



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:18 AM GMT

PDB ID : 4D8U
Title : Crystal structure of D-Cysteine desulfhydrase from Salmonella typhimurium
at 3.3 Å in monoclinic space group with 8 subunits in the asymmetric unit
Authors : Bharath, S.R.; Shveta, B.; Rajesh, K.H.; Savithri, H.S.; Murthy, M.R.N.
Deposited on : 2012-01-11
Resolution : 3.30 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>

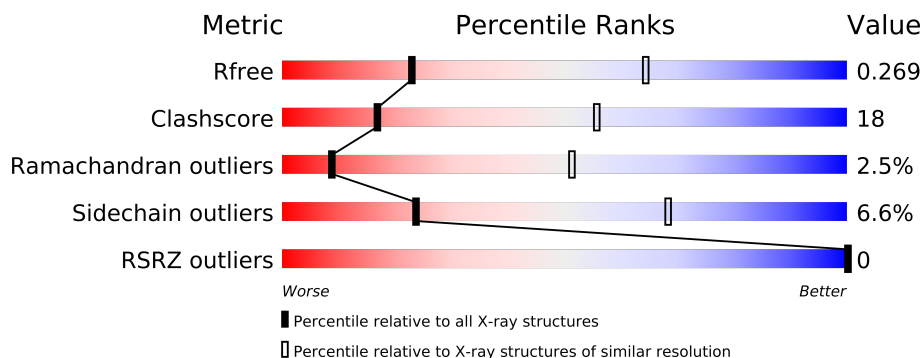
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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	342	
1	B	342	
1	C	342	
1	D	342	
1	E	342	
1	F	342	
1	G	342	
1	H	342	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19156 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 D-cysteine desulfhydrase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	P	S	0	0	0
			2466	1567	420	468	1	10			
1	B	323	Total	C	N	O	P	S	1	0	0
			2335	1485	388	452	1	9			
1	C	323	Total	C	N	O	P	S	0	0	0
			2361	1501	392	459	1	8			
1	D	329	Total	C	N	O	P	S	0	0	0
			2464	1567	420	466	1	10			
1	E	330	Total	C	N	O	P	S	0	0	0
			2450	1558	412	470	1	9			
1	F	318	Total	C	N	O	P	S	0	0	0
			2227	1405	375	438	1	8			
1	G	324	Total	C	N	O	P	S	0	0	0
			2341	1481	394	456	1	9			
1	H	331	Total	C	N	O	P	S	0	0	0
			2454	1559	418	466	1	10			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
A	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
A	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
A	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
A	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-7	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
A	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
A	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7
B	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
B	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
B	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
B	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
B	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-7	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
B	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
B	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7
B	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7
C	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
C	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
C	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
C	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
C	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-7	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
C	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
C	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7
C	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7
D	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
D	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
D	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
D	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
D	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-7	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
D	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
D	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7

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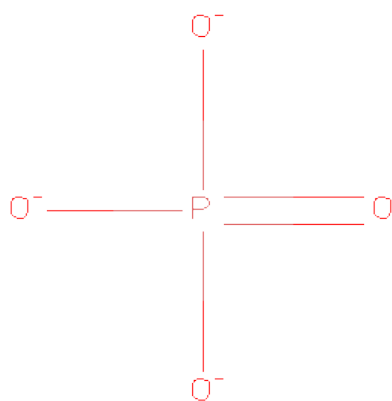
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7
E	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
E	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
E	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
E	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
E	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
E	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
E	-7	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
E	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
E	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
E	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
E	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
E	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
E	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7
E	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7
F	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
F	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
F	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
F	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
F	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
F	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
F	-7	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
F	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
F	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
F	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
F	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
F	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
F	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7
F	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7
G	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
G	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
G	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
G	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
G	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
G	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
G	-7	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
G	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
G	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
G	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
G	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
G	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
G	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7
H	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
H	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
H	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
H	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
H	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
H	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
H	-7	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
H	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
H	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
H	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
H	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
H	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
H	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7
H	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

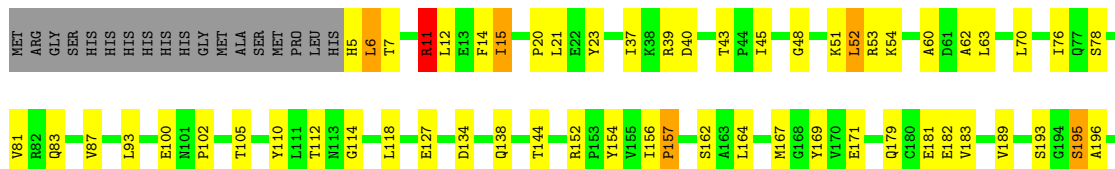
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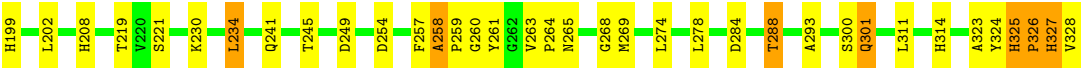
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

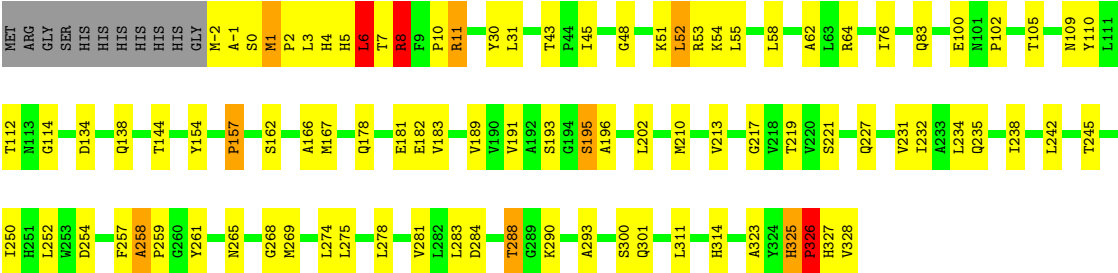
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	1	Total	O	0	0
			1	1		
3	C	1	Total	O	0	0
			1	1		
3	D	2	Total	O	0	0
			2	2		
3	E	1	Total	O	0	0
			1	1		
3	F	1	Total	O	0	0
			1	1		
3	H	6	Total	O	0	0
			6	6		





● Molecule 1: D-cysteine desulfhydrase

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.46Å 158.14Å 181.93Å 90.00° 94.10° 90.00°	Depositor
Resolution (Å)	52.04 – 3.30 52.04 – 3.30	Depositor EDS
% Data completeness (in resolution range)	90.4 (52.04-3.30) 90.4 (52.04-3.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.246 , 0.275 0.245 , 0.269	Depositor DCC
R_{free} test set	3499 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	74.8	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 69631 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	19156	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, IT1

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.67	1/2489 (0.0%)	0.79	5/3394 (0.1%)
1	B	0.67	0/2354	0.72	1/3220 (0.0%)
1	C	0.65	0/2380	0.74	3/3252 (0.1%)
1	D	0.66	0/2487	0.76	5/3391 (0.1%)
1	E	0.66	1/2473 (0.0%)	0.73	2/3376 (0.1%)
1	F	0.74	0/2241	0.73	0/3070
1	G	0.72	0/2361	0.75	2/3231 (0.1%)
1	H	0.67	2/2477 (0.1%)	0.74	3/3381 (0.1%)
All	All	0.68	4/19262 (0.0%)	0.75	21/26315 (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	E	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	326	PRO	N-CD	-5.48	1.40	1.47
1	E	95	CYS	CB-SG	-5.37	1.73	1.81
1	H	8	ARG	N-CA	-5.07	1.36	1.46
1	A	6	LEU	N-CA	-5.01	1.36	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	LEU	CB-CA-C	-7.56	95.83	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	269	MET	CB-CG-SD	7.19	133.98	112.40
1	D	6	LEU	CB-CG-CD1	7.13	123.11	111.00
1	D	269	MET	CB-CG-SD	7.09	133.67	112.40
1	H	8	ARG	N-CA-C	-6.96	92.20	111.00
1	A	6	LEU	CA-C-O	6.91	134.61	120.10
1	A	269	MET	CB-CG-SD	6.83	132.90	112.40
1	B	186	LEU	CB-CG-CD2	6.54	122.13	111.00
1	G	6	LEU	N-CA-C	6.51	128.57	111.00
1	A	5	HIS	CB-CA-C	-6.31	97.78	110.40
1	D	6	LEU	CA-CB-CG	-6.24	100.95	115.30
1	H	6	LEU	CB-CA-C	-5.87	99.04	110.20
1	E	4	HIS	N-CA-C	5.86	126.83	111.00
1	C	70	LEU	CA-CB-CG	5.86	128.77	115.30
1	D	269	MET	CA-CB-CG	5.67	122.94	113.30
1	D	5	HIS	CB-CA-C	-5.41	99.57	110.40
1	A	269	MET	CA-CB-CG	5.34	122.38	113.30
1	G	11	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	174	LEU	CA-CB-CG	5.20	127.25	115.30
1	H	8	ARG	N-CA-CB	5.18	119.92	110.60
1	C	252	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	0	SER	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	2466	0	2455	92	0
1	B	2335	0	2252	79	0
1	C	2361	0	2295	80	0
1	D	2464	0	2461	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2450	0	2421	91	0
1	F	2227	0	2063	73	0
1	G	2341	0	2236	84	0
1	H	2454	0	2424	109	0
2	A	5	0	0	2	0
2	B	5	0	0	0	0
2	C	5	0	0	2	0
2	D	5	0	0	0	0
2	E	5	0	0	2	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	6	0	0	1	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	H	6	0	0	1	0
All	All	19156	0	18607	670	0

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 18.

