



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:34 AM UTC

PDB ID : 4D8U / pdb_00004d8u
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

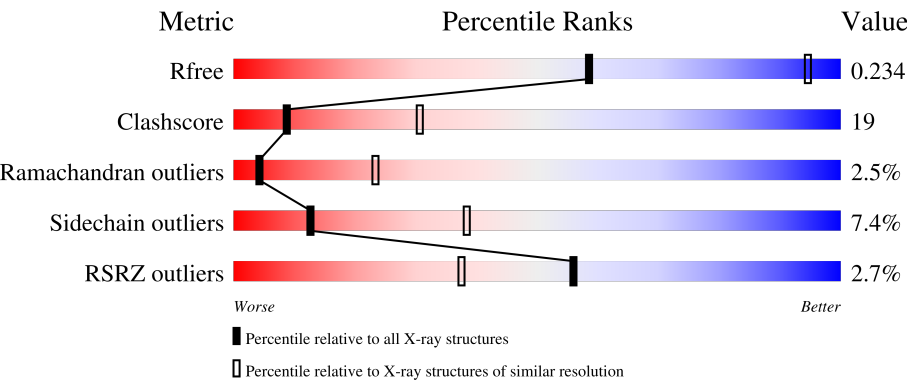
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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.



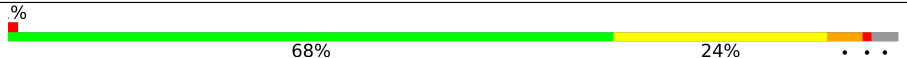
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	342	2% 65% 26% •••
1	B	342	4% 63% 26% 5% 6%
1	C	342	3% 65% 25% • 6%
1	D	342	2% 67% 23% 5% ••
1	E	342	2% 69% 22% 5% ••

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Mol	Chain	Length	Quality of chain
1	F	342	
1	G	342	
1	H	342	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	401	-	-	X	-
2	PO4	C	401	-	-	X	-
2	PO4	E	401	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19156 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 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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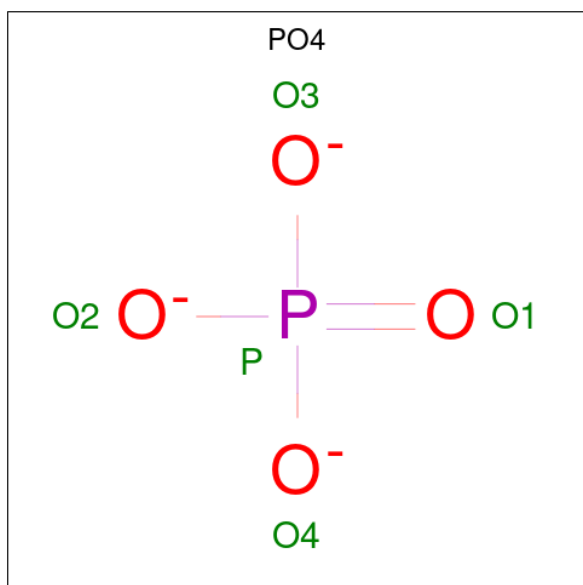
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP Q8ZNT7
E	-13	MET	-	expression tag	UNP Q8ZNT7
E	-12	ARG	-	expression tag	UNP Q8ZNT7
E	-11	GLY	-	expression tag	UNP Q8ZNT7
E	-10	SER	-	expression tag	UNP Q8ZNT7
E	-9	HIS	-	expression tag	UNP Q8ZNT7
E	-8	HIS	-	expression tag	UNP 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 (CCD ID: 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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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		

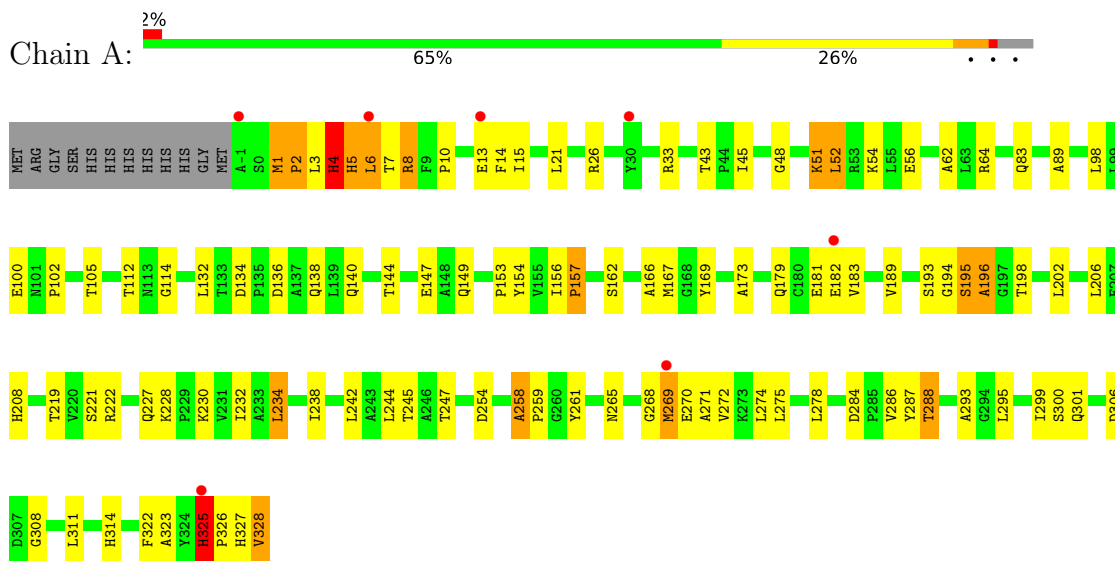
- Molecule 3 is water.

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		

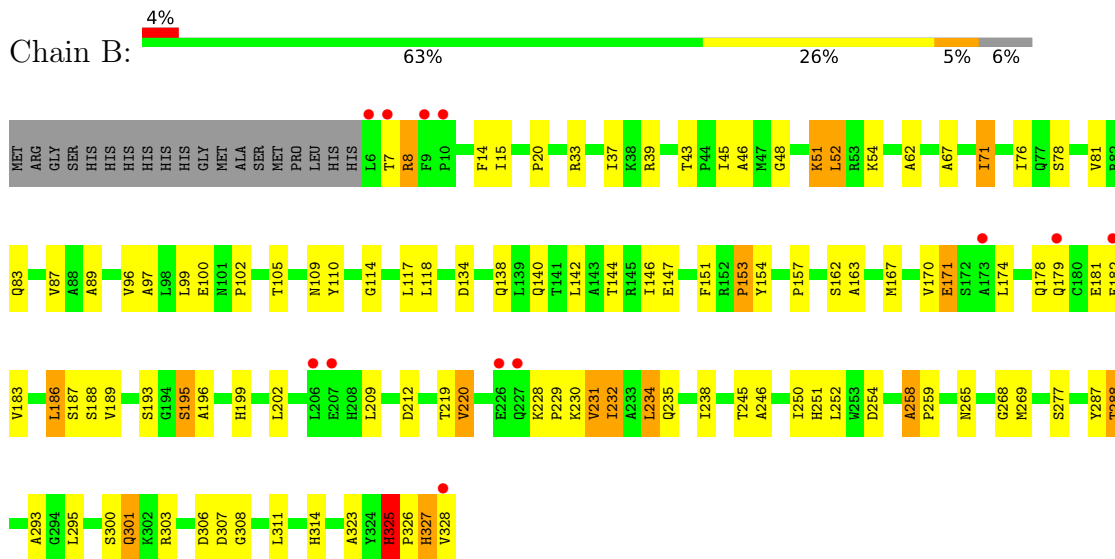
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: D-cysteine desulfhydrase

