD	CHA-C1A-NA	2.87	129.37	124.58
2	B	760[A]	HDD	CAA-CBA-CGA	-2.85	104.31	113.47
3	D	761[B]	HDE	CAA-C2A-C1A	-2.85	111.40	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	760[A]	HDD	C3C-C4C-NC	-2.85	105.87	108.64
2	C	760[A]	HDD	OND-C2D-C1D	-2.84	106.50	111.72
3	C	761[B]	HDE	C1B-NB-C4B	-2.83	102.56	106.67
2	A	760[A]	HDD	C4D-ND-C1D	2.82	109.85	107.94
2	D	760[A]	HDD	CHA-C1A-NA	2.79	129.24	124.58
3	B	761[B]	HDE	CAC-C3C-C2C	-2.74	121.14	127.81
3	A	761[B]	HDE	CMB-C2B-C3B	2.72	130.07	124.94
2	D	760[A]	HDD	CAA-CBA-CGA	-2.72	104.72	113.47
2	C	760[A]	HDD	CAD-C3D-C4D	-2.70	111.64	116.02
3	C	761[B]	HDE	CMD-C2D-C3D	2.69	130.02	124.94
3	A	761[B]	HDE	C2B-C1B-NB	2.69	111.44	109.41
3	B	761[B]	HDE	CAD-CBD-CGD	-2.69	104.83	113.47
3	B	761[B]	HDE	CMB-C2B-C3B	2.68	130.00	124.94
2	D	760[A]	HDD	CAD-C3D-C4D	-2.67	111.68	116.02
3	D	761[B]	HDE	CMB-C2B-C3B	2.67	129.97	124.94
3	C	761[B]	HDE	CMB-C2B-C1B	-2.66	124.53	128.62
2	D	760[A]	HDD	C3B-C4B-NB	-2.60	107.76	111.52
2	D	760[A]	HDD	C3D-C4D-ND	2.57	110.12	105.75
2	C	760[A]	HDD	C3D-C4D-ND	2.57	110.12	105.75
3	A	761[B]	HDE	C4D-CHA-C1A	-2.56	124.74	130.06
2	A	760[A]	HDD	CMD-C2D-C1D	-2.55	108.81	113.22
3	C	761[B]	HDE	O1A-CGA-O2A	2.55	123.33	120.81
2	D	760[A]	HDD	C2B-C3B-CAB	-2.55	122.11	127.33
2	D	760[A]	HDD	CHB-C4A-NA	2.54	128.83	124.58
2	B	760[A]	HDD	C1A-C2A-C3A	2.54	109.55	106.92
3	B	761[B]	HDE	C4D-ND-C1D	-2.52	103.00	106.67
2	A	760[A]	HDD	CAA-CBA-CGA	-2.51	105.39	113.47
3	B	761[B]	HDE	C4C-C3C-C2C	2.49	109.74	105.77
3	A	761[B]	HDE	ONA-C3A-CMA	-2.49	105.24	109.57
2	C	760[A]	HDD	C4C-NC-C1C	2.48	110.03	106.76
2	A	760[A]	HDD	C2B-C3B-CAB	-2.47	122.27	127.33
3	A	761[B]	HDE	C4D-ND-C1D	-2.47	103.08	106.67
3	B	761[B]	HDE	CBA-CAA-C2A	2.44	108.82	105.00
3	C	761[B]	HDE	CHC-C4B-C3B	-2.42	124.78	129.63
3	D	761[B]	HDE	O1A-CGA-O2A	2.40	123.18	120.81
2	A	760[A]	HDD	C3D-O1D-CGD	2.40	117.56	109.33
2	D	760[A]	HDD	C4C-NC-C1C	2.40	109.92	106.76
2	B	760[A]	HDD	C4C-NC-C1C	2.40	109.92	106.76
3	A	761[B]	HDE	O1A-CGA-O2A	2.39	123.17	120.81
3	A	761[B]	HDE	CBA-CAA-C2A	2.38	108.72	105.00
2	C	760[A]	HDD	C4A-C3A-C2A	2.38	108.65	107.00
3	D	761[B]	HDE	C3D-C4D-ND	2.38	113.04	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	760[A]	HDD	CHB-C4A-NA	2.38	128.55	124.58
3	D	761[B]	HDE	O1A-C2A-C3A	2.38	113.93	109.46
3	A	761[B]	HDE	CMB-C2B-C1B	-2.37	124.97	128.62
2	A	760[A]	HDD	C4A-C3A-C2A	2.36	108.64	107.00
3	C	761[B]	HDE	C4D-ND-C1D	-2.35	103.25	106.67
3	C	761[B]	HDE	CMB-C2B-C3B	2.35	129.36	124.94
3	C	761[B]	HDE	CBA-CAA-C2A	2.34	108.67	105.00
2	C	760[A]	HDD	CHB-C4A-NA	2.34	128.48	124.58
2	A	760[A]	HDD	C2C-C1C-NC	-2.33	107.65	109.41
2	C	760[A]	HDD	C4C-CHD-C1D	-2.33	125.21	130.06
3	D	761[B]	HDE	CBB-CAB-C3B	-2.33	104.13	111.99
2	D	760[A]	HDD	CHC-C1C-NC	2.32	128.46	124.58
2	D	760[A]	HDD	CMA-C3A-C4A	-2.30	125.08	128.62
2	C	760[A]	HDD	C4B-NB-C1B	2.29	109.01	105.58
2	B	760[A]	HDD	C3D-C4D-ND	2.28	109.64	105.75
2	C	760[A]	HDD	CMD-C2D-C1D	2.27	117.14	113.22
2	D	760[A]	HDD	C2D-C1D-CHD	2.27	129.03	123.22
3	A	761[B]	HDE	CMD-C2D-C3D	2.25	129.19	124.94
3	B	761[B]	HDE	C3D-C4D-ND	2.24	112.85	109.73
2	D	760[A]	HDD	CMC-C2C-C1C	-2.24	125.17	128.62
2	B	760[A]	HDD	CAD-C3D-C4D	-2.22	112.42	116.02
3	D	761[B]	HDE	CMB-C2B-C1B	-2.22	125.21	128.62
2	A	760[A]	HDD	C4B-C3B-C2B	2.22	108.42	106.87
2	C	760[A]	HDD	CMC-C2C-C3C	2.21	128.45	124.97
2	C	760[A]	HDD	C4C-C3C-C2C	2.21	109.64	106.97
3	D	761[B]	HDE	CMD-C2D-C1D	2.19	129.92	127.13
2	C	760[A]	HDD	CMB-C2B-C3B	2.19	128.42	124.97
3	C	761[B]	HDE	CAA-C2A-C1A	-2.19	112.47	116.02
2	C	760[A]	HDD	CAA-CBA-CGA	-2.17	106.48	113.47
3	C	761[B]	HDE	CAB-C3B-C4B	2.16	129.39	127.14
3	A	761[B]	HDE	C1D-C2D-C3D	-2.16	103.17	106.07
2	C	760[A]	HDD	C4C-C3C-CAC	-2.14	122.85	127.18
2	B	760[A]	HDD	CBD-CAD-C3D	-2.14	101.65	105.00
3	B	761[B]	HDE	O1A-CGA-O2A	2.12	122.90	120.81
3	D	761[B]	HDE	C2B-C1B-CHB	-2.10	122.02	126.00
3	D	761[B]	HDE	CBA-CAA-C2A	2.09	108.28	105.00
3	D	761[B]	HDE	C3C-C4C-NC	-2.09	107.86	110.07
2	D	760[A]	HDD	CAD-C3D-C2D	2.08	118.39	116.32
2	D	760[A]	HDD	C3D-O1D-CGD	2.07	116.43	109.33
2	A	760[A]	HDD	C2A-C1A-CHA	-2.04	122.13	126.00
3	C	761[B]	HDE	CAD-CBD-CGD	-2.04	106.92	113.47
3	D	761[B]	HDE	CHD-C4C-C3C	-2.02	125.58	129.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	761[B]	HDE	CHD-C4C-C3C	-2.02	125.59	129.63
2	A	760[A]	HDD	C3C-C2C-C1C	2.01	108.18	107.00
3	D	761[B]	HDE	C4D-ND-C1D	-2.00	103.76	106.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	761[B]	HDE	C2B-C3B-CAB-CBB
3	C	761[B]	HDE	C2B-C3B-CAB-CBB
3	B	761[B]	HDE	C2B-C3B-CAB-CBB
3	A	761[B]	HDE	C2B-C3B-CAB-CBB
3	A	761[B]	HDE	C2C-C3C-CAC-CBC