All (670) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:-2:MET:CB	1:H:-1:ALA:HA	1.53	1.36
1:H:6:LEU:O	1:H:6:LEU:CD1	1.75	1.34
1:G:325:HIS:HB3	1:G:326:PRO:CD	1.66	1.24
1:F:325:HIS:CD2	1:F:326:PRO:HD3	1.71	1.23
1:G:5:HIS:C	1:G:6:LEU:HD12	1.60	1.18
1:D:6:LEU:HD13	1:D:6:LEU:O	1.43	1.16
1:F:325:HIS:CG	1:F:326:PRO:CD	2.30	1.15
1:E:325:HIS:HB3	1:E:326:PRO:HD2	1.16	1.15
1:H:11:ARG:HG3	1:H:11:ARG:HH11	1.06	1.13
1:E:325:HIS:HB3	1:E:326:PRO:CD	1.79	1.13
1:D:1:MET:HB2	1:D:2:PRO:HA	1.25	1.12
1:F:325:HIS:CB	1:F:326:PRO:HD2	1.69	1.10
1:H:325:HIS:HB3	1:H:326:PRO:HD3	1.12	1.10
1:F:325:HIS:CB	1:F:326:PRO:CD	2.30	1.10
1:H:-2:MET:CB	1:H:-1:ALA:CA	2.30	1.09
1:G:325:HIS:HB3	1:G:326:PRO:HD2	1.10	1.09