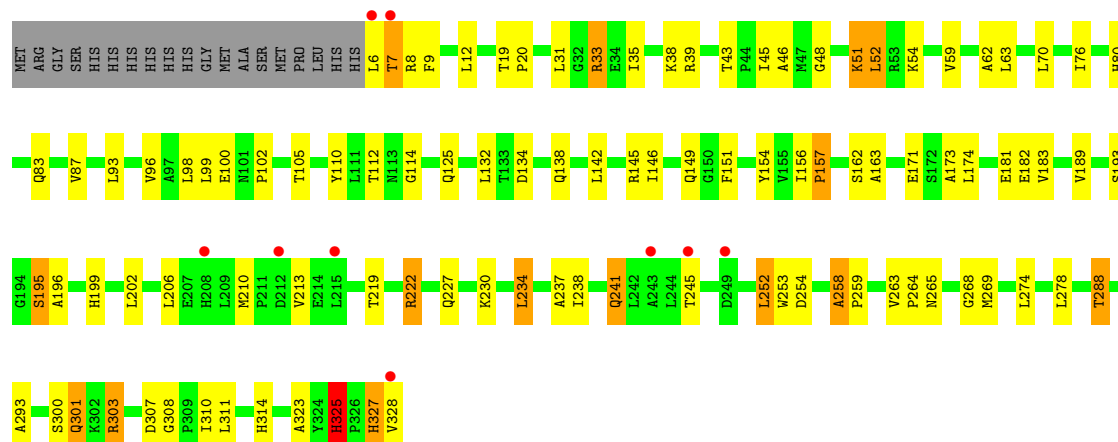


• Molecule 1: D-cysteine desulfhydrase



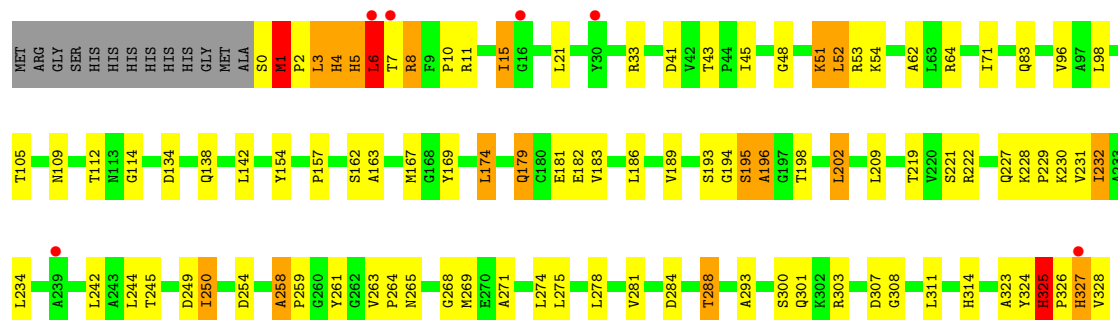
• Molecule 1: D-cysteine desulfhydrase

Chain C: 3% 65% 25% 6%



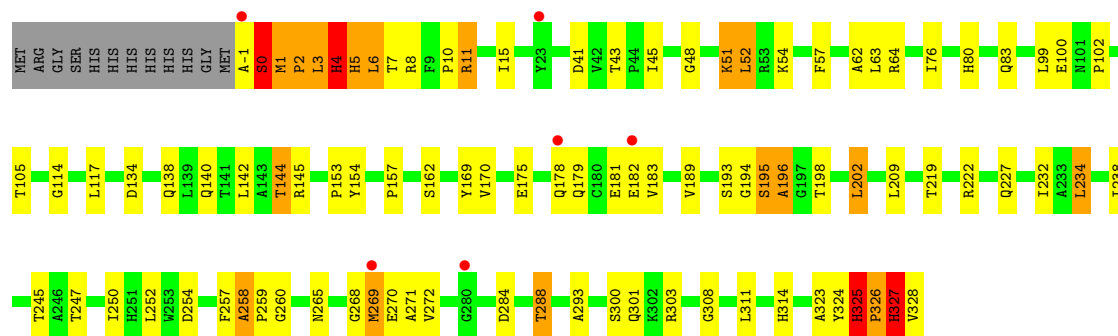
• Molecule 1: D-cysteine desulfhydrase

Chain D: 2% 67% 23% 5%



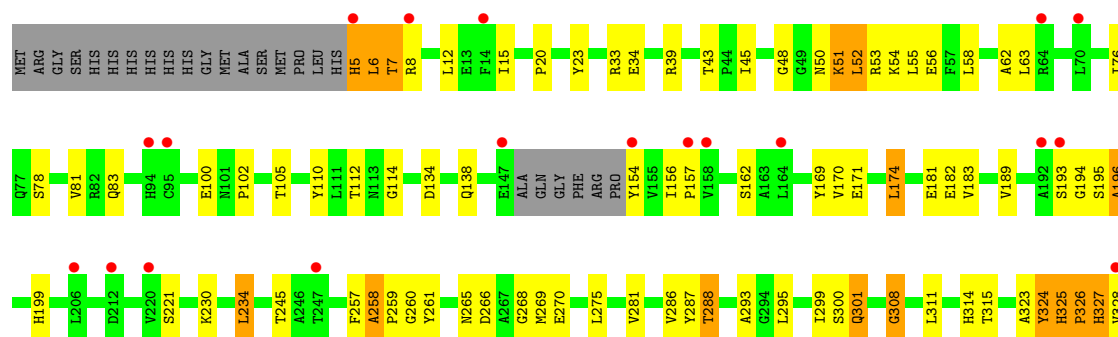
• Molecule 1: D-cysteine desulfhydrase

Chain E: 2% 69% 22% 5%

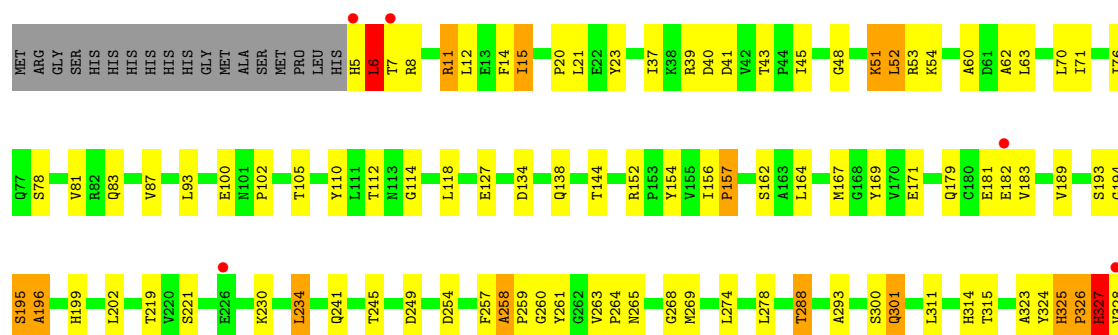


• Molecule 1: D-cysteine desulfhydrase

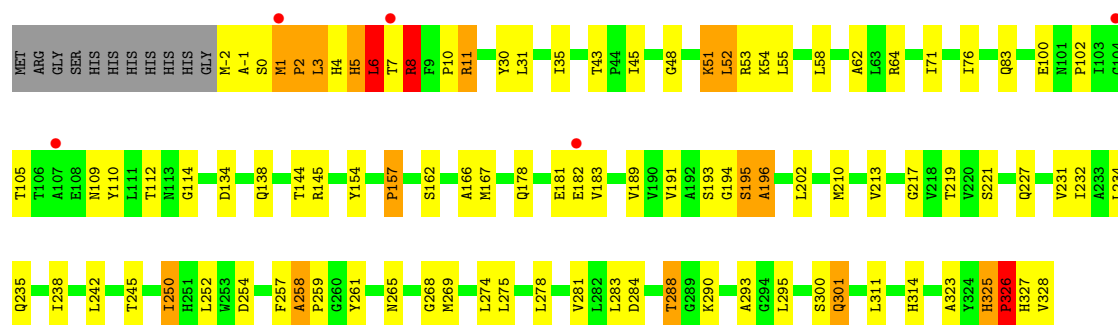
Chain F: 6% 68% 21% 5% 7%



- Molecule 1: D-cysteine desulfhydrase



- Molecule 1: D-cysteine desulfhydrase



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 (Not available) , 0.234	Depositor DCC
R_{free} test set	3868 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.92	3/2489 (0.1%)	1.15	16/3394 (0.5%)
1	B	0.84	0/2354	1.09	6/3220 (0.2%)
1	C	0.83	1/2380 (0.0%)	1.07	8/3252 (0.2%)
1	D	0.89	3/2487 (0.1%)	1.09	9/3391 (0.3%)
1	E	0.88	2/2473 (0.1%)	1.08	7/3376 (0.2%)
1	F	0.95	0/2241	1.10	6/3070 (0.2%)
1	G	0.88	1/2361 (0.0%)	1.09	3/3231 (0.1%)
1	H	0.91	5/2477 (0.2%)	1.08	6/3381 (0.2%)
All	All	0.89	15/19262 (0.1%)	1.09	61/26315 (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	E	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	5	HIS	CA-C	-8.18	1.41	1.52
1	A	6	LEU	N-CA	-8.01	1.36	1.46
1	H	8	ARG	N-CA	-7.74	1.36	1.46
1	C	8	ARG	N-CA	-6.73	1.40	1.46
1	D	8	ARG	N-CA	-6.68	1.37	1.46
1	A	6	LEU	CA-C	6.60	1.61	1.52
1	A	8	ARG	N-CA	-6.21	1.37	1.46
1	H	5	HIS	CA-C	-5.95	1.44	1.52
1	H	326	PRO	N-CD	-5.41	1.40	1.47
1	G	8	ARG	N-CA	-5.40	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	6	LEU	CB-CG	5.28	1.64	1.53
1	E	325	HIS	CG-ND1	-5.13	1.32	1.38
1	E	5	HIS	CA-C	-5.04	1.46	1.52
1	H	6	LEU	CA-C	-5.01	1.46	1.52
1	H	2	PRO	CA-C	-5.00	1.47	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	LEU	CA-C-O	12.73	134.61	119.59
1	D	5	HIS	N-CA-C	-9.94	100.94	112.87
1	A	6	LEU	CB-CA-C	-8.81	95.83	110.72
1	A	8	ARG	N-CA-C	-8.78	101.53	113.30
1	H	8	ARG	N-CA-C	-8.73	92.20	110.80
1	C	325	HIS	CA-C-N	-8.68	109.39	118.85
1	C	325	HIS	C-N-CA	-8.68	109.39	118.85
