



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:34 AM GMT

PDB ID : 3P9R  
Title : Structure of I274G variant of E. coli KatE  
Authors : Loewen, P.C.; Jha, V.; Louis, S.; Chelikani, P.; Carpena, X.; Fita, I.  
Deposited on : 2010-10-18  
Resolution : 1.90 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](mailto: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.

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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

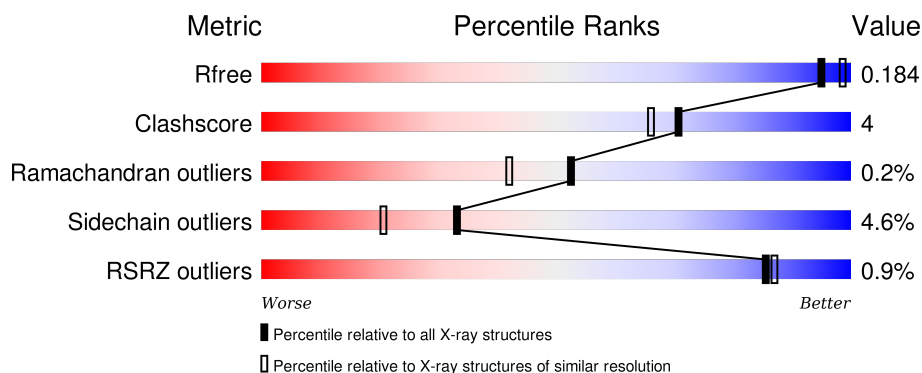
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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  $\geq 3$ , 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>87%</div> <div>8% . .</div> </div>
1	B	753	<div> <div>%</div> <div>85%</div> <div>10% . .</div> </div>
1	C	753	<div> <div>%</div> <div>83%</div> <div>12% . .</div> </div>
1	D	753	<div> <div>%</div> <div>86%</div> <div>9% . .</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26363 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.

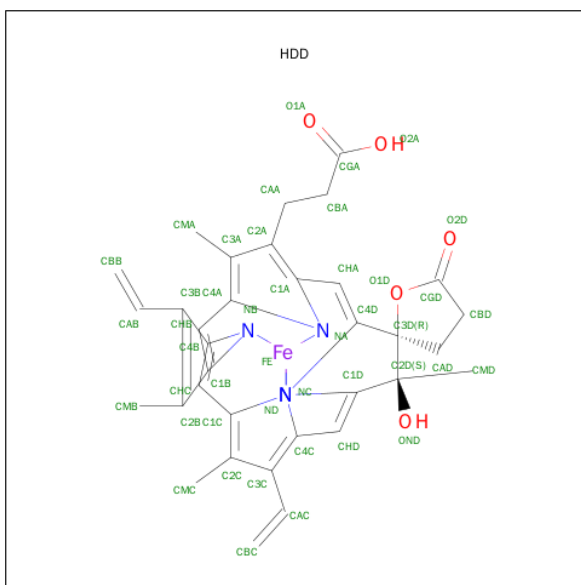
- Molecule 1 is a protein called Catalase HPIL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	4	0
			5748	3645	1006	1085	12			
1	B	726	Total	C	N	O	S	0	4	0
			5750	3645	1007	1086	12			
1	C	726	Total	C	N	O	S	0	3	0
			5744	3642	1006	1084	12			
1	D	726	Total	C	N	O	S	0	3	0
			5749	3645	1007	1085	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	GLY	ILE	ENGINEERED MUTATION	UNP P21179
B	274	GLY	ILE	ENGINEERED MUTATION	UNP P21179
C	274	GLY	ILE	ENGINEERED MUTATION	UNP P21179
D	274	GLY	ILE	ENGINEERED MUTATION	UNP P21179

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>5</sub>).



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

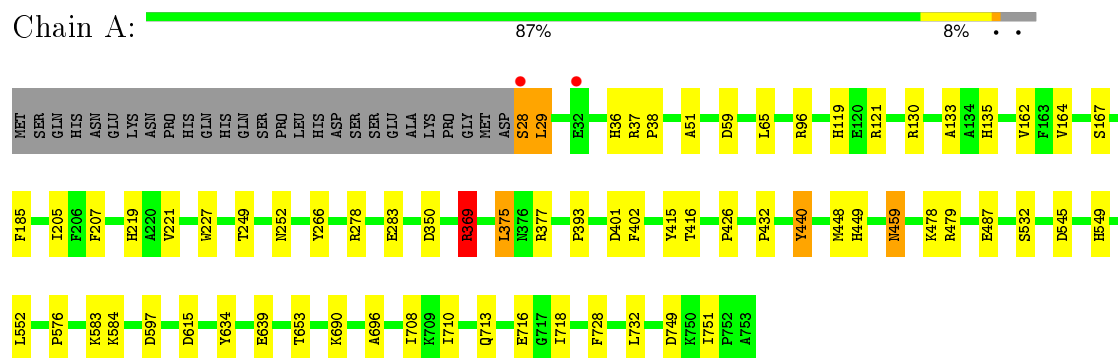
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	832	Total O 832 832	0	0
3	B	742	Total O 742 742	0	0
3	C	767	Total O 767 767	0	0
3	D	855	Total O 855 855	0	0