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:5:HIS:O	1:G:6:LEU:HG	1.53	1.09
1:H:325:HIS:HB3	1:H:326:PRO:CD	1.82	1.08
1:E:325:HIS:CB	1:E:326:PRO:CD	2.29	1.07
1:D:258:ALA:HB1	1:D:259:PRO:HD3	1.33	1.07
1:G:325:HIS:CB	1:G:326:PRO:CD	2.30	1.06
1:F:258:ALA:HB1	1:F:259:PRO:HD3	1.33	1.06
1:A:258:ALA:HB1	1:A:259:PRO:HD3	1.37	1.05
1:B:258:ALA:HB1	1:B:259:PRO:HD3	1.40	1.03
1:D:325:HIS:HB3	1:D:326:PRO:HD3	1.37	1.03
1:E:258:ALA:HB1	1:E:259:PRO:HD3	1.35	1.03
1:H:6:LEU:O	1:H:6:LEU:HD13	0.88	1.03
1:H:325:HIS:CB	1:H:326:PRO:HD3	1.90	1.02
1:C:258:ALA:HB1	1:C:259:PRO:HD3	1.37	1.01
1:H:258:ALA:HB1	1:H:259:PRO:HD3	1.41	1.01
1:B:167:MET:CE	1:B:238:ILE:HG23	1.91	1.01
1:G:5:HIS:C	1:G:6:LEU:CD1	2.29	1.00
1:F:325:HIS:HB3	1:F:326:PRO:CD	1.89	1.00
1:G:258:ALA:HB1	1:G:259:PRO:HD3	1.40	1.00
1:F:325:HIS:HB3	1:F:326:PRO:HD2	1.01	0.99
1:F:7:THR:HG23	1:F:7:THR:O	1.57	0.98
1:E:325:HIS:CG	1:E:326:PRO:CD	2.47	0.97
1:G:325:HIS:CB	1:G:326:PRO:HD2	1.90	0.96
1:G:5:HIS:CA	1:G:6:LEU:HD12	1.94	0.96
1:F:325:HIS:CG	1:F:326:PRO:HD3	1.99	0.95
1:F:105:THR:OG1	1:F:328:VAL:HG12	1.68	0.94
1:F:51:IT1:OP2	1:F:54:LYS:NZ	2.02	0.92
1:B:174:LEU:O	1:B:178:GLN:HG3	1.68	0.92
1:A:328:VAL:O	1:A:328:VAL:HG12	1.71	0.91
1:E:4:HIS:O	1:E:7:THR:HG23	1.71	0.90
1:G:324:TYR:O	1:G:325:HIS:O	1.88	0.90
1:B:76:ILE:HA	1:B:99:LEU:HD23	1.52	0.90
1:H:6:LEU:HD13	1:H:6:LEU:C	1.92	0.89
1:F:325:HIS:CD2	1:F:326:PRO:CD	2.52	0.89
1:G:11:ARG:HH11	1:G:11:ARG:HB3	1.35	0.89
1:H:258:ALA:CB	1:H:259:PRO:HD3	2.02	0.88
1:E:258:ALA:CB	1:E:259:PRO:HD3	2.02	0.88
1:B:167:MET:HE2	1:B:238:ILE:HG23	1.56	0.88
1:D:258:ALA:CB	1:D:259:PRO:HD3	2.02	0.88
1:G:6:LEU:HD12	1:G:6:LEU:N	1.89	0.87
1:A:10:PRO:HB3	1:D:10:PRO:HB3	1.54	0.87
1:G:219:THR:OG1	1:G:254:ASP:HA	1.75	0.87
1:H:0:SER:C	1:H:2:PRO:HD2	1.96	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:11:ARG:HG3	1:H:11:ARG:NH1	1.83	0.86
1:D:324:TYR:O	1:D:325:HIS:O	1.93	0.86
1:E:10:PRO:HB3	1:H:10:PRO:HB3	1.54	0.86
1:E:222:ARG:NH1	1:E:227:GLN:OE1	2.06	0.86
1:F:258:ALA:CB	1:F:259:PRO:HD3	2.05	0.86
1:E:325:HIS:CG	1:E:326:PRO:HD3	2.11	0.86
1:E:325:HIS:CG	1:E:326:PRO:N	2.40	0.85
1:A:258:ALA:CB	1:A:259:PRO:HD3	2.04	0.85
1:G:258:ALA:CB	1:G:259:PRO:HD3	2.07	0.85
1:H:52:LEU:HD12	1:H:83:GLN:HE21	1.42	0.85
1:A:52:LEU:HD12	1:A:83:GLN:HE21	1.41	0.85
1:F:258:ALA:CB	1:F:259:PRO:CD	2.54	0.85
1:D:325:HIS:HB3	1:D:326:PRO:CD	2.07	0.84
1:C:258:ALA:CB	1:C:259:PRO:HD3	2.06	0.84
1:E:258:ALA:CB	1:E:259:PRO:CD	2.56	0.84
1:B:167:MET:HE1	1:B:238:ILE:HG23	1.57	0.84
1:H:-2:MET:HA	1:H:0:SER:H	1.42	0.84
1:D:258:ALA:CB	1:D:259:PRO:CD	2.55	0.84
1:C:258:ALA:CB	1:C:259:PRO:CD	2.56	0.83
1:E:0:SER:CA	1:E:1:MET:CB	2.57	0.83
1:F:258:ALA:HB1	1:F:259:PRO:CD	2.09	0.83
1:B:51:IT1:OP2	1:B:54:LYS:NZ	2.12	0.82
1:G:258:ALA:CB	1:G:259:PRO:CD	2.57	0.82
1:B:146:ILE:HG22	1:B:151:PHE:HB2	1.61	0.82
1:B:258:ALA:CB	1:B:259:PRO:HD3	2.09	0.82
1:C:222:ARG:HB2	1:C:222:ARG:HH11	1.42	0.82
1:A:288:THR:HG21	1:A:314:HIS:HD2	1.44	0.81
1:C:76:ILE:HA	1:C:99:LEU:HD23	1.61	0.81
1:E:288:THR:HG21	1:E:314:HIS:HD2	1.44	0.81
1:G:134:ASP:O	1:G:138:GLN:HG3	1.80	0.81
1:A:258:ALA:CB	1:A:259:PRO:CD	2.59	0.81
1:F:134:ASP:O	1:F:138:GLN:HG3	1.81	0.81
1:C:134:ASP:O	1:C:138:GLN:HG3	1.81	0.81
1:C:222:ARG:NH1	1:C:227:GLN:OE1	2.13	0.80
1:G:5:HIS:O	1:G:6:LEU:CG	2.30	0.80
1:C:173:ALA:HB1	1:C:206:LEU:HD23	1.64	0.80
1:A:5:HIS:CE1	1:A:8:ARG:HE	2.00	0.80
1:H:6:LEU:HD22	1:H:167:MET:HE1	1.64	0.79
1:B:258:ALA:CB	1:B:259:PRO:CD	2.59	0.79
1:H:258:ALA:CB	1:H:259:PRO:CD	2.60	0.79
1:E:4:HIS:NE2	1:E:5:HIS:HD2	1.80	0.79
1:B:219:THR:OG1	1:B:254:ASP:HA	1.83	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:258:ALA:HB1	1:D:259:PRO:CD	2.12	0.79
1:F:5:HIS:O	1:F:6:LEU:CB	2.31	0.79
1:F:325:HIS:CG	1:F:326:PRO:N	2.50	0.79
1:E:258:ALA:HB1	1:E:259:PRO:CD	2.13	0.79
1:A:328:VAL:O	1:A:328:VAL:CG1	2.30	0.79
1:E:-1:ALA:O	1:E:0:SER:HB2	1.82	0.79
1:H:51:IT1:OP2	1:H:54:LYS:NZ	2.15	0.79
1:C:219:THR:OG1	1:C:254:ASP:HA	1.82	0.78
1:F:7:THR:O	1:F:7:THR:CG2	2.32	0.78
1:B:186:LEU:HD12	1:B:187:SER:N	1.99	0.78
1:C:258:ALA:HB1	1:C:259:PRO:CD	2.14	0.78
1:G:325:HIS:CG	1:G:326:PRO:CD	2.67	0.78
1:A:325:HIS:CE1	1:B:117:LEU:HD13	2.19	0.78
1:H:1:MET:N	1:H:2:PRO:CD	2.47	0.78
1:E:324:TYR:O	1:E:325:HIS:O	2.02	0.78
1:G:5:HIS:HA	1:G:6:LEU:HD12	1.67	0.77
1:E:326:PRO:O	1:E:327:HIS:HB3	1.84	0.77
1:D:52:LEU:HD12	1:D:83:GLN:HE21	1.50	0.77
1:F:114:GLY:HA3	1:F:323:ALA:HB2	1.65	0.77
1:C:52:LEU:HD12	1:C:83:GLN:HE21	1.48	0.77
1:G:5:HIS:C	1:G:6:LEU:CG	2.53	0.77
1:A:6:LEU:HA	1:A:242:LEU:CD2	2.14	0.77
1:D:228:LYS:HG3	1:D:250:ILE:HD11	1.66	0.77
1:G:288:THR:HG21	1:G:314:HIS:HD2	1.49	0.77
1:A:105:THR:HG21	1:A:328:VAL:HG13	1.65	0.77
1:C:51:IT1:OP2	1:C:54:LYS:NZ	2.19	0.76
1:B:52:LEU:HD12	1:B:83:GLN:HE21	1.50	0.76
1:G:114:GLY:HA3	1:G:323:ALA:HB2	1.68	0.75
1:F:52:LEU:HD12	1:F:83:GLN:HE21	1.52	0.75
1:D:325:HIS:O	1:D:326:PRO:C	2.23	0.75
1:H:114:GLY:HA3	1:H:323:ALA:HB2	1.68	0.74
1:E:51:IT1:OP2	1:E:54:LYS:NZ	2.19	0.74
1:H:288:THR:HG21	1:H:314:HIS:HD2	1.52	0.74
1:E:140:GLN:O	1:E:144:THR:HG23	1.87	0.74
1:E:4:HIS:NE2	1:E:5:HIS:CD2	2.55	0.74
1:F:288:THR:HG21	1:F:314:HIS:HD2	1.51	0.74
1:A:136:ASP:O	1:A:140:GLN:HG2	1.88	0.74
1:D:3:LEU:O	1:D:6:LEU:N	2.20	0.74
1:C:114:GLY:HA3	1:C:323:ALA:HB2	1.69	0.74
1:D:6:LEU:HD13	1:D:6:LEU:C	2.07	0.74
1:D:4:HIS:C	1:D:6:LEU:N	2.38	0.74
1:E:52:LEU:HD12	1:E:83:GLN:HE21	1.53	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:288:THR:HG21	1:D:314:HIS:HD2	1.52	0.74
1:H:-2:MET:CA	1:H:0:SER:H	2.00	0.73
1:D:51:IT1:OP2	1:D:54:LYS:NZ	2.20	0.73
1:B:258:ALA:HB1	1:B:259:PRO:CD	2.17	0.73
1:E:114:GLY:HA3	1:E:323:ALA:HB2	1.69	0.73
1:E:288:THR:HG21	1:E:314:HIS:CD2	2.24	0.73
1:A:4:HIS:CG	1:A:5:HIS:N	2.56	0.73
1:D:1:MET:HB2	1:D:2:PRO:CA	2.07	0.72
1:A:4:HIS:O	1:A:7:THR:HG22	1.89	0.72
1:C:33:ARG:HH12	1:C:307:ASP:HA	1.54	0.72
1:H:134:ASP:O	1:H:138:GLN:HG3	1.88	0.72
1:D:5:HIS:O	1:D:6:LEU:C	2.28	0.72
1:D:134:ASP:O	1:D:138:GLN:HG3	1.88	0.71
1:A:288:THR:HG21	1:A:314:HIS:CD2	2.25	0.71
1:G:14:PHE:CZ	1:G:87:VAL:HG13	2.24	0.71
1:G:325:HIS:HB3	1:G:326:PRO:HD3	1.72	0.71
1:A:258:ALA:HB1	1:A:259:PRO:CD	2.16	0.71
1:F:62:ALA:HA	1:F:154:TYR:CD1	2.26	0.71
1:E:5:HIS:C	1:E:7:THR:H	1.92	0.71
1:G:52:LEU:HD12	1:G:83:GLN:HE21	1.55	0.71
1:E:325:HIS:CD2	1:E:326:PRO:N	2.58	0.71
1:C:33:ARG:NH1	1:C:307:ASP:HA	2.06	0.70
1:D:114:GLY:HA3	1:D:323:ALA:HB2	1.71	0.70
1:E:134:ASP:O	1:E:138:GLN:HG3	1.91	0.70
1:H:166:ALA:HB3	1:H:238:ILE:HD11	1.73	0.70
1:C:288:THR:HG21	1:C:314:HIS:HD2	1.55	0.70
1:F:327:HIS:O	1:F:328:VAL:C	2.30	0.70
1:E:64:ARG:HB3	1:H:64:ARG:NH2	2.05	0.70
1:D:6:LEU:CD1	1:D:6:LEU:O	2.32	0.69
1:H:4:HIS:NE2	3:H:503:HOH:O	2.11	0.69
1:H:6:LEU:C	1:H:6:LEU:CD1	2.50	0.69
1:F:325:HIS:O	1:F:326:PRO:C	2.30	0.69
1:E:325:HIS:O	1:E:326:PRO:C	2.30	0.69
1:E:0:SER:N	1:E:1:MET:CB	2.56	0.69
1:D:219:THR:OG1	1:D:254:ASP:HA	1.91	0.69
1:A:134:ASP:O	1:A:138:GLN:HG3	1.91	0.69
1:B:288:THR:HG21	1:B:314:HIS:HD2	1.57	0.69
1:E:0:SER:HA	1:E:1:MET:CB	2.22	0.69
1:G:12:LEU:HG	1:G:60:ALA:HB2	1.74	0.69
1:H:3:LEU:HD12	1:H:3:LEU:N	2.07	0.69
1:H:219:THR:OG1	1:H:254:ASP:HA	1.92	0.69
1:G:51:IT1:OP2	1:G:54:LYS:NZ	2.25	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:325:HIS:ND1	1:E:326:PRO:HD3	2.06	0.68
1:A:1:MET:O	1:A:4:HIS:HB3	1.92	0.68
1:C:105:THR:OG1	1:C:328:VAL:HG12	1.93	0.68
1:G:325:HIS:O	1:G:326:PRO:C	2.32	0.68
1:F:324:TYR:O	1:F:325:HIS:O	2.12	0.68
1:D:325:HIS:CB	1:D:326:PRO:HD3	2.18	0.68
1:A:33:ARG:NH2	1:A:306:ASP:O	2.26	0.68
1:G:325:HIS:CG	1:G:326:PRO:N	2.62	0.68
1:B:151:PHE:O	1:B:153:PRO:HD3	1.93	0.68
1:A:51:IT1:OP2	1:A:54:LYS:NZ	2.27	0.68
1:H:6:LEU:HA	1:H:242:LEU:CD2	2.24	0.68
1:G:288:THR:HG21	1:G:314:HIS:CD2	2.29	0.67
1:A:114:GLY:HA3	1:A:323:ALA:HB2	1.74	0.67
1:C:134:ASP:H	1:C:138:GLN:HE21	1.43	0.67
1:H:105:THR:OG1	1:H:328:VAL:HG12	1.95	0.67
1:G:62:ALA:HA	1:G:154:TYR:CD1	2.29	0.67
1:D:198:THR:O	1:D:202:LEU:HD22	1.95	0.67
1:H:6:LEU:CD2	1:H:167:MET:HE1	2.24	0.67
1:G:70:LEU:HD21	1:G:93:LEU:HD13	1.77	0.67
1:D:105:THR:OG1	1:D:328:VAL:HG12	1.95	0.67
1:B:114:GLY:HA3	1:B:323:ALA:HB2	1.77	0.67
1:D:288:THR:HG21	1:D:314:HIS:CD2	2.29	0.66
1:E:105:THR:OG1	1:E:328:VAL:HG12	1.95	0.66
1:B:234:LEU:O	1:B:238:ILE:HG13	1.94	0.66
1:F:288:THR:HG21	1:F:314:HIS:CD2	2.30	0.66
1:E:51:IT1:H5A	1:E:51:IT1:NZ	2.09	0.66
1:G:134:ASP:H	1:G:138:GLN:HE21	1.43	0.66
1:G:325:HIS:CG	1:G:326:PRO:HD3	2.29	0.66
1:A:51:IT1:NZ	1:A:51:IT1:H5A	2.10	0.66
1:F:325:HIS:O	1:F:327:HIS:N	2.29	0.66
1:E:258:ALA:CB	1:E:265:ASN:HB3	2.26	0.65
1:G:51:IT1:H5A	1:G:51:IT1:NZ	2.10	0.65
1:E:5:HIS:O	1:E:7:THR:N	2.30	0.65
1:E:-1:ALA:O	1:E:0:SER:CB	2.42	0.65
1:H:288:THR:HG21	1:H:314:HIS:CD2	2.31	0.65
1:G:100:GLU:O	1:G:102:PRO:HD3	1.97	0.65
1:B:134:ASP:O	1:B:138:GLN:HG3	1.95	0.65
1:H:0:SER:C	1:H:2:PRO:CD	2.65	0.65
1:D:325:HIS:CB	1:D:326:PRO:CD	2.74	0.65
1:C:288:THR:HG21	1:C:314:HIS:CD2	2.31	0.65
1:A:7:THR:OG1	3:A:506:HOH:O	2.14	0.64
1:E:325:HIS:O	1:E:327:HIS:N	2.30	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:34:GLU:OE2	1:H:-1:ALA:N	2.30	0.64
1:H:5:HIS:C	1:H:7:THR:N	2.50	0.64
1:A:52:LEU:CD1	1:A:83:GLN:HE21	2.10	0.64
1:C:80:HIS:HB3	2:C:401:PO4:O1	1.97	0.64
1:B:105:THR:OG1	1:B:328:VAL:HG12	1.97	0.64
1:H:51:IT1:H5A	1:H:51:IT1:NZ	2.11	0.63
1:E:4:HIS:C	1:E:6:LEU:N	2.51	0.63