1	B	325	HIS	CA-C-N	-8.65	109.42	118.85
1	B	325	HIS	C-N-CA	-8.65	109.42	118.85
1	A	325	HIS	CA-C-N	-8.36	109.74	118.85
1	A	325	HIS	C-N-CA	-8.36	109.74	118.85
1	G	6	LEU	N-CA-C	8.35	128.57	110.80
1	A	2	PRO	N-CA-C	-8.15	104.00	114.03
1	H	2	PRO	N-CA-C	-7.90	103.44	114.98
1	D	8	ARG	N-CA-C	-7.69	102.17	114.09
1	E	4	HIS	N-CA-C	7.52	126.83	110.80
1	C	327	HIS	N-CA-C	7.11	119.17	107.73
1	E	269	MET	CB-CG-SD	7.09	133.98	112.70
1	D	269	MET	CB-CG-SD	6.99	133.67	112.70
1	F	7	THR	N-CA-C	6.84	119.99	108.23
1	A	269	MET	CB-CG-SD	6.73	132.90	112.70
1	A	5	HIS	CB-CA-C	-6.63	97.78	110.57
1	E	8	ARG	N-CA-C	-6.49	105.37	113.28
1	E	308	GLY	CA-C-N	6.35	126.37	119.90
1	E	308	GLY	C-N-CA	6.35	126.37	119.90
1	B	308	GLY	CA-C-N	6.32	126.34	119.90
1	B	308	GLY	C-N-CA	6.32	126.34	119.90
1	A	270	GLU	N-CA-C	-6.18	104.54	111.28
1	F	324	TYR	N-CA-C	-6.15	106.14	113.21
1	E	170	VAL	N-CA-C	-6.10	104.79	110.53
1	A	325	HIS	N-CA-C	6.01	123.09	109.81
1	C	308	GLY	CA-C-N	5.84	127.14	119.84
1	C	308	GLY	C-N-CA	5.84	127.14	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	327	HIS	N-CA-C	5.76	115.45	107.73
1	D	3	LEU	N-CA-C	-5.75	103.76	112.04
1	H	6	LEU	CB-CA-C	-5.72	99.04	110.42
1	H	3	LEU	N-CA-C	-5.72	106.91	112.97
1	H	35	ILE	N-CA-C	5.70	116.07	107.75
1	B	8	ARG	N-CA-C	-5.68	98.70	110.80
1	C	325	HIS	N-CA-C	5.65	122.30	109.81
1	F	308	GLY	CA-C-N	5.61	126.85	119.84
1	F	308	GLY	C-N-CA	5.61	126.85	119.84
1	H	8	ARG	N-CA-CB	5.58	119.92	110.49
1	D	308	GLY	CA-C-N	5.54	125.55	119.90
1	D	308	GLY	C-N-CA	5.54	125.55	119.90
1	F	8	ARG	N-CA-C	-5.46	105.41	113.61
1	E	270	GLU	N-CA-C	-5.45	105.34	111.28
1	A	308	GLY	CA-C-N	5.40	125.41	119.90
1	A	308	GLY	C-N-CA	5.40	125.41	119.90
1	B	327	HIS	N-CA-C	5.39	116.41	107.73
1	A	13	GLU	CA-CB-CG	-5.25	103.60	114.10
1	D	325	HIS	CA-C-N	-5.22	113.31	119.84
1	D	325	HIS	C-N-CA	-5.22	113.31	119.84
1	C	7	THR	N-CA-C	5.16	117.12	107.99
1	D	1	MET	N-CA-C	5.16	121.20	109.81
1	C	8	ARG	N-CA-C	-5.12	105.06	113.50
1	A	1	MET	CA-C-N	-5.09	114.58	119.87
1	A	1	MET	C-N-CA	-5.09	114.58	119.87
1	A	149	GLN	N-CA-C	-5.08	106.93	112.72
1	G	8	ARG	N-CA-C	-5.05	106.26	114.09
1	G	327	HIS	N-CA-C	5.03	115.83	107.73