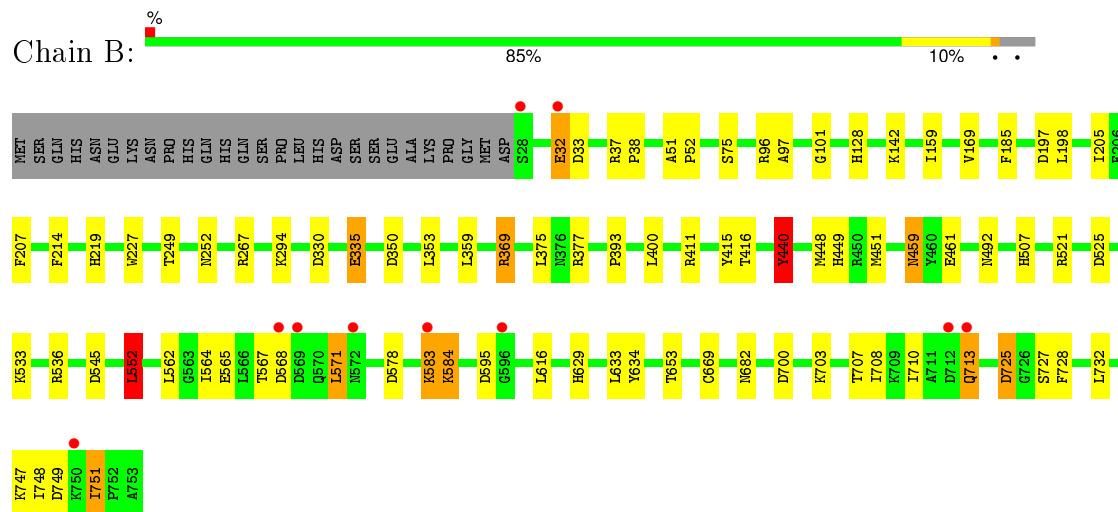
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

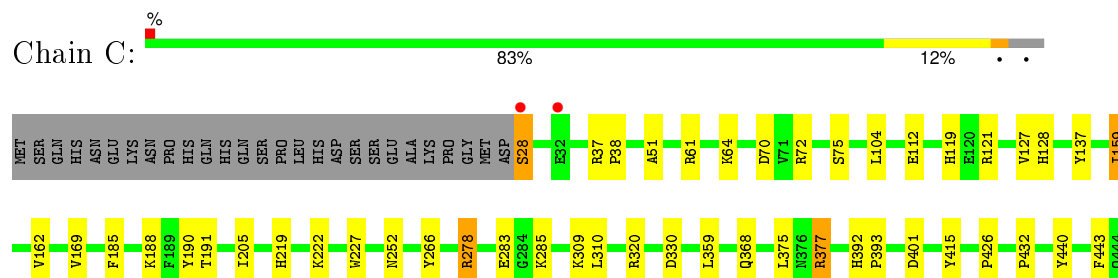
#### • Molecule 1: Catalase HP1I

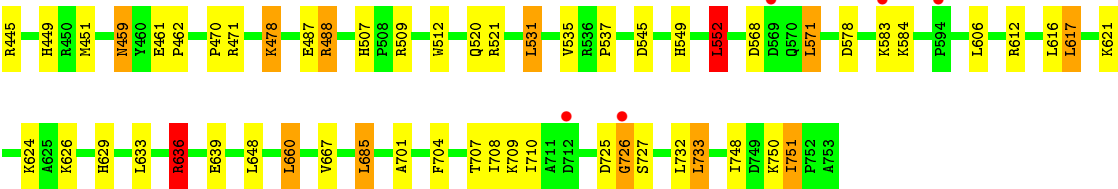


#### • Molecule 1: Catalase HP1I

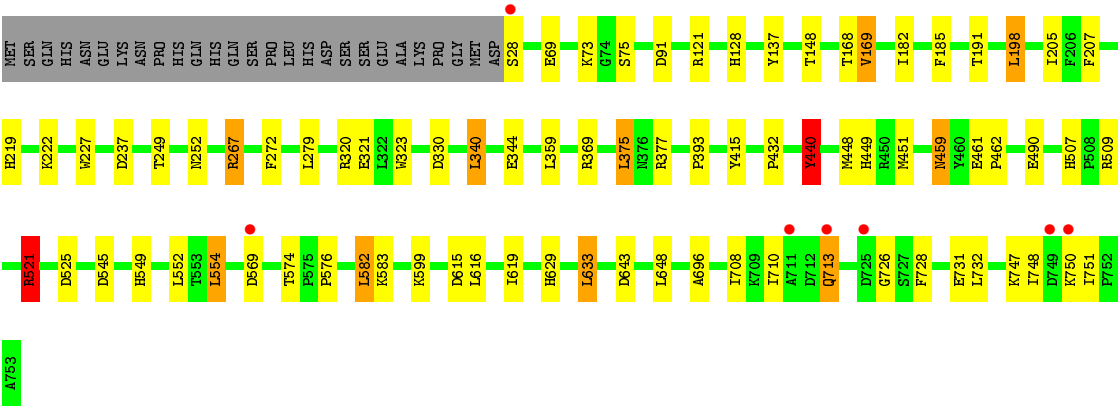
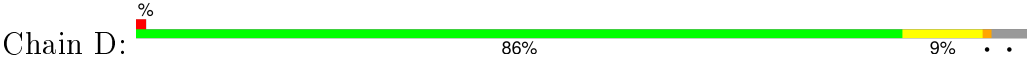


#### • Molecule 1: Catalase HP1I





• Molecule 1: Catalase HP11



A753

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.41Å 133.18Å 122.74Å 90.00° 109.21° 90.00°	Depositor
Resolution (Å)	35.24 – 1.90 35.24 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (35.24-1.90) 99.4 (35.24-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.133 , 0.184 0.133 , 0.184	Depositor DCC
$R_{free}$ test set	11178 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.8	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 221186 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	26363	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OCS, HDD