1:D:3:LEU:HD12	1:D:3:LEU:N	2.12	0.63
1:D:109:ASN:HD22	1:D:326:PRO:HD3	1.64	0.63
1:H:166:ALA:CB	1:H:238:ILE:HD11	2.28	0.63
1:H:5:HIS:O	1:H:7:THR:N	2.30	0.63
1:F:105:THR:HG1	1:F:328:VAL:HG12	1.64	0.63
1:B:258:ALA:CB	1:B:265:ASN:HB3	2.28	0.63
1:H:4:HIS:C	1:H:6:LEU:N	2.49	0.63
1:D:1:MET:HA	1:D:3:LEU:H	1.63	0.63
1:E:3:LEU:O	1:E:6:LEU:N	2.29	0.63
1:F:258:ALA:CB	1:F:265:ASN:HB3	2.29	0.62
1:D:258:ALA:CB	1:D:265:ASN:HB3	2.28	0.62
1:F:266:ASP:O	1:F:270:GLU:HG2	1.99	0.62
1:A:5:HIS:CE1	1:A:8:ARG:HH21	2.18	0.62
1:D:15:ILE:HD12	1:D:53:ARG:HD3	1.80	0.62
1:B:146:ILE:HG23	1:B:151:PHE:HD1	1.63	0.62
1:C:98:LEU:HD23	1:C:132:LEU:HD21	1.82	0.62
1:G:325:HIS:O	1:G:327:HIS:N	2.33	0.62
1:H:3:LEU:O	1:H:6:LEU:CB	2.48	0.62
1:A:105:THR:HB	1:A:328:VAL:HG11	1.80	0.61
1:A:134:ASP:H	1:A:138:GLN:HE21	1.48	0.61
1:D:222:ARG:NH1	1:D:227:GLN:OE1	2.33	0.61
1:E:80:HIS:CB	2:E:401:PO4:O4	2.48	0.61
1:E:5:HIS:C	1:E:7:THR:N	2.46	0.61
1:F:134:ASP:H	1:F:138:GLN:HE21	1.47	0.61
1:B:186:LEU:HD11	1:B:188:SER:O	2.00	0.61
1:C:258:ALA:CB	1:C:265:ASN:HB3	2.29	0.61
1:C:70:LEU:CD1	1:C:93:LEU:HD13	2.31	0.61
1:F:34:GLU:OE2	1:H:-1:ALA:HB2	1.99	0.61
1:D:0:SER:O	1:D:1:MET:O	2.19	0.61
1:A:105:THR:CG2	1:A:328:VAL:HG13	2.31	0.61
1:E:134:ASP:H	1:E:138:GLN:HE21	1.48	0.61
1:E:80:HIS:HB3	2:E:401:PO4:O4	2.01	0.61
1:D:71:ILE:HG12	1:D:96:VAL:HB	1.83	0.61
1:D:6:LEU:CD1	1:D:6:LEU:C	2.67	0.61
1:A:258:ALA:CB	1:A:265:ASN:HB3	2.30	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:105:THR:OG1	1:G:328:VAL:HG12	2.00	0.61
1:C:51:IT1:NZ	1:C:51:IT1:H5A	2.16	0.60
1:G:51:IT1:OP1	1:G:195:SER:N	2.34	0.60
1:H:3:LEU:O	1:H:6:LEU:HB2	2.00	0.60
1:H:258:ALA:CB	1:H:265:ASN:HB3	2.31	0.60
1:F:100:GLU:O	1:F:102:PRO:HD3	2.01	0.60
1:F:268:GLY:HA2	1:F:293:ALA:HB2	1.83	0.60
1:C:33:ARG:HE	1:C:310:ILE:HD11	1.66	0.60
1:H:6:LEU:HD22	1:H:167:MET:CE	2.30	0.60
1:E:269:MET:HA	1:E:272:VAL:HG23	1.83	0.60
1:H:325:HIS:CG	1:H:326:PRO:HD3	2.37	0.60
1:H:52:LEU:CD1	1:H:83:GLN:HE21	2.13	0.60
1:H:5:HIS:C	1:H:7:THR:H	2.04	0.60
1:E:325:HIS:CB	1:E:326:PRO:HD2	1.88	0.59
1:A:3:LEU:HD22	1:A:3:LEU:N	2.17	0.59
1:D:4:HIS:C	1:D:6:LEU:H	2.01	0.59
1:H:231:VAL:HG11	1:H:250:ILE:HG21	1.84	0.59
1:B:288:THR:HG21	1:B:314:HIS:CD2	2.37	0.59
1:C:98:LEU:HD23	1:C:132:LEU:CD2	2.33	0.59
1:D:325:HIS:O	1:D:327:HIS:N	2.35	0.59
1:D:109:ASN:HD22	1:D:326:PRO:CD	2.16	0.59
1:G:5:HIS:CA	1:G:6:LEU:CD1	2.74	0.59
1:G:157:PRO:HG3	1:G:162:SER:HB3	1.84	0.59
1:A:4:HIS:ND1	1:A:5:HIS:N	2.51	0.58
1:H:258:ALA:HB1	1:H:259:PRO:CD	2.22	0.58
1:E:4:HIS:C	1:E:6:LEU:H	2.05	0.58
1:B:62:ALA:HA	1:B:154:TYR:CD1	2.38	0.58
1:H:232:ILE:HG12	1:H:250:ILE:HG13	1.85	0.58
1:B:157:PRO:HG3	1:B:162:SER:HB3	1.84	0.58
1:F:157:PRO:HG3	1:F:162:SER:HB3	1.85	0.58
1:A:3:LEU:O	1:A:5:HIS:N	2.37	0.58
1:A:157:PRO:HG3	1:A:162:SER:HB3	1.86	0.58
1:E:157:PRO:HG3	1:E:162:SER:HB3	1.85	0.58
1:H:157:PRO:HG3	1:H:162:SER:HB3	1.85	0.58
1:H:268:GLY:HA2	1:H:293:ALA:HB2	1.86	0.58
1:H:134:ASP:H	1:H:138:GLN:HE21	1.52	0.57
1:E:1:MET:H	1:E:2:PRO:HD3	1.69	0.57
1:D:325:HIS:CG	1:D:326:PRO:N	2.72	0.57
1:G:43:THR:HB	1:G:48:GLY:HA3	1.85	0.57
1:E:258:ALA:HB3	1:E:259:PRO:CD	2.34	0.57
1:G:268:GLY:HA2	1:G:293:ALA:HB2	1.84	0.57
1:H:167:MET:CE	1:H:242:LEU:HD21	2.34	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:258:ALA:HB3	1:H:259:PRO:CD	2.35	0.57
1:G:258:ALA:CB	1:G:265:ASN:HB3	2.33	0.57
1:G:258:ALA:HB3	1:G:259:PRO:CD	2.35	0.57
1:E:4:HIS:CD2	1:E:5:HIS:HD2	2.22	0.57
1:B:52:LEU:CD1	1:B:83:GLN:HE21	2.16	0.57
1:C:62:ALA:HA	1:C:154:TYR:CD1	2.39	0.57
1:C:258:ALA:HB3	1:C:259:PRO:CD	2.35	0.57
1:D:3:LEU:O	1:D:5:HIS:N	2.37	0.56
1:D:134:ASP:H	1:D:138:GLN:HE21	1.53	0.56
1:A:208:HIS:CE1	1:A:244:LEU:HD13	2.40	0.56
1:G:258:ALA:HB1	1:G:259:PRO:CD	2.16	0.56
1:A:6:LEU:HA	1:A:242:LEU:HD23	1.85	0.56
1:B:268:GLY:HA2	1:B:293:ALA:HB2	1.87	0.56
1:C:219:THR:HG1	1:C:254:ASP:HA	1.70	0.56
1:A:140:GLN:O	1:A:144:THR:HG23	2.05	0.56
1:C:268:GLY:HA2	1:C:293:ALA:HB2	1.86	0.56
1:C:199:HIS:HE1	1:C:252:LEU:CD1	2.18	0.56
1:D:268:GLY:HA2	1:D:293:ALA:HB2	1.88	0.56
1:D:5:HIS:C	1:D:7:THR:N	2.55	0.56
1:F:52:LEU:CD1	1:F:83:GLN:HE21	2.19	0.56
1:F:258:ALA:HB3	1:F:259:PRO:CD	2.36	0.56
1:B:174:LEU:O	1:B:178:GLN:CG	2.49	0.55
1:A:4:HIS:C	1:A:6:LEU:H	2.08	0.55
1:A:1:MET:N	1:A:2:PRO:CD	2.69	0.55
1:E:219:THR:OG1	1:E:254:ASP:HA	2.07	0.55
1:B:51:IT1:NZ	1:B:51:IT1:H5A	2.22	0.55
1:D:51:IT1:OP1	1:D:195:SER:N	2.39	0.55
1:F:300:SER:C	1:F:301:GLN:HE21	2.10	0.55
1:E:268:GLY:HA2	1:E:293:ALA:HB2	1.89	0.55
1:C:157:PRO:HG3	1:C:162:SER:HB3	1.89	0.55
1:D:6:LEU:HA	1:D:242:LEU:HD22	1.89	0.55
1:E:175:GLU:O	1:E:179:GLN:HG3	2.06	0.55
1:F:51:IT1:H5A	1:F:51:IT1:NZ	2.20	0.54
1:B:100:GLU:O	1:B:102:PRO:HD3	2.06	0.54
1:H:7:THR:HG23	1:H:7:THR:O	2.07	0.54
1:C:80:HIS:CB	2:C:401:PO4:O1	2.55	0.54
1:D:157:PRO:HG3	1:D:162:SER:HB3	1.89	0.54
1:D:3:LEU:CD1	1:D:3:LEU:N	2.70	0.54
1:C:325:HIS:CD2	1:C:325:HIS:C	2.80	0.54
1:H:100:GLU:O	1:H:102:PRO:HD3	2.08	0.54
1:D:51:IT1:H5A	1:D:51:IT1:NZ	2.23	0.54
1:E:62:ALA:HA	1:E:154:TYR:CD1	2.43	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:33:ARG:NH2	1:B:306:ASP:O	2.40	0.54
1:D:258:ALA:HB3	1:D:259:PRO:CD	2.36	0.54
1:B:229:PRO:O	1:B:232:ILE:HG13	2.08	0.54
1:C:112:THR:HB	1:D:325:HIS:HE1	1.72	0.54
1:B:258:ALA:HB3	1:B:265:ASN:HB3	1.90	0.54
1:A:326:PRO:O	1:A:327:HIS:HB3	2.07	0.54
1:A:219:THR:OG1	1:A:254:ASP:HA	2.07	0.54
1:F:43:THR:HB	1:F:48:GLY:HA3	1.90	0.53
1:C:199:HIS:CE1	1:C:252:LEU:CD1	2.91	0.53
1:D:228:LYS:HG3	1:D:250:ILE:CD1	2.35	0.53
1:E:52:LEU:CD1	1:E:83:GLN:HE21	2.19	0.53
1:F:189:VAL:HG22	1:F:311:LEU:HB3	1.90	0.53
1:C:234:LEU:O	1:C:238:ILE:HG13	2.09	0.53
1:B:33:ARG:NE	1:B:307:ASP:O	2.42	0.53
1:E:63:LEU:HB3	1:H:8:ARG:HB3	1.90	0.53
1:H:109:ASN:HD22	1:H:326:PRO:CD	2.22	0.53
1:B:258:ALA:HB3	1:B:259:PRO:CD	2.39	0.53
1:B:300:SER:C	1:B:301:GLN:HE21	2.11	0.53
1:D:324:TYR:O	1:D:325:HIS:C	2.47	0.53
1:C:43:THR:HB	1:C:48:GLY:HA3	1.91	0.53
1:C:9:PHE:CD1	1:C:9:PHE:N	2.77	0.53
1:A:268:GLY:HA2	1:A:293:ALA:HB2	1.91	0.52
1:A:51:IT1:NZ	2:A:401:PO4:O3	2.42	0.52
1:D:21:LEU:HB2	1:D:179:GLN:OE1	2.10	0.52
1:B:134:ASP:H	1:B:138:GLN:HE21	1.57	0.52
1:D:3:LEU:C	1:D:6:LEU:H	2.11	0.52
1:D:300:SER:C	1:D:301:GLN:HE21	2.12	0.52
1:A:258:ALA:HB3	1:A:259:PRO:CD	2.38	0.52
1:G:12:LEU:HD11	1:G:63:LEU:HD12	1.92	0.52
1:G:53:ARG:HD2	1:G:169:TYR:CZ	2.44	0.52
1:A:62:ALA:HA	1:A:154:TYR:CD1	2.44	0.52
1:G:325:HIS:HE1	1:H:112:THR:HB	1.75	0.52
1:A:105:THR:HB	1:A:328:VAL:CG1	2.39	0.52
1:E:43:THR:HG22	1:E:45:ILE:H	1.75	0.52
1:D:174:LEU:HD13	1:D:209:LEU:HD11	1.92	0.52
1:G:12:LEU:HG	1:G:60:ALA:CB	2.40	0.52
1:H:6:LEU:CG	1:H:6:LEU:O	2.50	0.52
1:D:52:LEU:CD1	1:D:83:GLN:HE21	2.20	0.52
1:G:325:HIS:CD2	1:G:326:PRO:N	2.77	0.51
1:A:33:ARG:HH11	1:A:299:ILE:HG23	1.75	0.51
1:B:109:ASN:HD22	1:B:326:PRO:HD3	1.75	0.51
1:B:199:HIS:CE1	1:B:252:LEU:HD21	2.45	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:323:ALA:C	1:F:325:HIS:H	2.14	0.51
1:C:51:IT1:OP1	1:C:195:SER:N	2.44	0.51
1:H:6:LEU:HA	1:H:242:LEU:HD22	1.92	0.51
1:H:258:ALA:HB3	1:H:265:ASN:HB3	1.93	0.51
1:H:4:HIS:C	1:H:6:LEU:H	2.13	0.51
1:B:186:LEU:CD1	1:B:187:SER:N	2.73	0.51
1:H:325:HIS:O	1:H:326:PRO:C	2.47	0.51
1:E:76:ILE:HA	1:E:99:LEU:HD13	1.92	0.51
1:C:237:ALA:O	1:C:241:GLN:HG3	2.11	0.51
1:A:181:GLU:C	1:A:183:VAL:H	2.14	0.51
1:E:325:HIS:HB3	1:E:326:PRO:HD3	1.85	0.50
1:G:112:THR:HB	1:H:325:HIS:HE1	1.77	0.50
1:C:59:VAL:HG22	1:C:70:LEU:HD21	1.91	0.50
1:A:222:ARG:NH1	1:A:227:GLN:OE1	2.44	0.50
1:G:300:SER:C	1:G:301:GLN:HE21	2.14	0.50
1:D:231:VAL:HG12	1:D:250:ILE:HG21	1.93	0.50
1:D:4:HIS:CG	1:D:5:HIS:N	2.79	0.50
1:E:234:LEU:O	1:E:238:ILE:HD12	2.12	0.50
1:H:0:SER:HA	1:H:2:PRO:HD3	1.94	0.50
1:E:268:GLY:O	1:E:271:ALA:HB3	2.12	0.50
1:E:0:SER:H	1:E:1:MET:CB	2.25	0.50
1:C:325:HIS:CE1	1:D:112:THR:HB	2.47	0.50
1:C:146:ILE:HG22	1:C:151:PHE:HB2	1.94	0.50
1:C:181:GLU:C	1:C:183:VAL:H	2.15	0.50
1:E:300:SER:C	1:E:301:GLN:HE21	2.15	0.50
1:C:100:GLU:O	1:C:102:PRO:HD3	2.12	0.50
1:H:167:MET:HE2	1:H:242:LEU:HD21	1.95	0.49
1:D:5:HIS:CE1	1:D:8:ARG:HH21	2.30	0.49
1:C:134:ASP:H	1:C:138:GLN:NE2	2.09	0.49
1:C:70:LEU:HD23	1:C:156:ILE:CD1	2.42	0.49
1:G:15:ILE:HD12	1:G:43:THR:HG23	1.94	0.49
1:H:231:VAL:CG1	1:H:250:ILE:HG21	2.43	0.49
1:F:327:HIS:O	1:F:328:VAL:O	2.30	0.49
1:A:327:HIS:O	1:A:328:VAL:O	2.30	0.49
1:C:222:ARG:HB2	1:C:222:ARG:NH1	2.20	0.49
1:B:228:LYS:O	1:B:232:ILE:HG23	2.12	0.49
1:D:275:LEU:HB3	1:D:281:VAL:HG23	1.94	0.49
1:G:258:ALA:HB3	1:G:265:ASN:HB3	1.93	0.49
1:G:20:PRO:HG2	1:G:39:ARG:HB2	1.94	0.49
1:G:134:ASP:H	1:G:138:GLN:NE2	2.09	0.49
1:C:325:HIS:HE1	1:D:112:THR:HB	1.77	0.49
1:E:169:TYR:HB3	1:E:202:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:23:TYR:CE2	1:H:-2:MET:CB	2.95	0.49
1:G:78:SER:OG	1:G:81:VAL:HG23	2.12	0.48
1:D:2:PRO:O	1:D:244:LEU:HD21	2.13	0.48
1:C:146:ILE:CG2	1:C:151:PHE:HD1	2.26	0.48
1:F:199:HIS:O	1:F:199:HIS:HD2	1.96	0.48
1:A:258:ALA:HB3	1:A:265:ASN:HB3	1.95	0.48
1:H:51:IT1:OP1	1:H:195:SER:N	2.46	0.48
1:C:52:LEU:CD1	1:C:83:GLN:HE21	2.22	0.48
1:C:253:TRP:CD2	1:C:303:ARG:NH1	2.82	0.48
1:A:268:GLY:O	1:A:271:ALA:HB3	2.14	0.48
1:F:286:VAL:HG13	1:F:287:TYR:CD2	2.48	0.48
1:G:6:LEU:N	1:G:6:LEU:CD1	2.60	0.48
1:H:231:VAL:HG12	1:H:250:ILE:HD12	1.96	0.48
1:H:4:HIS:CG	1:H:5:HIS:N	2.81	0.48
1:B:43:THR:HG22	1:B:45:ILE:H	1.79	0.48
1:H:-2:MET:CA	1:H:0:SER:N	2.74	0.48