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	0	SER	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	2466	0	2456	97	0
1	B	2335	0	2253	84	0
1	C	2361	0	2296	82	0
1	D	2464	0	2462	95	0
1	E	2450	0	2422	95	0
1	F	2227	0	2064	78	0
1	G	2341	0	2237	89	0
1	H	2454	0	2425	113	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	18615	705	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (705) 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: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:G:5:HIS:C	1:G:6:LEU:HD12	1.60	1.23
1:F:325:HIS:CD2	1:F:326:PRO:HD3	1.71	1.23
1:D:6:LEU:HD13	1:D:6:LEU:O	1.43	1.16
1:E:325:HIS:HB3	1:E:326:PRO:HD2	1.16	1.15
1:F:325:HIS:CG	1:F:326:PRO:CD	2.30	1.15
1:H:11:ARG:HH11	1:H:11:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:167:MET:HE1	1:B:238:ILE:HG23	1.30	1.06
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:G:5:HIS:C	1:G:6:LEU:CD1	2.29	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	1.00
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:H:167:MET:HE1	1:H:242:LEU:HD21	1.47	0.95
1:H:6:LEU:HD13	1:H:6:LEU:C	1.92	0.94
1:F:105:THR:OG1	1:F:328:VAL:HG12	1.68	0.94
1:F:51:LLP: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:H:0:SER:C	1:H:2:PRO:HD2	1.96	0.91
1:A:328:VAL:HG12	1:A:328:VAL:O	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:F:325:HIS:CD2	1:F:326:PRO:CD	2.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:258:ALA:CB	1:D:259:PRO:HD3	2.02	0.88
1:A:10:PRO:HB3	1:D:10:PRO:HB3	1.54	0.87
1:G:6:LEU:HD12	1:G:6:LEU:N	1.89	0.87
1:G:219:THR:OG1	1:G:254:ASP:HA	1.75	0.87
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:H:11:ARG:HG3	1:H:11:ARG:NH1	1.83	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:A:258:ALA:CB	1:A:259:PRO:HD3	2.04	0.85
1:E:325:HIS:CG	1:E:326:PRO:N	2.40	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:C:258:ALA:CB	1:C:259:PRO:HD3	2.06	0.84
1:D:325:HIS:HB3	1:D:326:PRO:CD	2.07	0.84
1:E:258:ALA:CB	1:E:259:PRO:CD	2.56	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:LLP: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:HH11	1:C:222:ARG:HB2	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:5:HIS:C	1:G:6:LEU:CG	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:325:HIS:O	1:D:326:PRO:C	2.23	0.80
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
1:D:4:HIS:C	1:D:6:LEU:N	2.38	0.79
1:H:51:LLP:OP2	1:H:54:LYS:NZ	2.15	0.79
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:E:-1:ALA:O	1:E:0:SER:HB2	1.82	0.79
1:E:258:ALA:HB1	1:E:259:PRO:CD	2.13	0.79
1:F:325:HIS:CG	1:F:326:PRO:N	2.50	0.79
1:A:328:VAL:O	1:A:328:VAL:CG1	2.30	0.78
1:D:6:LEU:HD13	1:D:6:LEU:C	2.07	0.78
1:B:167:MET:HE1	1:B:238:ILE:CG2	2.13	0.78
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:E:324:TYR:O	1:E:325:HIS:O	2.02	0.78
1:H:1:MET:N	1:H:2:PRO:CD	2.47	0.78
1:E:326:PRO:O	1:E:327:HIS:HB3	1.84	0.77
1:G:5:HIS:HA	1:G:6:LEU:HD12	1.67	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: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:D:5:HIS:O	1:D:6:LEU:C	2.28	0.77
1:C:51:LLP: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:E:5:HIS:C	1:E:7:THR:H	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:327:HIS:O	1:F:328:VAL:C	2.30	0.75
1:H:114:GLY:HA3	1:H:323:ALA:HB2	1.68	0.74
1:E:51:LLP:OP2	1:E:54:LYS:NZ	2.19	0.74
1:E:140:GLN:O	1:E:144:THR:HG23	1.87	0.74
1:H:288:THR:HG21	1:H:314:HIS:HD2	1.52	0.74
1:F:325:HIS:O	1:F:326:PRO:C	2.30	0.74
1:A:136:ASP:O	1:A:140:GLN:HG2	1.88	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:H:6:LEU:CD1	1:H:6:LEU:C	2.50	0.74
1:E:325:HIS:O	1:E:326:PRO:C	2.30	0.74
1:C:114:GLY:HA3	1:C:323:ALA:HB2	1.69	0.74
1:D:3:LEU:O	1:D:6:LEU:N	2.20	0.74
1:D:51:LLP:OP2	1:D:54:LYS:NZ	2.20	0.74
1:D:288:THR:HG21	1:D:314:HIS:HD2	1.52	0.74
1:E:52:LEU:HD12	1:E:83:GLN:HE21	1.53	0.74
1:H:-2:MET:CA	1:H:0:SER:H	2.00	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:G:325:HIS:O	1:G:326:PRO:C	2.32	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:A:4:HIS:O	1:A:7:THR:HG22	1.89	0.72
1:D:1:MET:HB2	1:D:2:PRO:CA	2.07	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: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: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:G:325:HIS:HB3	1:G:326:PRO:HD3	1.72	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:E:64:ARG:HB3	1:H:64:ARG:NH2	2.05	0.70
1:D:6:LEU:O	1:D:6:LEU:CD1	2.32	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:0:SER:C	1:H:2:PRO:CD	2.65	0.69
1:H:4:HIS:NE2	3:H:503:HOH:O	2.11	0.69
1:E:0:SER:N	1:E:1:MET:CB	2.56	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:D:219:THR:OG1	1:D:254:ASP:HA	1.91	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:LLP:OP2	1:G:54:LYS:NZ	2.25	0.69
1:A:1:MET:O	1:A:4:HIS:HB3	1.92	0.68
1:E:325:HIS:ND1	1:E:326:PRO:HD3	2.06	0.68
1:C:105:THR:OG1	1:C:328:VAL:HG12	1.93	0.68
1:A:33:ARG:NH2	1:A:306:ASP:O	2.26	0.68
1:D:325:HIS:CB	1:D:326:PRO:HD3	2.18	0.68
1:F:324:TYR:O	1:F:325:HIS:O	2.12	0.68
1:A:51:LLP:OP2	1:A:54:LYS:NZ	2.27	0.68
1:B:151:PHE:O	1:B:153:PRO:HD3	1.93	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:4:HIS:C	1:H:6:LEU:N	2.49	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:D:105:THR:OG1	1:D:328:VAL:HG12	1.95	0.67
1:G:70:LEU:HD21	1:G:93:LEU:HD13	1.77	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:LLP:H5'1	1:E:51:LLP: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:H:5:HIS:C	1:H:7:THR:H	2.04	0.66
1:A:51:LLP:H5'1	1:A:51:LLP:NZ	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:LLP:NZ	1:G:51:LLP:H5'1	2.10	0.65
1:G:325:HIS:CG	1:G:326:PRO:N	2.62	0.65
1:D:6:LEU:C	1:D:6:LEU:CD1	2.67	0.65
1:E:5:HIS:O	1:E:7:THR:N	2.30	0.65
1:B:134:ASP:O	1:B:138:GLN:HG3	1.95	0.65
1:E:-1:ALA:O	1:E:0:SER:CB	2.42	0.65