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	1.15	7/5913 (0.1%)	0.97	13/8037 (0.2%)
1	B	1.12	2/5912 (0.0%)	0.96	14/8035 (0.2%)
1	C	1.12	2/5906 (0.0%)	1.00	20/8027 (0.2%)
1	D	1.16	9/5906 (0.2%)	0.96	15/8027 (0.2%)
All	All	1.14	20/23637 (0.1%)	0.97	62/32126 (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	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	266	TYR	CD1-CE1	6.69	1.49	1.39
1	A	162	VAL	CB-CG2	6.47	1.66	1.52
1	A	377	ARG	CZ-NH2	6.32	1.41	1.33
1	D	440	TYR	CE1-CZ	5.93	1.46	1.38
1	A	440	TYR	CE1-CZ	5.90	1.46	1.38
1	D	169	VAL	CB-CG1	5.88	1.65	1.52
1	A	266	TYR	CD1-CE1	5.62	1.47	1.39
1	B	440	TYR	CE1-CZ	5.57	1.45	1.38
1	D	272	PHE	CE2-CZ	5.46	1.47	1.37
1	D	69	GLU	CG-CD	5.39	1.60	1.51
1	B	335	GLU	CB-CG	-5.38	1.42	1.52
1	D	321	GLU	CD-OE1	5.30	1.31	1.25
1	A	402	PHE	CD2-CE2	5.30	1.49	1.39
1	A	221	VAL	CB-CG2	5.23	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	SER	CB-OG	5.21	1.49	1.42
1	C	112	GLU	CB-CG	5.14	1.61	1.52
1	D	323	TRP	CZ3-CH2	5.14	1.48	1.40
1	D	267	ARG	CG-CD	5.13	1.64	1.51
1	D	137	TYR	CD2-CE2	5.12	1.47	1.39
1	D	344	GLU	CD-OE2	5.03	1.31	1.25