1:H:62:ALA:HA	1:H:154:TYR:CD1	2.49	0.48
1:B:199:HIS:O	1:B:199:HIS:HD2	1.97	0.47
1:E:181:GLU:C	1:E:183:VAL:H	2.17	0.47
1:F:105:THR:OG1	1:F:328:VAL:CG1	2.53	0.47
1:E:7:THR:O	1:E:7:THR:OG1	2.30	0.47
1:B:146:ILE:CG2	1:B:151:PHE:HD1	2.26	0.47
1:A:3:LEU:O	1:A:6:LEU:CB	2.62	0.47
1:F:230:LYS:O	1:F:234:LEU:HD12	2.14	0.47
1:D:181:GLU:C	1:D:183:VAL:H	2.17	0.47
1:D:51:IT1:HA	1:D:51:IT1:HD	1.76	0.47
1:B:51:IT1:OP1	1:B:195:SER:N	2.47	0.47
1:H:300:SER:C	1:H:301:GLN:HE21	2.18	0.47
1:A:325:HIS:C	1:A:325:HIS:ND1	2.66	0.47
1:A:269:MET:HA	1:A:272:VAL:HG23	1.96	0.47
1:H:43:THR:HB	1:H:48:GLY:HA3	1.96	0.47
1:H:257:PHE:HA	1:H:290:LYS:HD3	1.97	0.47
1:A:112:THR:HB	1:B:325:HIS:CE1	2.49	0.47
1:G:40:ASP:OD2	1:G:53:ARG:NE	2.37	0.47
1:H:4:HIS:O	1:H:6:LEU:N	2.48	0.47
1:G:7:THR:O	1:G:7:THR:HG23	2.15	0.47
1:E:4:HIS:CE1	1:E:5:HIS:HD2	2.31	0.47
1:D:189:VAL:HG22	1:D:311:LEU:HB3	1.96	0.47
1:G:76:ILE:HB	1:G:110:TYR:CE1	2.50	0.47
1:A:100:GLU:O	1:A:102:PRO:HD3	2.14	0.47
1:E:227:GLN:HG2	1:E:252:LEU:HD13	1.96	0.47
1:E:51:IT1:HD	1:E:51:IT1:HA	1.71	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:142:LEU:O	1:C:146:ILE:HG12	2.15	0.47
1:H:227:GLN:HG2	1:H:252:LEU:HD22	1.95	0.47
1:E:250:ILE:O	1:E:250:ILE:HD12	2.15	0.47
1:E:43:THR:HB	1:E:48:GLY:HA3	1.97	0.47
1:C:189:VAL:HG22	1:C:311:LEU:HB3	1.97	0.47
1:H:167:MET:HE1	1:H:242:LEU:HD21	1.97	0.46
1:B:230:LYS:O	1:B:234:LEU:HD12	2.15	0.46
1:A:112:THR:HB	1:B:325:HIS:HE1	1.80	0.46
1:E:117:LEU:HD13	1:F:325:HIS:CE1	2.50	0.46
1:G:181:GLU:C	1:G:183:VAL:H	2.19	0.46
1:E:4:HIS:CE1	1:E:5:HIS:CD2	3.04	0.46
1:E:169:TYR:CD1	1:E:198:THR:HG23	2.50	0.46
1:B:325:HIS:CD2	1:B:325:HIS:C	2.89	0.46
1:A:300:SER:C	1:A:301:GLN:HE21	2.19	0.46
1:A:43:THR:HB	1:A:48:GLY:HA3	1.98	0.46
1:H:181:GLU:C	1:H:183:VAL:H	2.18	0.46
1:B:181:GLU:C	1:B:183:VAL:H	2.18	0.46
1:E:258:ALA:HB3	1:E:265:ASN:HB3	1.96	0.46
1:C:325:HIS:HE1	1:D:112:THR:C	2.19	0.46
1:A:51:IT1:HD	1:A:51:IT1:HA	1.77	0.46
1:C:274:LEU:O	1:C:278:LEU:HB2	2.16	0.46
1:D:274:LEU:O	1:D:278:LEU:HB2	2.16	0.46
1:B:189:VAL:HG22	1:B:311:LEU:HB3	1.97	0.46
1:B:140:GLN:HE21	1:B:144:THR:HG23	1.81	0.46
1:E:51:IT1:OP1	1:E:195:SER:N	2.49	0.45
1:H:189:VAL:HG22	1:H:311:LEU:HB3	1.97	0.45
1:A:43:THR:HG22	1:A:45:ILE:H	1.81	0.45
1:A:51:IT1:C4A	2:A:401:PO4:O3	2.63	0.45
1:G:76:ILE:HB	1:G:110:TYR:HE1	1.80	0.45
1:C:171:GLU:O	1:C:174:LEU:HB3	2.16	0.45
1:F:51:IT1:HA	1:F:51:IT1:HD	1.65	0.45
1:G:274:LEU:O	1:G:278:LEU:HB2	2.16	0.45
1:F:171:GLU:O	1:F:174:LEU:HB3	2.16	0.45
1:C:173:ALA:CB	1:C:206:LEU:HD23	2.42	0.45
1:D:186:LEU:HD11	1:D:311:LEU:HB2	1.99	0.45
1:F:181:GLU:C	1:F:183:VAL:H	2.20	0.45
1:D:62:ALA:HA	1:D:154:TYR:CD1	2.52	0.45
1:C:300:SER:C	1:C:301:GLN:HE21	2.20	0.45
1:B:220:VAL:HG11	1:B:287:TYR:HA	1.98	0.45
1:A:1:MET:H	1:A:2:PRO:CD	2.30	0.45
1:A:169:TYR:CD1	1:A:198:THR:HG23	2.52	0.45
1:B:71:ILE:HG23	1:B:96:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:3:LEU:HD13	1:A:3:LEU:HA	1.44	0.45
1:E:325:HIS:HE1	1:F:112:THR:HB	1.83	0.44
1:C:258:ALA:HB3	1:C:265:ASN:HB3	1.98	0.44
1:C:76:ILE:HB	1:C:110:TYR:HE1	1.82	0.44
1:E:189:VAL:HG22	1:E:311:LEU:HB3	1.99	0.44
1:B:76:ILE:HB	1:B:110:TYR:HE1	1.83	0.44
1:E:1:MET:H	1:E:2:PRO:CD	2.29	0.44
1:H:275:LEU:HB3	1:H:281:VAL:HG23	1.99	0.44
1:A:322:PHE:CE2	1:B:118:LEU:HD11	2.52	0.44
1:H:3:LEU:CD1	1:H:3:LEU:N	2.77	0.44
1:E:175:GLU:O	1:E:179:GLN:CG	2.65	0.44
1:H:43:THR:HG22	1:H:45:ILE:H	1.81	0.44
1:G:230:LYS:O	1:G:234:LEU:HD12	2.18	0.44
1:B:167:MET:HE1	1:B:238:ILE:CG2	2.37	0.44
1:G:52:LEU:CD1	1:G:83:GLN:HE21	2.27	0.44
1:F:156:ILE:HA	1:F:157:PRO:HD2	1.85	0.44
1:F:258:ALA:HB3	1:F:265:ASN:HB3	1.99	0.44
1:H:274:LEU:O	1:H:278:LEU:HB2	2.17	0.44
1:E:4:HIS:O	1:E:6:LEU:N	2.50	0.44
1:G:37:ILE:HG12	1:G:39:ARG:HD2	2.00	0.44
1:B:43:THR:HB	1:B:48:GLY:HA3	2.00	0.44
1:A:274:LEU:O	1:A:278:LEU:HB2	2.18	0.44
1:F:134:ASP:H	1:F:138:GLN:NE2	2.15	0.44
1:B:78:SER:OG	1:B:81:VAL:HG23	2.17	0.44
1:B:76:ILE:HB	1:B:110:TYR:CE1	2.53	0.44
1:C:96:VAL:HG22	1:C:125:GLN:HB2	1.99	0.44
1:B:14:PHE:CZ	1:B:87:VAL:HG13	2.52	0.44
1:G:199:HIS:HD2	1:G:199:HIS:O	2.01	0.44
1:B:235:GLN:HE21	1:B:246:ALA:HB1	1.83	0.44
1:F:221:SER:HB3	1:F:261:TYR:HB2	2.00	0.43
1:B:51:IT1:HA	1:B:51:IT1:HD	1.72	0.43
1:D:263:VAL:HA	1:D:264:PRO:HD3	1.86	0.43
1:A:1:MET:C	1:A:3:LEU:N	2.71	0.43
1:A:3:LEU:CD2	1:A:3:LEU:N	2.81	0.43
1:F:20:PRO:HG2	1:F:39:ARG:HB2	2.00	0.43
1:H:11:ARG:NH1	1:H:11:ARG:CG	2.65	0.43
1:H:51:IT1:HA	1:H:51:IT1:HD	1.76	0.43
1:C:43:THR:HG22	1:C:45:ILE:H	1.83	0.43
1:A:5:HIS:CE1	1:A:8:ARG:NE	2.79	0.43
1:C:51:IT1:HD	1:C:51:IT1:HA	1.68	0.43
1:D:268:GLY:O	1:D:271:ALA:HB3	2.19	0.43
1:A:14:PHE:CD2	1:A:56:GLU:HG2	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:189:VAL:HG22	1:G:311:LEU:HB3	2.00	0.43
1:H:5:HIS:O	1:H:6:LEU:C	2.55	0.43
1:C:45:ILE:HB	1:C:52:LEU:HD11	2.00	0.43
1:D:169:TYR:CD1	1:D:198:THR:HG23	2.54	0.43
1:D:221:SER:HB3	1:D:261:TYR:HB2	2.00	0.43
1:D:43:THR:HB	1:D:48:GLY:HA3	2.00	0.43
1:F:33:ARG:HH21	1:F:299:ILE:HG23	1.83	0.43
1:H:30:TYR:CD2	1:H:31:LEU:CD1	3.02	0.43
1:H:3:LEU:O	1:H:6:LEU:N	2.44	0.43
1:G:43:THR:HG22	1:G:45:ILE:H	1.84	0.43
1:C:199:HIS:HE1	1:C:252:LEU:HD12	1.82	0.43
1:F:34:GLU:OE2	1:H:-1:ALA:CB	2.67	0.43
1:C:76:ILE:HB	1:C:110:TYR:CE1	2.54	0.43
1:F:43:THR:HG21	1:F:52:LEU:HD22	2.01	0.43
1:G:21:LEU:HB2	1:G:179:GLN:OE1	2.19	0.43
1:G:263:VAL:HA	1:G:264:PRO:HD3	1.88	0.42
1:D:33:ARG:HD2	1:D:307:ASP:O	2.19	0.42
1:F:78:SER:OG	1:F:81:VAL:HG23	2.19	0.42
1:A:98:LEU:HD23	1:A:132:LEU:CD2	2.49	0.42
1:C:230:LYS:O	1:C:234:LEU:HD12	2.19	0.42
1:A:51:IT1:OP1	1:A:195:SER:N	2.52	0.42
1:F:50:ASN:HA	1:F:169:TYR:OH	2.19	0.42
1:A:167:MET:SD	1:A:242:LEU:HD11	2.59	0.42
1:C:59:VAL:HG21	1:C:87:VAL:HG11	2.01	0.42
1:C:199:HIS:O	1:C:199:HIS:HD2	2.03	0.42
1:C:145:ARG:O	1:C:149:GLN:HG3	2.19	0.42
1:D:43:THR:HG22	1:D:45:ILE:H	1.84	0.42
1:A:21:LEU:HB2	1:A:179:GLN:OE1	2.19	0.42
1:G:219:THR:HG1	1:G:254:ASP:HA	1.79	0.42
1:C:70:LEU:HD11	1:C:93:LEU:HD13	2.01	0.42
1:F:12:LEU:HD11	1:F:63:LEU:HD12	2.01	0.42
1:B:97:ALA:HB1	1:B:99:LEU:HD11	2.02	0.42
1:C:12:LEU:HD11	1:C:63:LEU:HD12	2.02	0.42
1:H:2:PRO:HG2	1:H:3:LEU:HD12	2.02	0.42
1:D:15:ILE:CD1	1:D:53:ARG:HD3	2.47	0.42
1:A:322:PHE:HE2	1:B:118:LEU:HD11	1.83	0.42
1:F:55:LEU:HA	1:F:58:LEU:HB2	2.01	0.42
1:F:76:ILE:HB	1:F:110:TYR:HE1	1.85	0.42
1:C:210:MET:HB3	1:C:213:VAL:HG23	2.02	0.42
1:F:275:LEU:HB3	1:F:281:VAL:HG23	2.02	0.42
1:A:286:VAL:HG13	1:A:287:TYR:CD2	2.55	0.42
1:F:257:PHE:HD1	1:F:260:GLY:HA2	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:258:ALA:HB3	1:D:265:ASN:HB3	1.98	0.42
1:D:174:LEU:HD13	1:D:209:LEU:CD1	2.50	0.42
1:C:146:ILE:O	1:C:149:GLN:N	2.52	0.42
1:A:112:THR:C	1:B:325:HIS:HE1	2.22	0.42
1:H:191:VAL:O	1:H:217:GLY:HA2	2.19	0.42
1:A:230:LYS:O	1:A:234:LEU:HD12	2.20	0.42
1:B:231:VAL:HG12	1:B:250:ILE:HD13	2.02	0.42
1:A:242:LEU:HA	1:A:242:LEU:HD23	1.80	0.42
1:E:257:PHE:HD1	1:E:260:GLY:HA2	1.85	0.42
1:A:1:MET:N	1:A:2:PRO:HD2	2.35	0.41
1:B:186:LEU:C	1:B:186:LEU:HD12	2.40	0.41
1:F:199:HIS:C	1:F:199:HIS:CD2	2.92	0.41
1:A:26:ARG:NH1	1:B:89:ALA:O	2.52	0.41
1:E:3:LEU:HD22	1:E:209:LEU:HD11	2.02	0.41
1:G:114:GLY:O	1:G:118:LEU:HD12	2.19	0.41
1:E:100:GLU:O	1:E:102:PRO:HD3	2.20	0.41
1:A:64:ARG:HG2	1:D:64:ARG:NE	2.35	0.41
1:H:1:MET:N	1:H:2:PRO:HD3	2.31	0.41
1:H:325:HIS:CG	1:H:326:PRO:CD	3.02	0.41
1:G:257:PHE:HD1	1:G:260:GLY:HA2	1.84	0.41
1:H:55:LEU:HA	1:H:58:LEU:HB2	2.03	0.41
1:E:327:HIS:O	1:E:328:VAL:C	2.59	0.41
1:A:89:ALA:HB1	1:B:277:SER:O	2.19	0.41
1:G:152:ARG:HB3	1:G:152:ARG:HE	1.46	0.41
1:G:6:LEU:HB3	1:G:7:THR:H	1.49	0.41
1:G:221:SER:HB3	1:G:261:TYR:HB2	2.01	0.41
1:A:189:VAL:HG22	1:A:311:LEU:HB3	2.03	0.41
1:H:11:ARG:HH11	1:H:11:ARG:CG	1.97	0.41
1:D:231:VAL:CG1	1:D:250:ILE:HG21	2.51	0.41
1:B:199:HIS:C	1:B:199:HIS:CD2	2.94	0.41
1:G:164:LEU:O	1:G:167:MET:HB2	2.21	0.41
1:H:221:SER:HB3	1:H:261:TYR:HB2	2.02	0.41
1:H:76:ILE:HB	1:H:110:TYR:HE1	1.85	0.41
1:H:4:HIS:O	1:H:5:HIS:C	2.58	0.41
1:D:1:MET:HB3	1:D:4:HIS:HB3	2.02	0.41
1:B:171:GLU:O	1:B:174:LEU:HB3	2.21	0.41
1:D:250:ILE:H	1:D:250:ILE:HG13	1.69	0.41
1:E:11:ARG:HB2	1:E:57:PHE:CE2	2.56	0.41
1:H:242:LEU:HA	1:H:242:LEU:HD23	1.84	0.41
1:G:156:ILE:HA	1:G:157:PRO:HD2	1.84	0.41
1:D:98:LEU:HD13	1:D:142:LEU:HD22	2.03	0.41
1:H:210:MET:HB3	1:H:213:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:4:HIS:O	1:H:7:THR:HG22	2.21	0.41
1:D:229:PRO:O	1:D:232:ILE:HG22	2.21	0.41
1:A:221:SER:HB3	1:A:261:TYR:HB2	2.03	0.41
1:E:327:HIS:ND1	1:E:327:HIS:C	2.73	0.41
1:B:67:ALA:CB	1:B:153:PRO:O	2.69	0.41
1:C:263:VAL:HA	1:C:264:PRO:HD3	1.89	0.41
1:C:31:LEU:HD12	1:C:35:ILE:CD1	2.51	0.41
1:F:43:THR:HG22	1:F:45:ILE:H	1.86	0.40
1:H:275:LEU:HD22	1:H:283:LEU:HD11	2.03	0.40
1:A:173:ALA:HB1	1:A:206:LEU:HD12	2.02	0.40
1:C:19:THR:OG1	1:C:38:LYS:HE3	2.21	0.40
1:G:112:THR:HB	1:H:325:HIS:CE1	2.55	0.40
1:E:-1:ALA:O	1:G:23:TYR:CE2	2.73	0.40
1:A:112:THR:CB	1:B:325:HIS:HE1	2.35	0.40
1:B:37:ILE:HG12	1:B:39:ARG:HD2	2.02	0.40
1:C:20:PRO:HG2	1:C:39:ARG:HB2	2.03	0.40
1:G:51:IT1:HD	1:G:51:IT1:HA	1.63	0.40
1:A:156:ILE:HA	1:A:157:PRO:HD2	1.89	0.40
1:B:20:PRO:HG2	1:B:39:ARG:HB2	2.04	0.40
1:F:53:ARG:O	1:F:56:GLU:HB2	2.22	0.40
1:A:228:LYS:HB3	1:A:228:LYS:HE2	1.96	0.40
1:A:166:ALA:HB3	1:A:238:ILE:HD11	2.03	0.40
1:E:134:ASP:H	1:E:138:GLN:NE2	2.17	0.40
1:B:251:HIS:C	1:B:252:LEU:HG	2.42	0.40