1:G:100:GLU:O	1:G:102:PRO:HD3	1.97	0.65
1:H:288:THR:HG21	1:H:314:HIS:CD2	2.31	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:5:HIS:C	1:E:7:THR:N	2.46	0.64
1:E:325:HIS:O	1:E:327:HIS:N	2.30	0.64
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:B:105:THR:OG1	1:B:328:VAL:HG12	1.97	0.64
1:C:80:HIS:HB3	2:C:401:PO4:O2	1.97	0.64
1:H:51:LLP:H5'1	1:H:51:LLP:NZ	2.11	0.63
1:D:4:HIS:C	1:D:6:LEU:H	2.01	0.63
1:D:3:LEU:N	1:D:3:LEU:HD12	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:B:258:ALA:CB	1:B:265:ASN:HB3	2.28	0.63
1:F:105:THR:HG1	1:F:328:VAL:HG12	1.64	0.63
1:H:5:HIS:O	1:H:7:THR:N	2.30	0.63
1:D:1:MET:HA	1:D:3:LEU:H	1.63	0.63
1:E:4:HIS:C	1:E:6:LEU:H	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:HIS:CB	2:E:401:PO4:O4	2.48	0.61
1:A:4:HIS:C	1:A:6:LEU:H	2.08	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:70:LEU:CD1	1:C:93:LEU:HD13	2.31	0.61
1:C:258:ALA:CB	1:C:265:ASN:HB3	2.29	0.61
1:A:105:THR:CG2	1:A:328:VAL:HG13	2.31	0.61
1:D:0:SER:O	1:D:1:MET:O	2.19	0.61
1:E:80:HIS:HB3	2:E:401:PO4:O4	2.01	0.61
1:E:134:ASP:H	1:E:138:GLN:HE21	1.48	0.61
1:F:34:GLU:OE2	1:H:-1:ALA:HB2	1.99	0.61
1:D:71:ILE:HG12	1:D:96:VAL:HB	1.83	0.61
1:A:258:ALA:CB	1:A:265:ASN:HB3	2.30	0.61
1:G:105:THR:OG1	1:G:328:VAL:HG12	2.00	0.61
1:C:51:LLP:H5'1	1:C:51:LLP:NZ	2.16	0.60
1:G:51:LLP:OP1	1:G:195:SER:N	2.34	0.60
1:D:5:HIS:C	1:D:7:THR:N	2.55	0.60
1:H:3:LEU:O	1:H:6:LEU:HB2	2.00	0.60
1:H:6:LEU:HD22	1:H:167:MET:CE	2.30	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:H:258:ALA:CB	1:H:265:ASN:HB3	2.31	0.60
1:C:33:ARG:HE	1:C:310:ILE:HD11	1.66	0.60
1:E:4:HIS:C	1:E:6:LEU:N	2.51	0.60
1:E:269:MET:HA	1:E:272:VAL:HG23	1.83	0.60
1:H:52:LEU:CD1	1:H:83:GLN:HE21	2.13	0.60
1:H:325:HIS:CG	1:H:326:PRO:HD3	2.37	0.60
1:F:300:SER:C	1:F:301:GLN:HE21	2.10	0.59
1:A:3:LEU:N	1:A:3:LEU:HD22	2.17	0.59
1:E:325:HIS:CB	1:E:326:PRO:HD2	1.88	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:C:325:HIS:C	1:C:325:HIS:CD2	2.80	0.59
1:D:109:ASN:HD22	1:D:326:PRO:CD	2.16	0.59
1:D:325:HIS:O	1:D:327:HIS:N	2.35	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:6:LEU:HD22	1:H:167:MET:HE1	1.86	0.58
1:H:258:ALA:HB1	1:H:259:PRO:CD	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ALA:HA	1:B:154:TYR:CD1	2.38	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:H:232:ILE:HG12	1:H:250:ILE:HG13	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:B:300:SER:C	1:B:301:GLN:HE21	2.11	0.57
1:E:1:MET:H	1:E:2:PRO:HD3	1.69	0.57
1:G:43:THR:HB	1:G:48:GLY:HA3	1.85	0.57
1:D:3:LEU:C	1:D:6:LEU:H	2.11	0.57
1:D:324:TYR:O	1:D:325:HIS:C	2.47	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:258:ALA:HB3	1:H:259:PRO:CD	2.35	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:D:300:SER:C	1:D:301:GLN:HE21	2.12	0.57
1:E:4:HIS:CD2	1:E:5:HIS:HD2	2.22	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:C:258:ALA:HB3	1:C:259:PRO:CD	2.35	0.57
1:A:208:HIS:CE1	1:A:244:LEU:HD13	2.40	0.56
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: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:G:258:ALA:HB1	1:G:259:PRO:CD	2.16	0.56
1:A:140:GLN:O	1:A:144:THR:HG23	2.05	0.56
1:F:323:ALA:C	1:F:325:HIS:H	2.14	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: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:H:4:HIS:C	1:H:6:LEU:H	2.13	0.55
1:A:1:MET:N	1:A:2:PRO:CD	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:300:SER:C	1:G:301:GLN:HE21	2.14	0.55
1:H:325:HIS:O	1:H:326:PRO:C	2.47	0.55
1:A:181:GLU:C	1:A:183:VAL:H	2.14	0.55
1:B:167:MET:HE2	1:B:238:ILE:HG23	1.83	0.55
1:E:219:THR:OG1	1:E:254:ASP:HA	2.07	0.55
1:B:51:LLP:NZ	1:B:51:LLP:H5'1	2.22	0.55
1:D:51:LLP:OP1	1:D:195:SER:N	2.39	0.55
1:C:181:GLU:C	1:C:183:VAL:H	2.15	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:B:100:GLU:O	1:B:102:PRO:HD3	2.06	0.54
1:F:51:LLP:H5'1	1:F:51:LLP:NZ	2.20	0.54
1:E:300:SER:C	1:E:301:GLN:HE21	2.15	0.54
1:C:80:HIS:CB	2:C:401:PO4:O2	2.55	0.54
1:D:157:PRO:HG3	1:D:162:SER:HB3	1.89	0.54
1:D:3:LEU:N	1:D:3:LEU:CD1	2.70	0.54
1:H:100:GLU:O	1:H:102:PRO:HD3	2.08	0.54
1:B:33:ARG:NH2	1:B:306:ASP:O	2.40	0.54
1:D:51:LLP:H5'1	1:D:51:LLP:NZ	2.23	0.54
1:E:62:ALA:HA	1:E:154:TYR:CD1	2.43	0.54
1:B:229:PRO:O	1:B:232:ILE:HG13	2.08	0.54
1:D:258:ALA:HB3	1:D:259:PRO:CD	2.36	0.54
1:C:112:THR:HB	1:D:325:HIS:HE1	1.72	0.54
1:H:7:THR:HG23	1:H:7:THR:O	2.07	0.54
1:A:219:THR:OG1	1:A:254:ASP:HA	2.07	0.54
1:A:326:PRO:O	1:A:327:HIS:HB3	2.07	0.54
1:B:258:ALA:HB3	1:B:265:ASN:HB3	1.90	0.54
1:C:199:HIS:CE1	1:C:252:LEU:CD1	2.91	0.53
1:F:43:THR:HB	1:F:48:GLY:HA3	1.90	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:B:258:ALA:HB3	1:B:259:PRO:CD	2.39	0.53
1:H:109:ASN:HD22	1:H:326:PRO:CD	2.22	0.53
1:C:9:PHE:N	1:C:9:PHE:CD1	2.77	0.53
1:C:43:THR:HB	1:C:48:GLY:HA3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLY:HA2	1:A:293:ALA:HB2	1.91	0.52
1:A:51:LLP: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:E:181:GLU:C	1:E:183:VAL:H	2.17	0.52
1:B:134:ASP:H	1:B:138:GLN:HE21	1.57	0.52
1:D:181:GLU:C	1:D:183:VAL:H	2.17	0.52
1:A:62:ALA:HA	1:A:154:TYR:CD1	2.44	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: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:G:325:HIS:HE1	1:H:112:THR:HB	1.75	0.52
1:A:325:HIS:ND1	1:A:325:HIS:C	2.66	0.52
1:D:174:LEU:HD13	1:D:209:LEU:HD11	1.92	0.52
1:H:300:SER:C	1:H:301:GLN:HE21	2.18	0.52
1:G:12:LEU:HG	1:G:60:ALA:CB	2.40	0.52
1:D:52:LEU:CD1	1:D:83:GLN:HE21	2.20	0.52
1:H:6:LEU:O	1:H:6:LEU:CG	2.50	0.52
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
1:G:325:HIS:CD2	1:G:326:PRO:N	2.77	0.51
1:C:51:LLP: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:G:181:GLU:C	1:G:183:VAL:H	2.19	0.51
1:A:300:SER:C	1:A:301:GLN:HE21	2.19	0.51
1:B:181:GLU:C	1:B:183:VAL:H	2.18	0.51
1:B:186:LEU:CD1	1:B:187:SER:N	2.73	0.51