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	636	ARG	NE-CZ-NH2	-12.45	114.08	120.30
1	C	636	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	B	521	ARG	NE-CZ-NH2	9.02	124.81	120.30
1	A	615	ASP	CB-CG-OD2	8.10	125.59	118.30
1	C	121	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	B	536	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	C	37	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	D	633	LEU	CB-CG-CD1	7.65	124.00	111.00
1	A	121	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	C	320	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	C	471	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	A	350	ASP	CB-CG-OD1	-7.14	111.87	118.30
1	B	96	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	D	582	LEU	CB-CG-CD1	6.97	122.84	111.00
1	C	531	LEU	CB-CG-CD1	6.87	122.68	111.00
1	C	70	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	96	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	C	733	LEU	CA-CB-CG	6.41	130.04	115.30
1	B	350	ASP	CB-CG-OD1	-6.35	112.58	118.30
1	D	554	LEU	CB-CG-CD2	6.33	121.77	111.00
1	D	222	LYS	CD-CE-NZ	-6.31	97.19	111.70
1	C	377	ARG	NE-CZ-NH1	-6.29	117.16	120.30
1	D	521	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	C	445	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	B	521	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	D	375	LEU	CB-CG-CD1	6.04	121.26	111.00
1	B	400	LEU	CB-CG-CD2	-5.94	100.90	111.00
1	C	72	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	D	121	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	D	320	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	D	377	ARG	CG-CD-NE	-5.75	99.73	111.80
1	B	96	ARG	NE-CZ-NH1	5.71	123.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	636	ARG	CG-CD-NE	-5.65	99.93	111.80
1	A	350	ASP	CB-CA-C	5.60	121.59	110.40
1	A	29	LEU	CA-CB-CG	5.59	128.15	115.30
1	D	643	ASP	CB-CG-OD1	5.57	123.31	118.30
1	D	377	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	197	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	B	552	LEU	CA-CB-CG	5.33	127.57	115.30
1	A	479	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	130	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	615	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	A	369	ARG	NE-CZ-NH1	-5.31	117.65	120.30
1	C	685	LEU	CB-CG-CD1	5.28	119.98	111.00
1	C	552	LEU	CA-CB-CG	5.25	127.38	115.30
1	B	267	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	C	401	ASP	CB-CG-OD2	5.24	123.02	118.30
1	D	521	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	C	278	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	D	377	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	C	509	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	D	198	LEU	CA-CB-CG	5.18	127.20	115.30
1	B	353	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	B	536	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	401	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	33	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	375	LEU	CB-CG-CD2	5.07	119.62	111.00
1	C	222	LYS	CD-CE-NZ	-5.07	100.04	111.70
1	C	445	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	29	LEU	CB-CA-C	5.05	119.79	110.20
1	D	340	LEU	CB-CG-CD1	5.05	119.59	111.00
1	B	595	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	726	GLY	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	5748	0	5577	43	1
1	B	5750	0	5573	57	1
1	C	5744	0	5569	59	0
1	D	5749	0	5572	37	0
2	A	44	0	31	5	0
2	B	44	0	31	6	0
2	C	44	0	31	3	0
2	D	44	0	31	3	0
3	A	832	0	0	17	0
3	B	742	0	0	18	0
3	C	767	0	0	23	0
3	D	855	0	0	18	1
All	All	26363	0	22415	201	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 (201) 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:B:449[A]:HIS:CE1	3:B:3405:HOH:O	1.70	1.26
1:D:549:HIS:HE1	3:D:3214:HOH:O	1.04	1.26
1:C:449[B]:HIS:CD2	3:C:3402:HOH:O	1.70	1.24
1:B:416:THR:HG21	3:D:2464:HOH:O	1.39	1.18
1:A:549:HIS:HE1	3:A:3355:HOH:O	1.29	1.15
1:C:451:MET:SD	3:C:3402:HOH:O	2.08	1.10
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.88	1.08
1:C:392:HIS:CG	1:C:415:TYR:HB2	1.89	1.08
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.74	1.06
2:A:760:HDD:HMB1	2:A:760:HDD:HBB1	1.41	1.01
1:B:451:MET:SD	3:B:3409:HOH:O	2.19	1.00
2:D:760:HDD:HBB1	2:D:760:HDD:HMB1	1.44	0.99
1:C:751:ILE:HB	3:C:2367:HOH:O	1.63	0.98
1:B:449[A]:HIS:NE2	3:B:3405:HOH:O	1.76	0.97
1:B:369:ARG:HG2	3:B:1639:HOH:O	1.63	0.95
1:C:727:SER:HA	3:C:2714:HOH:O	1.72	0.88
1:B:545:ASP:OD1	3:B:3218:HOH:O	1.91	0.86
1:D:731:GLU:OE2	3:D:3028:HOH:O	1.95	0.85
2:B:760:HDD:HBB1	2:B:760:HDD:HMB1	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2649:HOH:O	1:C:28:SER:HA	1.76	0.84
1:D:748:ILE:O	1:D:751:ILE:HG22	1.77	0.84
1:B:294:LYS:HB2	3:B:1097:HOH:O	1.78	0.84
2:C:760:HDD:HBB1	2:C:760:HDD:HMB1	1.61	0.83
1:C:549:HIS:HE1	3:C:2940:HOH:O	1.61	0.82
1:B:578:ASP:HB2	3:B:2590:HOH:O	1.81	0.81
1:C:545:ASP:OD1	3:C:3210:HOH:O	2.00	0.79
1:A:532[A]:SER:OG	3:A:3278:HOH:O	1.99	0.78
1:C:449[B]:HIS:HD2	3:C:3402:HOH:O	1.23	0.77
1:D:549:HIS:CE1	3:D:3214:HOH:O	1.93	0.77
1:D:267:ARG:HG3	3:D:1920:HOH:O	1.85	0.77
1:B:748:ILE:O	1:B:751:ILE:HG22	1.86	0.75
1:B:37:ARG:NH1	3:B:2886:HOH:O	2.21	0.74
1:B:37:ARG:NH2	3:B:3231:HOH:O	2.20	0.73
1:A:549:HIS:CE1	3:A:3355:HOH:O	2.16	0.72
1:B:583:LYS:NZ	1:B:583:LYS:H	1.90	0.70
1:A:710:ILE:CD1	1:A:718:ILE:HG13	2.22	0.70
1:A:639:GLU:HG3	3:A:2414:HOH:O	1.93	0.69
1:D:545:ASP:OD1	3:D:3214:HOH:O	2.10	0.69
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.74	0.68
1:D:629:HIS:HD2	3:D:1554:HOH:O	1.77	0.68
1:A:710:ILE:HD13	1:A:718:ILE:HG13	1.75	0.67
1:A:545:ASP:OD1	3:A:2770:HOH:O	2.11	0.67
1:D:726:GLY:O	3:D:2447:HOH:O	2.14	0.66
1:B:525:ASP:OD2	3:B:819:HOH:O	2.14	0.65
1:D:449[A]:HIS:HD2	3:D:3408:HOH:O	1.79	0.65
1:D:451:MET:SD	3:D:3406:HOH:O	2.54	0.64
1:C:725:ASP:HB2	1:C:726:GLY:HA3	1.79	0.64
1:C:725:ASP:HB2	1:C:726:GLY:CA	2.28	0.64
1:B:629:HIS:HD2	3:B:1060:HOH:O	1.80	0.63
1:C:748:ILE:O	1:C:751:ILE:HG23	1.99	0.62
1:A:708:ILE:HD12	1:A:710:ILE:HD11	1.79	0.62
1:B:449[B]:HIS:HE1	3:D:1789:HOH:O	1.81	0.62
1:A:449[B]:HIS:HD2	3:A:3404:HOH:O	1.82	0.62
2:A:760:HDD:HMB1	2:A:760:HDD:CBB	2.25	0.61
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.83	0.61
1:C:392:HIS:ND1	1:C:415:TYR:CG	2.65	0.60
1:A:416[B]:THR:HG22	3:A:901:HOH:O	2.01	0.59
1:C:704:PHE:O	1:C:707:THR:HG22	2.02	0.59
1:A:478:LYS:HG2	3:A:1955:HOH:O	2.01	0.59
2:D:760:HDD:HMB1	2:D:760:HDD:CBB	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LEU:HB2	3:C:2405:HOH:O	2.01	0.59