There are no symmetry-related clashes.

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	327/342 (96%)	297 (91%)	22 (7%)	8 (2%)	9 53
1	B	320/342 (94%)	288 (90%)	25 (8%)	7 (2%)	10 55
1	C	320/342 (94%)	292 (91%)	22 (7%)	6 (2%)	12 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	326/342 (95%)	293 (90%)	26 (8%)	7 (2%)	11	56
1	E	327/342 (96%)	292 (89%)	22 (7%)	13 (4%)	5	36
1	F	313/342 (92%)	277 (88%)	28 (9%)	8 (3%)	8	50
1	G	321/342 (94%)	285 (89%)	29 (9%)	7 (2%)	10	55
1	H	328/342 (96%)	297 (90%)	22 (7%)	9 (3%)	8	49
All	All	2582/2736 (94%)	2321 (90%)	196 (8%)	65 (2%)	9	51

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	258	ALA
1	B	258	ALA
1	C	258	ALA
1	D	1	MET
1	D	4	HIS
1	D	258	ALA
1	D	325	HIS
1	E	0	SER
1	E	1	MET
1	E	258	ALA
1	E	325	HIS
1	E	326	PRO
1	F	6	LEU
1	F	258	ALA
1	F	325	HIS
1	F	326	PRO
1	G	258	ALA
1	G	325	HIS
1	G	326	PRO
1	H	258	ALA
1	H	325	HIS
1	B	8	ARG
1	B	195	SER
1	E	4	HIS
1	A	182	GLU
1	A	195	SER
1	B	182	GLU
1	B	196	ALA
1	C	182	GLU