1:B:325:HIS:C	1:B:325:HIS:CD2	2.89	0.51
1:E:76:ILE:HA	1:E:99:LEU:HD13	1.92	0.51
1:H:181:GLU:C	1:H:183:VAL:H	2.18	0.51
1:C:237:ALA:O	1:C:241:GLN:HG3	2.11	0.51
1:A:222:ARG:NH1	1:A:227:GLN:OE1	2.44	0.50
1:C:59:VAL:HG22	1:C:70:LEU:HD21	1.91	0.50
1:C:325:HIS:HE1	1:D:112:THR:C	2.19	0.50
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:D:231:VAL:HG12	1:D:250:ILE:HG21	1.93	0.50
1:E:234:LEU:O	1:E:238:ILE:HD12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:HIS:CG	1:D:5:HIS:N	2.79	0.50
1:E:268:GLY:O	1:E:271:ALA:HB3	2.12	0.50
1:H:0:SER:HA	1:H:2:PRO:HD3	1.94	0.50
1:C:146:ILE:HG22	1:C:151:PHE:HB2	1.94	0.50
1:C:325:HIS:CE1	1:D:112:THR:HB	2.47	0.50
1:E:0:SER:H	1:E:1:MET:CB	2.25	0.50
1:C:100:GLU:O	1:C:102:PRO:HD3	2.12	0.50
1:C:300:SER:C	1:C:301:GLN:HE21	2.20	0.50
1:F:181:GLU:C	1:F:183:VAL:H	2.20	0.50
1:C:134:ASP:H	1:C:138:GLN:NE2	2.09	0.49
1:D:5:HIS:CE1	1:D:8:ARG:HH21	2.30	0.49
1:H:167:MET:HE1	1:H:242:LEU:CD2	2.33	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:A:327:HIS:O	1:A:328:VAL:O	2.30	0.49
1:F:327:HIS:O	1:F:328:VAL:O	2.30	0.49
1:B:228:LYS:O	1:B:232:ILE:HG23	2.12	0.49
1:C:222:ARG:HB2	1:C:222:ARG:NH1	2.20	0.49
1:D:275:LEU:HB3	1:D:281:VAL:HG23	1.94	0.49
1:G:20:PRO:HG2	1:G:39:ARG:HB2	1.94	0.49
1:G:258:ALA:HB3	1:G:265:ASN:HB3	1.93	0.49
1:C:325:HIS:HE1	1:D:112:THR:HB	1.77	0.49
1:G:134:ASP:H	1:G:138:GLN:NE2	2.09	0.49
1:E:169:TYR:HB3	1:E:202:LEU:HD22	1.95	0.49
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:C:146:ILE:CG2	1:C:151:PHE:HD1	2.26	0.48
1:D:2:PRO:O	1:D:244:LEU:HD21	2.13	0.48
1:D:325:HIS:CG	1:D:326:PRO:N	2.72	0.48
1:F:199:HIS:HD2	1:F:199:HIS:O	1.96	0.48
1:A:258:ALA:HB3	1:A:265:ASN:HB3	1.95	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:H:51:LLP:OP1	1:H:195:SER:N	2.46	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:CD1	1:G:6:LEU:N	2.60	0.48
1:H:231:VAL:HG12	1:H:250:ILE:HD12	1.96	0.48
1:B:43:THR:HG22	1:B:45:ILE:H	1.79	0.48
1:H:4:HIS:CG	1:H:5:HIS:N	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:HIS:O	1:H:6:LEU:C	2.55	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:HD2	1:B:199:HIS:O	1.97	0.47
1:A:3:LEU:O	1:A:6:LEU:CB	2.62	0.47
1:B:146:ILE:CG2	1:B:151:PHE:HD1	2.26	0.47
1:E:7:THR:O	1:E:7:THR:OG1	2.30	0.47
1:F:105:THR:OG1	1:F:328:VAL:CG1	2.53	0.47
1:F:230:LYS:O	1:F:234:LEU:HD12	2.14	0.47
1:D:51:LLP:HA	1:D:51:LLP:HD2	1.76	0.47
1:B:51:LLP:OP1	1:B:195:SER:N	2.47	0.47
1:A:112:THR:HB	1:B:325:HIS:CE1	2.49	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:G:40:ASP:OD2	1:G:53:ARG:NE	2.37	0.47
1:A:100:GLU:O	1:A:102:PRO:HD3	2.14	0.47
1:D:167:MET:HE1	1:D:242:LEU:HG	1.96	0.47
1:D:189:VAL:HG22	1:D:311:LEU:HB3	1.96	0.47
1:E:4:HIS:CE1	1:E:5:HIS:HD2	2.31	0.47
1:G:7:THR:HG23	1:G:7:THR:O	2.15	0.47
1:G:76:ILE:HB	1:G:110:TYR:CE1	2.50	0.47
1:C:142:LEU:O	1:C:146:ILE:HG12	2.15	0.47
1:E:51:LLP:HD2	1:E:51:LLP:HA	1.71	0.47
1:E:227:GLN:HG2	1:E:252:LEU:HD13	1.96	0.47
1:E:250:ILE:O	1:E:250:ILE:HD12	2.15	0.47
1:H:227:GLN:HG2	1:H:252:LEU:HD22	1.95	0.47
1:A:1:MET:C	1:A:3:LEU:N	2.71	0.47
1:C:189:VAL:HG22	1:C:311:LEU:HB3	1.97	0.47
1:E:43:THR:HB	1:E:48:GLY:HA3	1.97	0.47
1:A:112:THR:C	1:B:325:HIS:HE1	2.22	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:B:186:LEU:HD12	1:B:186:LEU:C	2.40	0.46
1:F:199:HIS:C	1:F:199:HIS:CD2	2.92	0.46
1:E:117:LEU:HD13	1:F:325:HIS:CE1	2.50	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:E:327:HIS:O	1:E:328:VAL:C	2.59	0.46
1:H:4:HIS:O	1:H:6:LEU:N	2.48	0.46
1:A:43:THR:HB	1:A:48:GLY:HA3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:ALA:HB3	1:E:265:ASN:HB3	1.96	0.46
1:A:51:LLP:HA	1:A:51:LLP:HD2	1.77	0.46
1:B:189:VAL:HG22	1:B:311:LEU:HB3	1.97	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:H:4:HIS:O	1:H:5:HIS:C	2.58	0.46
1:B:140:GLN:HE21	1:B:144:THR:HG23	1.81	0.46
1:E:51:LLP: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:LLP:C4'	2:A:401:PO4:O3	2.63	0.45
1:C:171:GLU:O	1:C:174:LEU:HB3	2.16	0.45
1:E:327:HIS:ND1	1:E:327:HIS:C	2.73	0.45
1:G:76:ILE:HB	1:G:110:TYR:HE1	1.80	0.45
1:F:51:LLP:HA	1:F:51:LLP:HD2	1.65	0.45
1:F:171:GLU:O	1:F:174:LEU:HB3	2.16	0.45
1:G:274:LEU:O	1:G:278:LEU:HB2	2.16	0.45
1:B:199:HIS:CD2	1:B:199:HIS:C	2.94	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:D:62:ALA:HA	1:D:154:TYR:CD1	2.52	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:B:251:HIS:C	1:B:252:LEU:HG	2.42	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
1:A:3:LEU:HA	1:A:3:LEU:HD13	1.44	0.45
1:C:162:SER:O	1:C:163:ALA:C	2.60	0.45
1:A:194:GLY:C	1:A:196:ALA:N	2.74	0.44
1:C:76:ILE:HB	1:C:110:TYR:HE1	1.82	0.44
1:C:258:ALA:HB3	1:C:265:ASN:HB3	1.98	0.44
1:E:5:HIS:O	1:E:6:LEU:C	2.56	0.44
1:E:189:VAL:HG22	1:E:311:LEU:HB3	1.99	0.44
1:E:325:HIS:HE1	1:F:112:THR:HB	1.83	0.44
1:H:194:GLY:C	1:H:196:ALA:N	2.76	0.44
1:A:322:PHE:CE2	1:B:118:LEU:HD11	2.52	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:E:175:GLU:O	1:E:179:GLN:CG	2.65	0.44
1:E:325:HIS:CD2	1:E:325:HIS:C	2.92	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:230:LYS:O	1:G:234:LEU:HD12	2.18	0.44
1:H:3:LEU:N	1:H:3:LEU:CD1	2.77	0.44
1:H:43:THR:HG22	1:H:45:ILE:H	1.81	0.44
1:F:156:ILE:HA	1:F:157:PRO:HD2	1.85	0.44
1:G:52:LEU:CD1	1:G:83:GLN:HE21	2.27	0.44
1:B:295:LEU:C	1:B:295:LEU:HD23	2.43	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:A:274:LEU:O	1:A:278:LEU:HB2	2.18	0.44
1:B:43:THR:HB	1:B:48:GLY:HA3	2.00	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:78:SER:OG	1:B:81:VAL:HG23	2.17	0.44
1:F:134:ASP:H	1:F:138:GLN:NE2	2.15	0.44
1:B:14:PHE:CZ	1:B:87:VAL:HG13	2.52	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: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:327:HIS:ND1	1:F:327:HIS:C	2.76	0.44
1:F:221:SER:HB3	1:F:261:TYR:HB2	2.00	0.43
1:B:51:LLP:HD2	1:B:51:LLP:HA	1.72	0.43