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.18	0.59
1:A:29:LEU:HD22	3:C:2405:HOH:O	2.03	0.58
1:A:36:HIS:CD2	1:A:36:HIS:H	2.21	0.58
1:B:533:LYS:HE2	3:B:3100:HOH:O	2.02	0.58
1:D:440:TYR:HD1	3:D:3139:HOH:O	1.86	0.57
1:C:392:HIS:ND1	1:C:415:TYR:CA	2.65	0.57
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.87	0.57
1:A:716:GLU:HG3	3:A:2227:HOH:O	2.03	0.57
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.85	0.57
1:C:629:HIS:HD2	3:C:1129:HOH:O	1.88	0.56
2:B:760:HDD:CBB	2:B:760:HDD:HMB1	2.33	0.56
1:D:448:MET:O	1:D:449[A]:HIS:HB2	2.06	0.56
1:C:549:HIS:CE1	3:C:2940:HOH:O	2.43	0.56
1:D:449[A]:HIS:HE1	3:D:1789:HOH:O	1.89	0.55
1:A:545:ASP:O	1:A:549:HIS:HD2	1.89	0.55
1:B:214:PHE:CD1	2:B:760:HDD:HAC	2.41	0.55
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.90	0.54
2:C:760:HDD:HBB1	2:C:760:HDD:CMB	2.36	0.54
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.91	0.54
1:B:583:LYS:O	1:B:584:LYS:HB3	2.07	0.54
2:B:760:HDD:HBB1	2:B:760:HDD:CMB	2.36	0.54
1:B:583:LYS:HZ2	1:B:583:LYS:H	1.56	0.54
1:C:359:LEU:H	1:C:507:HIS:HD2	1.56	0.54
1:C:392:HIS:CG	1:C:415:TYR:CB	2.69	0.53
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.12	0.53
1:B:294:LYS:HE2	3:B:3346:HOH:O	2.08	0.53
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.39	0.53
1:D:599:LYS:HD3	3:D:2048:HOH:O	2.07	0.53
1:B:369:ARG:CG	3:B:1639:HOH:O	2.39	0.52
1:D:359:LEU:H	1:D:507:HIS:HD2	1.56	0.52
1:B:708:ILE:HG13	1:B:710:ILE:HG12	1.91	0.52
1:B:335:GLU:OE1	1:B:369:ARG:HD2	2.10	0.52
1:C:478:LYS:HB3	3:C:3101:HOH:O	2.09	0.52
2:A:760:HDD:HMC1	2:A:760:HDD:CBC	2.39	0.52
1:D:713:GLN:O	1:D:713:GLN:HG2	2.10	0.52
1:B:583:LYS:HZ3	1:B:583:LYS:H	1.58	0.51
1:C:368:GLN:NE2	3:C:1787:HOH:O	2.23	0.51
1:B:440:TYR:CE1	1:D:73:LYS:HE3	2.46	0.51
1:A:426:PRO:HG3	1:C:119:HIS:HB2	1.92	0.51
1:A:597:ASP:OD1	3:A:2719:HOH:O	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:760:HDD:HMB1	2:C:760:HDD:CBB	2.35	0.50
1:D:509:ARG:HD2	1:D:576:PRO:HD2	1.92	0.50
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.28	0.49
1:A:36:HIS:HE1	3:A:1872:HOH:O	1.94	0.49
1:B:411:ARG:HG2	2:B:760:HDD:C2C	2.42	0.49
1:B:533:LYS:CE	3:C:2623:HOH:O	2.60	0.49
1:C:636:ARG:HD3	3:C:2717:HOH:O	2.12	0.49
1:B:564:ILE:O	3:B:2603:HOH:O	2.20	0.49
1:A:28:SER:OG	1:A:28:SER:O	2.29	0.48
1:C:359:LEU:H	1:C:507:HIS:CD2	2.31	0.48
1:C:488:ARG:NH1	3:C:2379:HOH:O	2.18	0.48
1:C:583:LYS:O	1:C:584:LYS:HB3	2.13	0.48
1:B:533:LYS:HD2	3:C:2623:HOH:O	2.14	0.48
2:A:760:HDD:HMC1	2:A:760:HDD:HBC1	1.96	0.48
1:B:38:PRO:HG2	1:B:51:ALA:HB2	1.96	0.48
1:B:669:OCS:OD2	1:B:700:ASP:HB2	2.14	0.47
1:B:634:TYR:O	1:B:653:THR:HA	2.14	0.47
1:A:448:MET:O	1:A:449[B]:HIS:HB2	2.15	0.47
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.50	0.47
1:D:521:ARG:HD2	1:D:525:ASP:OD1	2.15	0.47
1:A:583:LYS:O	1:A:584:LYS:HB3	2.14	0.47
1:C:667:VAL:CG1	1:C:701:ALA:HB1	2.44	0.47
1:B:448:MET:O	1:B:449[B]:HIS:HB2	2.15	0.46
1:C:535:VAL:O	1:C:537:PRO:HD3	2.15	0.46
1:A:708:ILE:CD1	1:A:710:ILE:HD11	2.44	0.46
3:A:2649:HOH:O	1:C:28:SER:CA	2.51	0.46
1:A:710:ILE:HD11	1:A:718:ILE:HG13	1.97	0.46
1:D:583:LYS:HD3	3:D:3374:HOH:O	2.15	0.46
2:D:760:HDD:HBB1	2:D:760:HDD:CMB	2.31	0.45
1:C:667:VAL:HG12	1:C:701:ALA:CB	2.46	0.45
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.51	0.45
1:C:725:ASP:HB2	1:C:726:GLY:C	2.37	0.45
1:D:615:ASP:O	1:D:619:ILE:HG13	2.17	0.45
2:A:760:HDD:CMB	2:A:760:HDD:HBB1	2.29	0.45
1:B:294:LYS:NZ	3:B:2778:HOH:O	2.49	0.45
1:D:128:HIS:HA	1:D:168:THR:O	2.17	0.45
1:C:748:ILE:O	1:C:751:ILE:CG2	2.63	0.45
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.32	0.45
1:D:169:VAL:HG21	1:D:182:ILE:HB	1.99	0.45
1:C:309:LYS:CE	3:C:1232:HOH:O	2.64	0.45
1:C:309:LYS:HE3	3:C:1232:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLU:OE1	1:B:32:GLU:HA	2.16	0.44
1:C:38:PRO:HG2	1:C:51:ALA:HB2	1.99	0.44
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.52	0.44
1:B:214:PHE:CD2	2:B:760:HDD:HMC2	2.52	0.44
1:C:617:LEU:HD12	3:C:2230:HOH:O	2.17	0.44
1:D:549:HIS:HD2	3:D:2205:HOH:O	2.00	0.44
1:C:310:LEU:HD13	1:C:660:LEU:HB3	2.00	0.44
1:A:369:ARG:HG2	3:A:2410:HOH:O	2.17	0.44
1:A:549:HIS:O	1:A:576:PRO:HD3	2.17	0.44
1:A:29:LEU:CB	3:C:2405:HOH:O	2.61	0.44
1:B:492:ASN:CG	3:B:2605:HOH:O	2.56	0.44
1:D:461:GLU:HA	1:D:462:PRO:C	2.38	0.44
1:C:461:GLU:HA	1:C:462:PRO:C	2.37	0.44
1:B:207:PHE:O	1:B:249:THR:HA	2.18	0.44
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.52	0.44
1:B:52:PRO:HG3	3:D:1451:HOH:O	2.17	0.43
1:D:207:PHE:O	1:D:249:THR:HA	2.17	0.43
1:B:725:ASP:OD2	1:B:727:SER:HB3	2.18	0.43
1:B:552:LEU:HB2	3:B:3202:HOH:O	2.17	0.43
1:D:393:PRO:HD2	1:D:415:TYR:CG	2.53	0.43
1:A:634:TYR:O	1:A:653:THR:HA	2.18	0.43
1:A:133:ALA:HA	1:A:164:VAL:O	2.18	0.43
1:D:708:ILE:HG13	1:D:710:ILE:HG12	2.00	0.43
1:A:690:LYS:HG3	3:A:3093:HOH:O	2.19	0.43
1:C:392:HIS:HB2	1:C:415:TYR:HB3	2.01	0.43
1:C:127:VAL:O	1:C:128:HIS:HB2	2.19	0.43
1:A:207:PHE:O	1:A:249:THR:HA	2.19	0.42
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.95	0.42
1:A:65:LEU:HD21	1:A:135:HIS:CG	2.54	0.42
1:B:567:THR:O	1:B:571:LEU:HD22	2.19	0.42
1:B:359:LEU:H	1:B:507:HIS:HD2	1.66	0.42
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.55	0.42
3:A:1016:HOH:O	1:C:104:LEU:HB3	2.19	0.42
1:C:330:ASP:OD1	1:C:629:HIS:HE1	2.01	0.42
1:C:393:PRO:HD2	1:C:415:TYR:CG	2.55	0.42
1:C:278:ARG:HH12	1:C:487:GLU:CD	2.23	0.42
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.55	0.42
1:D:148:THR:HB	1:D:279:LEU:HB3	2.02	0.41
1:D:521:ARG:HG2	3:D:2917:HOH:O	2.20	0.41
1:C:128:HIS:CE1	1:C:169:VAL:HG22	2.55	0.41
1:B:97:ALA:O	1:B:101:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:621:LYS:HG2	3:C:3116:HOH:O	2.21	0.41
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.36	0.41
1:A:459:ASN:HD22	1:A:459:ASN:H	1.68	0.41
1:C:64:LYS:HE2	1:C:190:TYR:CZ	2.55	0.41
1:A:369:ARG:NH1	3:A:3347:HOH:O	2.49	0.41
1:B:459:ASN:H	1:B:459:ASN:HD22	1.68	0.41
1:A:119:HIS:HB2	1:C:426:PRO:HG3	2.02	0.41
1:C:512:TRP:CH2	1:C:520:GLN:HB3	2.55	0.41
1:D:448:MET:O	1:D:449[A]:HIS:CB	2.68	0.41
1:B:533:LYS:CD	3:C:2623:HOH:O	2.69	0.41
1:A:393:PRO:HD2	1:A:415:TYR:CD2	2.55	0.41
1:B:747:LYS:HE3	1:B:747:LYS:HB3	1.89	0.41
1:B:713:GLN:H	1:B:713:GLN:HG3	1.55	0.41
1:B:451:MET:HE1	1:D:451:MET:HE2	2.02	0.40
1:C:28:SER:OG	1:C:28:SER:O	2.37	0.40
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.03	0.40
1:C:162:VAL:HA	1:C:188:LYS:O	2.21	0.40
1:B:461:GLU:OE1	1:D:91:ASP:OD1	2.40	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:NH2[2_545]	2.07	0.13
3:D:2178:HOH:O	3:D:2976:HOH:O[1_655]	2.18	0.02