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Mol	Chain	Res	Type
1	C	196	ALA
1	D	182	GLU
1	D	195	SER
1	D	196	ALA
1	E	195	SER
1	E	327	HIS
1	F	195	SER
1	G	182	GLU
1	G	196	ALA
1	H	6	LEU
1	H	182	GLU
1	H	195	SER
1	A	196	ALA
1	A	325	HIS
1	B	325	HIS
1	C	195	SER
1	E	6	LEU
1	E	182	GLU
1	E	196	ALA
1	F	182	GLU
1	F	196	ALA
1	G	195	SER
1	H	8	ARG
1	H	196	ALA
1	A	157	PRO
1	C	325	HIS
1	G	157	PRO
1	B	153	PRO
1	A	153	PRO
1	H	326	PRO
1	F	308	GLY
1	C	157	PRO
1	E	2	PRO
1	E	153	PRO
1	H	157	PRO

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	251/266 (94%)	239 (95%)	12 (5%)	35	79
1	B	227/266 (85%)	209 (92%)	18 (8%)	18	59
1	C	233/266 (88%)	216 (93%)	17 (7%)	20	63
1	D	252/266 (95%)	237 (94%)	15 (6%)	27	72
1	E	248/266 (93%)	230 (93%)	18 (7%)	20	63
1	F	203/266 (76%)	192 (95%)	11 (5%)	31	76
1	G	227/266 (85%)	209 (92%)	18 (8%)	18	59
1	H	247/266 (93%)	231 (94%)	16 (6%)	24	69
All	All	1888/2128 (89%)	1763 (93%)	125 (7%)	24	68

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	52	LEU
1	A	193	SER
1	A	202	LEU
1	A	212	ASP
1	A	232	ILE
1	A	234	LEU
1	A	245	THR
1	A	247	THR
1	A	284	ASP
1	A	288	THR
1	A	328	VAL
1	B	7	THR
1	B	15	ILE
1	B	52	LEU
1	B	71	ILE
1	B	142	LEU
1	B	186	LEU
1	B	193	SER
1	B	202	LEU
1	B	209	LEU
1	B	212	ASP
1	B	220	VAL
1	B	234	LEU
1	B	245	THR
1	B	269	MET
1	B	284	ASP

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Mol	Chain	Res	Type
1	B	288	THR
1	B	301	GLN
1	B	327	HIS
1	C	6	LEU
1	C	7	THR
1	C	33	ARG
1	C	52	LEU
1	C	193	SER
1	C	202	LEU
1	C	222	ARG
1	C	234	LEU
1	C	241	GLN
1	C	245	THR
1	C	252	LEU
1	C	269	MET
1	C	284	ASP
1	C	288	THR
1	C	301	GLN
1	C	303	ARG
1	C	327	HIS
1	D	11	ARG
1	D	15	ILE
1	D	33	ARG
1	D	52	LEU
1	D	174	LEU
1	D	193	SER
1	D	202	LEU
1	D	230	LYS
1	D	234	LEU
1	D	245	THR
1	D	249	ASP
1	D	284	ASP
1	D	288	THR
1	D	303	ARG
1	D	327	HIS
1	E	3	LEU
1	E	11	ARG
1	E	15	ILE
1	E	33	ARG
1	E	52	LEU
1	E	142	LEU
1	E	144	THR

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Mol	Chain	Res	Type
1	E	178	GLN
1	E	193	SER
1	E	202	LEU
1	E	209	LEU
1	E	234	LEU
1	E	245	THR
1	E	247	THR
1	E	284	ASP
1	E	288	THR
1	E	303	ARG
1	E	327	HIS
1	F	5	HIS
1	F	15	ILE
1	F	52	LEU
1	F	174	LEU
1	F	193	SER
1	F	234	LEU
1	F	245	THR
1	F	269	MET
1	F	288	THR
1	F	301	GLN
1	F	327	HIS
1	G	11	ARG
1	G	15	ILE
1	G	52	LEU
1	G	127	GLU
1	G	144	THR
1	G	171	GLU
1	G	193	SER
1	G	202	LEU
1	G	208	HIS
1	G	234	LEU
1	G	241	GLN
1	G	245	THR
1	G	249	ASP
1	G	269	MET
1	G	284	ASP
1	G	288	THR
1	G	301	GLN
1	G	327	HIS
1	H	1	MET
1	H	8	ARG

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Mol	Chain	Res	Type
1	H	11	ARG
1	H	52	LEU
1	H	53	ARG
1	H	144	THR
1	H	178	GLN
1	H	193	SER
1	H	202	LEU
1	H	234	LEU
1	H	235	GLN
1	H	245	THR
1	H	269	MET
1	H	284	ASP
1	H	288	THR
1	H	327	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	80	HIS
1	A	83	GLN
1	A	138	GLN
1	A	208	HIS
1	A	301	GLN
1	A	314	HIS
1	B	80	HIS
1	B	83	GLN
1	B	94	HIS
1	B	138	GLN
1	B	140	GLN
1	B	235	GLN
1	B	301	GLN
1	B	325	HIS
1	C	80	HIS
1	C	83	GLN
1	C	138	GLN
1	C	140	GLN
1	C	241	GLN
1	C	301	GLN
1	C	325	HIS
1	D	5	HIS
1	D	80	HIS

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Mol	Chain	Res	Type
1	D	83	GLN
1	D	138	GLN
1	D	208	HIS
1	D	301	GLN
1	D	325	HIS
1	E	5	HIS
1	E	80	HIS
1	E	83	GLN
1	E	138	GLN
1	E	149	GLN
1	E	236	GLN
1	E	301	GLN
1	E	325	HIS
1	F	80	HIS
1	F	83	GLN
1	F	138	GLN
1	F	301	GLN
1	F	325	HIS
1	G	80	HIS
1	G	83	GLN
1	G	138	GLN
1	G	301	GLN
1	G	325	HIS
1	H	80	HIS
1	H	83	GLN
1	H	138	GLN
1	H	208	HIS
1	H	241	GLN
1	H	301	GLN
1	H	314	HIS
1	H	325	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

8 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	IT1	A	51	1	24,24,25	3.74	7 (29%)	30,32,34	1.29	4 (13%)
1	IT1	B	51	1	24,24,25	3.88	5 (20%)	30,32,34	1.38	6 (20%)
1	IT1	C	51	1	24,24,25	4.15	7 (29%)	30,32,34	1.32	6 (20%)
1	IT1	D	51	1	24,24,25	3.71	6 (25%)	30,32,34	1.40	4 (13%)
1	IT1	E	51	1	24,24,25	4.09	6 (25%)	30,32,34	1.37	4 (13%)
1	IT1	F	51	1	24,24,25	4.06	6 (25%)	30,32,34	1.24	4 (13%)
1	IT1	G	51	1	24,24,25	3.92	5 (20%)	30,32,34	1.36	4 (13%)
1	IT1	H	51	1	24,24,25	3.97	7 (29%)	30,32,34	1.54	7 (23%)