1:D:263:VAL:HA	1:D:264:PRO:HD3	1.86	0.43
1:A:3:LEU:N	1:A:3:LEU:CD2	2.81	0.43
1:F:20:PRO:HG2	1:F:39:ARG:HB2	2.00	0.43
1:C:43:THR:HG22	1:C:45:ILE:H	1.83	0.43
1:H:11:ARG:NH1	1:H:11:ARG:CG	2.65	0.43
1:H:51:LLP:HD2	1:H:51:LLP:HA	1.76	0.43
1:A:5:HIS:CE1	1:A:8:ARG:NE	2.79	0.43
1:C:51:LLP:HD2	1:C:51:LLP:HA	1.68	0.43
1:G:324:TYR:O	1:G:325:HIS:C	2.54	0.43
1:A:14:PHE:CD2	1:A:56:GLU:HG2	2.53	0.43
1:D:268:GLY:O	1:D:271:ALA:HB3	2.19	0.43
1:G:189:VAL:HG22	1:G:311:LEU:HB3	2.00	0.43
1:B:45:ILE:O	1:B:46:ALA:C	2.61	0.43
1:C:45:ILE:HB	1:C:52:LEU:HD11	2.00	0.43
1:D:43:THR:HB	1:D:48:GLY:HA3	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:41:ASP:CG	1:D:314:HIS:ND1	2.77	0.43
1:F:33:ARG:HH21	1:F:299:ILE:HG23	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:30:TYR:CD2	1:H:31:LEU:CD1	3.02	0.43
1:A:325:HIS:C	1:A:325:HIS:HD1	2.27	0.43
1:C:199:HIS:HE1	1:C:252:LEU:HD12	1.82	0.43
1:G:40:ASP:CG	1:G:53:ARG:HH11	2.27	0.43
1:G:43:THR:HG22	1:G:45:ILE:H	1.84	0.43
1:H:3:LEU:O	1:H:6:LEU:N	2.44	0.43
1:H:167:MET:CE	1:H:242:LEU:HD21	2.34	0.43
1:C:76:ILE:HB	1:C:110:TYR:CE1	2.54	0.43
1:F:34:GLU:OE2	1:H:-1:ALA:CB	2.67	0.43
1:F:43:THR:HG21	1:F:52:LEU:HD22	2.01	0.43
1:F:324:TYR:C	1:F:325:HIS:O	2.62	0.43
1:G:21:LEU:HB2	1:G:179:GLN:OE1	2.19	0.43
1:A:98:LEU:HD23	1:A:132:LEU:CD2	2.49	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:G:263:VAL:HA	1:G:264:PRO:HD3	1.88	0.42
1:C:230:LYS:O	1:C:234:LEU:HD12	2.19	0.42
1:A:51:LLP: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:21:LEU:HB2	1:A:179:GLN:OE1	2.19	0.42
1:A:167:MET:SD	1:A:242:LEU:HD11	2.59	0.42
1:C:45:ILE:O	1:C:46:ALA:C	2.62	0.42
1:C:59:VAL:HG21	1:C:87:VAL:HG11	2.01	0.42
1:C:145:ARG:O	1:C:149:GLN:HG3	2.19	0.42
1:C:199:HIS:HD2	1:C:199:HIS:O	2.03	0.42
1:D:43:THR:HG22	1:D:45:ILE:H	1.84	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:F:295:LEU:HD23	1:F:295:LEU:C	2.44	0.42
1:A:194:GLY:C	1:A:196:ALA:H	2.28	0.42
1:A:322:PHE:HE2	1:B:118:LEU:HD11	1.83	0.42
1:C:210:MET:HB3	1:C:213:VAL:HG23	2.02	0.42
1:D:15:ILE:CD1	1:D:53:ARG:HD3	2.47	0.42
1:D:51:LLP:OP1	1:D:195:SER:OG	2.33	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:H:2:PRO:HG2	1:H:3:LEU:HD12	2.02	0.42
1:A:3:LEU:O	1:A:4:HIS:C	2.63	0.42
1:A:286:VAL:HG13	1:A:287:TYR:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LLP:OP1	1:B:195:SER:OG	2.37	0.42
1:F:257:PHE:HD1	1:F:260:GLY:HA2	1.84	0.42
1:F:275:LEU:HB3	1:F:281:VAL:HG23	2.02	0.42
1:G:199:HIS:CD2	1:G:199:HIS:C	2.96	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:C:146:ILE:O	1:C:149:GLN:N	2.52	0.42
1:D:174:LEU:HD13	1:D:209:LEU:CD1	2.50	0.42
1:D:258:ALA:HB3	1:D:265:ASN:HB3	1.98	0.42
1:E:194:GLY:C	1:E:196:ALA:N	2.78	0.42
1:F:51:LLP:H2'2	1:F:315:THR:C	2.45	0.42
1:G:219:THR:HG1	1:G:254:ASP:HA	1.78	0.42
1:H:191:VAL:O	1:H:217:GLY:HA2	2.19	0.42
1:A:242:LEU:HD23	1:A:242:LEU:HA	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:A:26:ARG:NH1	1:B:89:ALA:O	2.52	0.41
1:A:64:ARG:HG2	1:D:64:ARG:NE	2.35	0.41
1:E:3:LEU:HD22	1:E:209:LEU:HD11	2.02	0.41
1:E:100:GLU:O	1:E:102:PRO:HD3	2.20	0.41
1:G:114:GLY:O	1:G:118:LEU:HD12	2.19	0.41
1:E:41:ASP:CG	1:E:314:HIS:ND1	2.77	0.41
1:G:257:PHE:HD1	1:G:260:GLY:HA2	1.84	0.41
1:H:1:MET:N	1:H:2:PRO:HD3	2.31	0.41
1:H:55:LEU:HA	1:H:58:LEU:HB2	2.03	0.41
1:H:325:HIS:CG	1:H:326:PRO:CD	3.02	0.41
1:A:89:ALA:HB1	1:B:277:SER:O	2.19	0.41
1:G:152:ARG:HE	1:G:152:ARG:HB3	1.46	0.41
1:A:189:VAL:HG22	1:A:311:LEU:HB3	2.03	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:D:231:VAL:CG1	1:D:250:ILE:HG21	2.51	0.41
1:G:164:LEU:O	1:G:167:MET:HB2	2.21	0.41
1:H:11:ARG:HH11	1:H:11:ARG:CG	1.97	0.41
1:H:76:ILE:HB	1:H:110:TYR:HE1	1.85	0.41
1:H:221:SER:HB3	1:H:261:TYR:HB2	2.02	0.41
1:B:171:GLU:O	1:B:174:LEU:HB3	2.21	0.41
1:D:1:MET:HB3	1:D:4:HIS:HB3	2.02	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:D:98:LEU:HD13	1:D:142:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:ILE:HA	1:G:157:PRO:HD2	1.84	0.41
1:H:210:MET:HB3	1:H:213:VAL:HG23	2.03	0.41
1:H:242:LEU:HD23	1:H:242:LEU:HA	1.84	0.41
1:H:295:LEU:C	1:H:295:LEU:HD23	2.45	0.41
1:A:221:SER:HB3	1:A:261:TYR:HB2	2.03	0.41
1:D:229:PRO:O	1:D:232:ILE:HG22	2.21	0.41
1:F:194:GLY:C	1:F:196:ALA:N	2.79	0.41
1:G:41:ASP:CG	1:G:314:HIS:ND1	2.79	0.41
1:H:4:HIS:O	1:H:7:THR:HG22	2.21	0.41
1:A:295:LEU:HD23	1:A:295:LEU:C	2.46	0.41
1:B:67:ALA:CB	1:B:153:PRO:O	2.69	0.41
1:B:178:GLN:O	1:B:179:GLN:C	2.62	0.41
1:C:31:LEU:HD12	1:C:35:ILE:CD1	2.51	0.41
1:C:199:HIS:CD2	1:C:199:HIS:C	2.97	0.41
1:C:263:VAL:HA	1:C:264:PRO:HD3	1.89	0.41
1:D:194:GLY:C	1:D:196:ALA:N	2.78	0.40
1:H:51:LLP:OP1	1:H:195:SER:OG	2.36	0.40
1:H:194:GLY:C	1:H:196:ALA:H	2.28	0.40
1:A:173:ALA:HB1	1:A:206:LEU:HD12	2.02	0.40
1:B:162:SER:O	1:B:163:ALA:C	2.64	0.40
1:C:19:THR:OG1	1:C:38:LYS:HE3	2.21	0.40
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: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:D:162:SER:O	1:D:163:ALA:C	2.62	0.40
1:E:-1:ALA:O	1:G:23:TYR:CE2	2.73	0.40
1:G:112:THR:HB	1:H:325:HIS:CE1	2.55	0.40
1:G:194:GLY:C	1:G:196:ALA:N	2.78	0.40
1:A:156:ILE:HA	1:A:157:PRO:HD2	1.89	0.40
1:A:166:ALA:HB3	1:A:238:ILE:HD11	2.03	0.40
1:A:228:LYS:HE2	1:A:228:LYS:HB3	1.96	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:G:51:LLP:HA	1:G:51:LLP:HD2	1.63	0.40
1:E:134:ASP:H	1:E:138:GLN:NE2	2.17	0.40
1:H:6:LEU:CD2	1:H:167:MET:CE	2.99	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%)	4	24
1	B	320/342 (94%)	288 (90%)	25 (8%)	7 (2%)	5	26
1	C	320/342 (94%)	292 (91%)	22 (7%)	6 (2%)	6	28
1	D	326/342 (95%)	293 (90%)	26 (8%)	7 (2%)	5	26
1	E	327/342 (96%)	292 (89%)	22 (7%)	13 (4%)	2	15
1	F	313/342 (92%)	277 (88%)	28 (9%)	8 (3%)	4	23
1	G	321/342 (94%)	285 (89%)	29 (9%)	7 (2%)	5	26
1	H	328/342 (96%)	297 (90%)	22 (7%)	9 (3%)	4	22
All	All	2582/2736 (94%)	2321 (90%)	196 (8%)	65 (2%)	4	23