## 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	727/753 (96%)	706 (97%)	21 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	727/753 (96%)	706 (97%)	18 (2%)	3 (0%)	39	27
1	C	726/753 (96%)	707 (97%)	18 (2%)	1 (0%)	56	46
1	D	726/753 (96%)	709 (98%)	16 (2%)	1 (0%)	56	46
All	All	2906/3012 (96%)	2828 (97%)	73 (2%)	5 (0%)	52	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	B	75	SER
1	B	584	LYS
1	C	75	SER
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	613/634 (97%)	597 (97%)	16 (3%)	54	45
1	B	613/634 (97%)	586 (96%)	27 (4%)	35	22
1	C	612/634 (96%)	572 (94%)	40 (6%)	21	10
1	D	612/634 (96%)	584 (95%)	28 (5%)	33	21
All	All	2450/2536 (97%)	2339 (96%)	111 (4%)	33	21

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	185	PHE
1	A	205	ILE
1	A	227	TRP
1	A	252	ASN
1	A	283	GLU

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Mol	Chain	Res	Type
1	A	369	ARG
1	A	375	LEU
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	713	GLN
1	A	732	LEU
1	A	749	ASP
1	A	751	ILE
1	B	32	GLU
1	B	142	LYS
1	B	159	ILE
1	B	185	PHE
1	B	198	LEU
1	B	205	ILE
1	B	227	TRP
1	B	252	ASN
1	B	369	ARG
1	B	375	LEU
1	B	377	ARG
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	616	LEU
1	B	633	LEU
1	B	703	LYS
1	B	713	GLN
1	B	728	PHE
1	B	732	LEU
1	B	749	ASP
1	B	751	ILE
1	C	28	SER
1	C	61	ARG
1	C	159	ILE
1	C	185	PHE
1	C	191	THR

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Mol	Chain	Res	Type
1	C	205	ILE
1	C	227	TRP
1	C	252	ASN
1	C	283	GLU
1	C	285	LYS
1	C	375	LEU
1	C	377	ARG
1	C	432	PRO
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	521	ARG
1	C	531	LEU
1	C	552	LEU
1	C	568	ASP
1	C	571	LEU
1	C	578	ASP
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	617	LEU
1	C	624	LYS
1	C	626	LYS
1	C	633	LEU
1	C	636	ARG
1	C	639	GLU
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	709	LYS
1	C	732	LEU
1	C	733	LEU
1	C	750	LYS
1	C	751	ILE
1	D	28	SER
1	D	185	PHE
1	D	191	THR
1	D	198	LEU
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP

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Mol	Chain	Res	Type
1	D	252	ASN
1	D	340	LEU
1	D	369	ARG
1	D	375	LEU
1	D	432	PRO
1	D	440	TYR
1	D	459	ASN
1	D	490	GLU
1	D	521	ARG
1	D	552	LEU
1	D	554	LEU
1	D	569	ASP
1	D	574	THR
1	D	582	LEU
1	D	616	LEU
1	D	633	LEU
1	D	648	LEU
1	D	713	GLN
1	D	732	LEU
1	D	747	LYS
1	D	750	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) 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	549	HIS
1	A	713	GLN
1	B	157	ASN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	252	ASN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	572	ASN
1	C	629	HIS

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Mol	Chain	Res	Type
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	549	HIS
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	3.95	2 (28%)	7,11,13	2.65	3 (42%)
1	OCS	B	669	1	7,8,9	2.65	1 (14%)	7,11,13	2.13	3 (42%)
1	OCS	C	669	1	7,8,9	2.45	1 (14%)	7,11,13	1.58	1 (14%)
1	OCS	D	669	1	7,8,9	4.72	2 (28%)	7,11,13	5.73	5 (71%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	669	OCS	CB-CA	2.37	1.59	1.51
1	D	669	OCS	CB-CA	2.59	1.60	1.51
1	C	669	OCS	CB-SG	6.16	1.87	1.77
1	B	669	OCS	CB-SG	6.73	1.87	1.77
1	A	669	OCS	CB-SG	10.08	1.92	1.77
1	D	669	OCS	CB-SG	12.08	1.95	1.77

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	669	OCS	OD1-SG-CB	-3.72	103.81	106.94
1	D	669	OCS	OD2-SG-OD3	-2.84	105.00	111.61
1	D	669	OCS	OD3-SG-OD1	-2.69	103.67	113.48
1	D	669	OCS	OD2-SG-OD1	-2.55	105.68	111.61
1	B	669	OCS	OD2-SG-OD3	-2.31	106.24	111.61
1	A	669	OCS	OD2-SG-OD1	-2.24	106.40	111.61
1	A	669	OCS	OD3-SG-CB	2.52	109.07	106.94
1	B	669	OCS	OD3-SG-CB	3.02	109.49	106.94
1	C	669	OCS	OD3-SG-CB	3.15	109.59	106.94
1	A	669	OCS	OD1-SG-CB	5.78	111.82	106.94
1	D	669	OCS	OD1-SG-CB	6.24	112.20	106.94
1	D	669	OCS	OD3-SG-CB	12.93	117.84	106.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	669	OCS	1	0

## 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	HDD	A	760	1,3	30,52,52	2.23	11 (36%)	20,89,89	3.42	8 (40%)
2	HDD	B	760	1,3	30,52,52	2.00	10 (33%)	20,89,89	3.87	12 (60%)
2	HDD	C	760	1,3	30,52,52	2.09	8 (26%)	20,89,89	4.07	11 (55%)
2	HDD	D	760	1	30,52,52	2.15	10 (33%)	20,89,89	3.33	6 (30%)

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	1,3	-	0/3/89/89	0/1/9/9
2	HDD	B	760	1,3	-	0/3/89/89	0/1/9/9
2	HDD	C	760	1,3	-	0/3/89/89	0/1/9/9
2	HDD	D	760	1	-	0/3/89/89	0/1/9/9

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	760	HDD	C3C-C2C	-4.70	1.34	1.40
2	B	760	HDD	C3C-C2C	-4.38	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HDD	C3C-C2C	-4.12	1.34	1.40
2	C	760	HDD	C3B-C2B	-4.09	1.34	1.40
2	C	760	HDD	C3C-C2C	-3.99	1.35	1.40
2	B	760	HDD	C3B-C2B	-3.88	1.35	1.40
2	A	760	HDD	C3B-C2B	-3.87	1.35	1.40
2	D	760	HDD	C3B-C2B	-3.15	1.36	1.40
2	A	760	HDD	O1D-C3D	-2.88	1.41	1.46
2	C	760	HDD	O1D-C3D	-2.72	1.42	1.46
2	B	760	HDD	O1D-C3D	-2.46	1.42	1.46
2	B	760	HDD	O2D-CGD	2.04	1.28	1.22
2	B	760	HDD	CMC-C2C	2.06	1.55	1.51
2	A	760	HDD	C3C-CAC	2.09	1.52	1.47
2	D	760	HDD	CMB-C2B	2.18	1.56	1.51
2	A	760	HDD	CMA-C3A	2.18	1.56	1.51
2	B	760	HDD	O1D-CGD	2.21	1.39	1.35
2	B	760	HDD	C4D-ND	2.25	1.41	1.38
2	C	760	HDD	C4B-NB	2.41	1.39	1.36
2	C	760	HDD	CMB-C2B	2.48	1.57	1.51
2	A	760	HDD	OND-C2D	2.51	1.47	1.42
2	D	760	HDD	C1B-NB	2.54	1.40	1.36
2	A	760	HDD	C1B-NB	2.70	1.40	1.36
2	D	760	HDD	C3C-CAC	2.73	1.53	1.47
2	D	760	HDD	CMD-C2D	2.83	1.57	1.53
2	D	760	HDD	CAA-C2A	2.84	1.56	1.52
2	C	760	HDD	CMC-C2C	3.00	1.57	1.51
2	A	760	HDD	CMB-C2B	3.03	1.58	1.51
2	D	760	HDD	OND-C2D	3.07	1.49	1.42
2	B	760	HDD	CAA-C2A	3.34	1.57	1.52
2	C	760	HDD	C3B-CAB	3.38	1.54	1.47
2	B	760	HDD	C3B-CAB	3.74	1.55	1.47
2	D	760	HDD	C3B-CAB	3.98	1.56	1.47
2	A	760	HDD	CMC-C2C	4.06	1.60	1.51
2	A	760	HDD	C3B-CAB	4.10	1.56	1.47
2	B	760	HDD	FE-ND	4.11	2.12	1.95
2	D	760	HDD	FE-ND	5.26	2.16	1.95
2	A	760	HDD	FE-ND	5.38	2.17	1.95
2	C	760	HDD	FE-ND	5.39	2.17	1.95