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	726/753 (96%)	-0.65	3 (0%) 90 89	3, 9, 26, 43	2 (0%)
1	B	726/753 (96%)	-0.51	8 (1%) 77 73	4, 11, 32, 47	2 (0%)
1	C	726/753 (96%)	-0.54	4 (0%) 86 85	4, 11, 31, 46	2 (0%)
1	D	726/753 (96%)	-0.64	3 (0%) 90 89	3, 9, 27, 43	1 (0%)
All	All	2904/3012 (96%)	-0.58	18 (0%) 86 85	3, 10, 30, 47	7 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	28	SER	3.8
1	B	726	GLY	3.7
1	A	28	SER	3.2
1	B	713	GLN	3.1
1	B	32	GLU	3.1
1	D	749	ASP	3.0
1	B	673	ALA	2.8
1	B	28	SER	2.8
1	A	713	GLN	2.7
1	C	726	GLY	2.4
1	A	32	GLU	2.4
1	B	583	LYS	2.3
1	C	750	LYS	2.2
1	D	713	GLN	2.2
1	C	712	ASP	2.2
1	C	713	GLN	2.1
1	B	706	ALA	2.0
1	B	647	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	H2S	C	754	1/1	0.35	16.33	26,26,26,26	1
4	H2S	D	754	1/1	0.26	12.27	20,20,20,20	1
4	H2S	B	754	1/1	0.25	11.48	22,22,22,22	1
4	H2S	A	754	1/1	0.23	9.99	24,24,24,24	1
2	HDD	C	760[A]	44/44	0.06	0.41	2,4,10,12	44
3	HDE	C	761[B]	44/44	0.06	0.32	3,9,12,14	44
2	HDD	B	760[A]	44/44	0.06	0.30	2,4,6,10	44
2	HDD	D	760[A]	44/44	0.06	0.27	2,3,8,12	44
3	HDE	B	761[B]	44/44	0.06	0.24	3,10,12,14	44
3	HDE	A	761[B]	44/44	0.06	0.18	2,7,11,11	44
2	HDD	A	760[A]	44/44	0.06	0.09	2,3,8,10	44
3	HDE	D	761[B]	44/44	0.05	-0.06	2,8,11,16	44

6.5 Other polymers ⓘ

There are no such residues in this entry.