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	IT1	A	51	1	-	1/15/17/19	0/1/1/1
1	IT1	B	51	1	-	1/15/17/19	0/1/1/1
1	IT1	C	51	1	-	1/15/17/19	0/1/1/1
1	IT1	D	51	1	-	1/15/17/19	0/1/1/1
1	IT1	E	51	1	-	1/15/17/19	0/1/1/1
1	IT1	F	51	1	-	1/15/17/19	0/1/1/1
1	IT1	G	51	1	-	1/15/17/19	0/1/1/1
1	IT1	H	51	1	-	1/15/17/19	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	51	IT1	O-C	18.34	1.24	1.11
1	E	51	IT1	O-C	18.17	1.23	1.11
1	F	51	IT1	O-C	18.00	1.23	1.11
1	H	51	IT1	O-C	17.43	1.23	1.11
1	G	51	IT1	O-C	17.24	1.23	1.11
1	B	51	IT1	O-C	17.08	1.23	1.11
1	D	51	IT1	O-C	16.08	1.22	1.11
1	A	51	IT1	O-C	16.08	1.22	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	51	IT1	O3-C3	-5.59	1.23	1.37
1	A	51	IT1	O3-C3	-5.55	1.23	1.37
1	B	51	IT1	O3-C3	-5.31	1.24	1.37
1	G	51	IT1	O3-C3	-5.29	1.24	1.37
1	D	51	IT1	O3-C3	-5.18	1.24	1.37
1	H	51	IT1	O3-C3	-5.11	1.24	1.37
1	E	51	IT1	O3-C3	-5.09	1.24	1.37
1	F	51	IT1	O3-C3	-5.06	1.24	1.37
1	H	51	IT1	C4-C4A	3.70	1.53	1.46
1	D	51	IT1	C4-C4A	3.59	1.53	1.46
1	A	51	IT1	C3-C2	-3.55	1.38	1.40
1	F	51	IT1	C4-C4A	3.24	1.52	1.46
1	E	51	IT1	C4-C4A	3.15	1.52	1.46
1	F	51	IT1	C2-N1	3.01	1.39	1.33
1	G	51	IT1	C4-C4A	3.00	1.52	1.46
1	E	51	IT1	C2-N1	2.99	1.39	1.33
1	B	51	IT1	C2-N1	2.99	1.39	1.33
1	H	51	IT1	C2-N1	2.95	1.39	1.33
1	F	51	IT1	C4A-NZ	2.87	1.36	1.27
1	A	51	IT1	C4-C4A	2.85	1.51	1.46
1	B	51	IT1	C4-C4A	2.81	1.51	1.46
1	G	51	IT1	C2-N1	2.76	1.39	1.33
1	C	51	IT1	C4A-NZ	2.73	1.35	1.27
1	G	51	IT1	C4A-NZ	2.72	1.35	1.27
1	D	51	IT1	C4A-NZ	2.69	1.35	1.27
1	H	51	IT1	C4A-NZ	2.68	1.35	1.27
1	C	51	IT1	C4-C4A	2.66	1.51	1.46
1	D	51	IT1	C2-N1	2.63	1.38	1.33
1	B	51	IT1	C4A-NZ	2.58	1.35	1.27
1	E	51	IT1	C4A-NZ	2.52	1.35	1.27
1	C	51	IT1	CB-CA	-2.46	1.51	1.53
1	A	51	IT1	P-OP2	-2.39	1.46	1.54
1	F	51	IT1	CE-NZ	2.36	1.51	1.46
1	A	51	IT1	C4A-NZ	2.30	1.34	1.27
1	H	51	IT1	CA-C	2.24	1.52	1.48
1	E	51	IT1	P-OP2	-2.24	1.46	1.54
1	A	51	IT1	C2-N1	2.21	1.38	1.33
1	D	51	IT1	P-OP2	-2.15	1.46	1.54
1	C	51	IT1	C3-C2	-2.15	1.39	1.40
1	C	51	IT1	C2-N1	2.09	1.37	1.33
1	H	51	IT1	P-OP2	-2.07	1.47	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	51	IT1	C3-C4-C4A	-3.65	115.67	120.19
1	H	51	IT1	C3-C4-C4A	-3.50	115.86	120.19
1	D	51	IT1	C5-C4-C4A	3.10	125.86	121.53
1	H	51	IT1	C5-C4-C4A	3.07	125.81	121.53
1	A	51	IT1	C3-C4-C4A	-2.78	116.75	120.19
1	C	51	IT1	OP3-P-OP1	2.68	119.19	110.44
1	E	51	IT1	C5-C6-N1	-2.67	119.05	123.86
1	F	51	IT1	OP3-P-OP2	2.65	117.92	107.61
1	E	51	IT1	C2A-C2-C3	-2.61	117.84	121.02
1	E	51	IT1	C3-C4-C4A	-2.61	116.97	120.19
1	G	51	IT1	OP3-P-OP2	2.60	117.73	107.61
1	H	51	IT1	C2A-C2-C3	-2.59	117.87	121.02
1	C	51	IT1	C3-C4-C4A	-2.59	116.99	120.19
1	C	51	IT1	OP3-P-OP2	2.57	117.60	107.61
1	G	51	IT1	C5-C6-N1	-2.52	119.32	123.86
1	H	51	IT1	C5-C6-N1	-2.50	119.36	123.86
1	B	51	IT1	OP3-P-OP1	2.47	118.50	110.44
1	F	51	IT1	C3-C4-C4A	-2.37	117.25	120.19
1	B	51	IT1	C3-C4-C4A	-2.37	117.25	120.19
1	A	51	IT1	OP3-P-OP1	2.37	118.18	110.44
1	D	51	IT1	C5-C6-N1	-2.36	119.61	123.86
1	H	51	IT1	O3-C3-C2	2.35	121.78	117.61
1	A	51	IT1	C5-C6-N1	-2.33	119.66	123.86
1	B	51	IT1	OP3-P-OP2	2.32	116.64	107.61
1	B	51	IT1	OP3-P-OP4	-2.27	100.39	106.65
1	G	51	IT1	OP3-P-OP1	2.23	117.75	110.44
1	B	51	IT1	OP4-P-OP1	-2.18	100.31	106.71
1	E	51	IT1	OP3-P-OP1	2.18	117.56	110.44
1	C	51	IT1	C5-C4-C4A	2.15	124.53	121.53
1	H	51	IT1	OP3-P-OP2	2.13	115.91	107.61
1	A	51	IT1	OP4-P-OP1	-2.13	100.46	106.71
1	G	51	IT1	OP2-P-OP4	-2.13	100.78	106.65
1	C	51	IT1	OP3-P-OP4	-2.12	100.79	106.65
1	B	51	IT1	C5-C6-N1	-2.10	120.08	123.86
1	F	51	IT1	C5-C6-N1	-2.09	120.08	123.86
1	D	51	IT1	OP3-P-OP4	-2.06	100.97	106.65
1	C	51	IT1	C5-C6-N1	-2.05	120.16	123.86
1	F	51	IT1	OP3-P-OP4	-2.03	101.05	106.65
1	H	51	IT1	C4-C3-C2	-2.01	118.83	120.18

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	51	IT1	C4-C4A-NZ-CE
1	B	51	IT1	C4-C4A-NZ-CE
1	C	51	IT1	C4-C4A-NZ-CE
1	G	51	IT1	C4-C4A-NZ-CE
1	D	51	IT1	C4-C4A-NZ-CE
1	A	51	IT1	C4-C4A-NZ-CE
1	E	51	IT1	C4-C4A-NZ-CE
1	H	51	IT1	C4-C4A-NZ-CE

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 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	PO4	A	401	-	4,4,4	0.41	0	6,6,6	0.32	0
2	PO4	B	401	-	4,4,4	0.25	0	6,6,6	0.32	0
2	PO4	C	401	-	4,4,4	0.19	0	6,6,6	0.33	0
2	PO4	D	401	-	4,4,4	0.20	0	6,6,6	0.32	0
2	PO4	E	401	-	4,4,4	0.46	0	6,6,6	0.32	0
2	PO4	F	401	-	4,4,4	0.30	0	6,6,6	0.31	0
2	PO4	G	401	-	4,4,4	0.23	0	6,6,6	0.32	0
2	PO4	H	401	-	4,4,4	0.22	0	6,6,6	0.30	0

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	PO4	A	401	-	-	0/0/0/0	0/0/0/0
2	PO4	B	401	-	-	0/0/0/0	0/0/0/0
2	PO4	C	401	-	-	0/0/0/0	0/0/0/0
2	PO4	D	401	-	-	0/0/0/0	0/0/0/0
2	PO4	E	401	-	-	0/0/0/0	0/0/0/0
2	PO4	F	401	-	-	0/0/0/0	0/0/0/0
2	PO4	G	401	-	-	0/0/0/0	0/0/0/0
2	PO4	H	401	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	330/342 (96%)	0.02	0 100 100	53, 68, 80, 87	0
1	B	323/342 (94%)	-0.11	0 100 100	55, 68, 81, 86	1 (0%)
1	C	323/342 (94%)	-0.08	0 100 100	55, 68, 81, 87	0
1	D	329/342 (96%)	-0.01	0 100 100	53, 68, 80, 86	0
1	E	330/342 (96%)	-0.03	0 100 100	53, 68, 80, 86	0
1	F	318/342 (92%)	-0.13	0 100 100	55, 68, 80, 88	0
1	G	324/342 (94%)	-0.13	0 100 100	55, 68, 81, 86	0
1	H	331/342 (96%)	-0.04	0 100 100	54, 68, 81, 87	0
All	All	2608/2736 (95%)	-0.06	0 100 100	53, 68, 80, 88	1 (0%)

There are no RSRZ outliers to report.

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

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
1	IT1	G	51	24/25	0.21	0.29	55,56,57,58	0
1	IT1	B	51	24/25	0.21	0.08	55,56,57,58	0
1	IT1	C	51	24/25	0.22	-0.13	55,56,57,58	0
1	IT1	D	51	24/25	0.22	-0.19	55,56,57,58	0
1	IT1	A	51	24/25	0.23	-0.21	55,56,57,58	0
1	IT1	F	51	24/25	0.20	-0.33	55,57,57,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	IT1	H	51	24/25	0.20	-0.68	55,56,57,58	0
1	IT1	E	51	24/25	0.20	-1.07	55,56,57,58	0

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(\AA^2)	Q<0.9
2	PO4	G	401	5/5	0.19	0.07	108,108,109,109	0
2	PO4	F	401	5/5	0.18	-0.40	154,154,155,155	0
2	PO4	E	401	5/5	0.17	-1.20	75,76,76,77	0
2	PO4	C	401	5/5	0.15	-1.21	97,98,98,98	0
2	PO4	D	401	5/5	0.17	-1.32	83,85,85,85	0
2	PO4	H	401	5/5	0.18	-1.33	112,113,113,113	0
2	PO4	B	401	5/5	0.18	-1.36	123,123,124,124	0
2	PO4	A	401	5/5	0.19	-1.69	81,81,82,83	0

6.5 Other polymers

There are no such residues in this entry.