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	760	HDD	O1D-CGD-CBD	-6.52	102.57	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	760	HDD	C3C-CAC-CBC	-6.32	113.39	126.32
2	A	760	HDD	O1D-CGD-CBD	-6.25	102.88	110.20
2	C	760	HDD	OND-C2D-CMD	-5.99	98.59	109.41
2	C	760	HDD	O1D-CGD-CBD	-5.76	103.45	110.20
2	D	760	HDD	CAA-CBA-CGA	-5.71	102.28	112.75
2	D	760	HDD	OND-C2D-CMD	-5.57	99.36	109.41
2	B	760	HDD	CAA-CBA-CGA	-5.32	103.00	112.75
2	B	760	HDD	O1D-CGD-CBD	-5.24	104.06	110.20
2	A	760	HDD	C3C-CAC-CBC	-4.99	116.12	126.32
2	A	760	HDD	CAA-CBA-CGA	-4.38	104.71	112.75
2	B	760	HDD	OND-C2D-CMD	-4.01	102.17	109.41
2	C	760	HDD	C3B-CAB-CBB	-3.67	118.80	126.32
2	C	760	HDD	CAA-CBA-CGA	-3.42	106.48	112.75
2	C	760	HDD	CMA-C3A-C4A	-3.38	122.78	128.36
2	B	760	HDD	C3C-CAC-CBC	-3.35	119.47	126.32
2	B	760	HDD	CMC-C2C-C1C	-3.18	123.10	128.36
2	D	760	HDD	C3C-CAC-CBC	-2.88	120.43	126.32
2	B	760	HDD	C3B-CAB-CBB	-2.87	120.45	126.32
2	A	760	HDD	CMA-C3A-C4A	-2.85	123.65	128.36
2	B	760	HDD	C3C-C4C-NC	-2.77	105.63	109.21
2	C	760	HDD	CAA-C2A-C1A	-2.52	124.27	127.01
2	A	760	HDD	C3C-C4C-NC	-2.52	105.96	109.21
2	B	760	HDD	CAA-C2A-C1A	-2.51	124.29	127.01
2	B	760	HDD	CMA-C3A-C4A	-2.44	124.32	128.36
2	A	760	HDD	CAA-C2A-C1A	-2.34	124.47	127.01
2	B	760	HDD	C3B-C4B-NB	-2.32	106.56	110.94
2	C	760	HDD	C3C-C4C-NC	-2.28	106.26	109.21
2	C	760	HDD	CMA-C3A-C2A	2.06	129.54	125.24
2	D	760	HDD	C4D-ND-C1D	3.10	109.36	107.36
2	B	760	HDD	C4D-ND-C1D	4.55	110.29	107.36
2	A	760	HDD	C4D-ND-C1D	4.71	110.40	107.36
2	C	760	HDD	C4D-ND-C1D	6.12	111.31	107.36
2	D	760	HDD	O1D-CGD-O2D	8.59	128.97	120.80
2	A	760	HDD	O1D-CGD-O2D	10.07	130.37	120.80
2	C	760	HDD	O1D-CGD-O2D	10.93	131.19	120.80
2	B	760	HDD	O1D-CGD-O2D	11.87	132.09	120.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	760	HDD	5	0
2	B	760	HDD	6	0
2	C	760	HDD	3	0
2	D	760	HDD	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	725/753 (96%)	-0.74	2 (0%) 94 94	5, 11, 27, 43	0
1	B	725/753 (96%)	-0.65	10 (1%) 78 80	6, 13, 33, 47	0
1	C	725/753 (96%)	-0.67	7 (0%) 84 86	5, 13, 33, 47	0
1	D	725/753 (96%)	-0.72	7 (0%) 84 86	5, 11, 29, 44	0
All	All	2900/3012 (96%)	-0.70	26 (0%) 85 87	5, 12, 31, 47	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	726	GLY	5.0
1	A	28	SER	4.0
1	C	28	SER	3.3
1	B	28	SER	3.3
1	D	28	SER	2.9
1	B	713	GLN	2.8
1	A	32	GLU	2.7
1	B	32	GLU	2.7
1	D	750	LYS	2.6
1	B	572	ASN	2.6
1	B	712	ASP	2.5
1	B	568	ASP	2.5
1	D	713	GLN	2.4
1	C	594	PRO	2.4
1	C	583	LYS	2.3
1	C	569	ASP	2.3
1	D	725	ASP	2.3
1	D	711	ALA	2.3
1	B	596	GLY	2.2
1	D	569	ASP	2.2
1	C	32	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	569	ASP	2.1
1	B	750	LYS	2.1
1	D	749	ASP	2.1
1	B	583	LYS	2.1
1	C	712	ASP	2.1

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	OCS	A	669	9/10	0.92	0.11	-	20,24,39,42	0
1	OCS	C	669	9/10	0.91	0.18	-	30,33,48,48	0
1	OCS	B	669	9/10	0.92	0.18	-	30,33,49,49	0
1	OCS	D	669	9/10	0.90	0.15	-	23,27,43,45	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	HDD	B	760	44/44	0.98	0.07	0.28	5,11,19,22	0
2	HDD	A	760	44/44	0.99	0.09	0.27	3,10,17,22	0
2	HDD	D	760	44/44	0.98	0.07	0.01	3,10,16,24	0
2	HDD	C	760	44/44	0.99	0.07	-0.13	4,10,18,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.