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	237 (94%)	14 (6%)	19	47
1	B	227/266 (85%)	204 (90%)	23 (10%)	7	26
1	C	233/266 (88%)	217 (93%)	16 (7%)	14	41
1	D	252/266 (95%)	234 (93%)	18 (7%)	13	40
1	E	248/266 (93%)	230 (93%)	18 (7%)	13	39
1	F	203/266 (76%)	192 (95%)	11 (5%)	20	49
1	G	227/266 (85%)	208 (92%)	19 (8%)	10	34
1	H	247/266 (93%)	226 (92%)	21 (8%)	10	33
All	All	1888/2128 (89%)	1748 (93%)	140 (7%)	13	38

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	15	ILE
1	A	52	LEU
1	A	147	GLU
1	A	193	SER
1	A	202	LEU
1	A	232	ILE
1	A	234	LEU
1	A	245	THR

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Mol	Chain	Res	Type
1	A	247	THR
1	A	275	LEU
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	147	GLU
1	B	170	VAL
1	B	171	GLU
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	231	VAL
1	B	232	ILE
1	B	234	LEU
1	B	245	THR
1	B	269	MET
1	B	288	THR
1	B	301	GLN
1	B	303	ARG
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	288	THR
1	C	301	GLN

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Mol	Chain	Res	Type
1	C	303	ARG
1	C	327	HIS
1	D	6	LEU
1	D	11	ARG
1	D	15	ILE
1	D	52	LEU
1	D	174	LEU
1	D	179	GLN
1	D	193	SER
1	D	202	LEU
1	D	230	LYS
1	D	232	ILE
1	D	234	LEU
1	D	245	THR
1	D	249	ASP
1	D	250	ILE
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	52	LEU
1	E	142	LEU
1	E	144	THR
1	E	145	ARG
1	E	178	GLN
1	E	193	SER
1	E	202	LEU
1	E	232	ILE
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	170	VAL

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Mol	Chain	Res	Type
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	G	6	LEU
1	G	11	ARG
1	G	15	ILE
1	G	52	LEU
1	G	71	ILE
1	G	127	GLU
1	G	144	THR
1	G	171	GLU
1	G	193	SER
1	G	202	LEU
1	G	234	LEU
1	G	241	GLN
1	G	245	THR
1	G	249	ASP
1	G	269	MET
1	G	288	THR
1	G	301	GLN
1	G	315	THR
1	G	327	HIS
1	H	1	MET
1	H	6	LEU
1	H	8	ARG
1	H	11	ARG
1	H	52	LEU
1	H	53	ARG
1	H	71	ILE
1	H	144	THR
1	H	145	ARG
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	250	ILE

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Mol	Chain	Res	Type
1	H	269	MET
1	H	284	ASP
1	H	288	THR
1	H	301	GLN
1	H	327	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) 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	B	80	HIS
1	B	83	GLN
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	94	HIS
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
1	D	83	GLN
1	D	138	GLN
1	D	178	GLN
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	236	GLN

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Mol	Chain	Res	Type
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	140	GLN
1	G	301	GLN
1	G	325	HIS
1	H	80	HIS
1	H	83	GLN
1	H	138	GLN
1	H	140	GLN
1	H	208	HIS
1	H	241	GLN
1	H	301	GLN
1	H	325	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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	LLP	A	51	1	23,24,25	1.80	6 (26%)	25,32,34	1.31	3 (12%)
1	LLP	F	51	1	23,24,25	1.76	6 (26%)	25,32,34	1.31	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	C	51	1	23,24,25	1.78	4 (17%)	25,32,34	1.38	4 (16%)
1	LLP	D	51	1	23,24,25	1.77	5 (21%)	25,32,34	1.40	4 (16%)
1	LLP	B	51	1	23,24,25	1.73	5 (21%)	25,32,34	1.42	5 (20%)
1	LLP	H	51	1	23,24,25	1.75	5 (21%)	25,32,34	1.59	8 (32%)
1	LLP	G	51	1	23,24,25	1.73	4 (17%)	25,32,34	1.45	3 (12%)
1	LLP	E	51	1	23,24,25	1.73	5 (21%)	25,32,34	1.45	3 (12%)

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	LLP	A	51	1	-	6/16/17/19	0/1/1/1
1	LLP	F	51	1	-	8/16/17/19	0/1/1/1
1	LLP	C	51	1	-	5/16/17/19	0/1/1/1
1	LLP	D	51	1	-	5/16/17/19	0/1/1/1
1	LLP	B	51	1	-	8/16/17/19	0/1/1/1
1	LLP	H	51	1	-	6/16/17/19	0/1/1/1
1	LLP	G	51	1	-	5/16/17/19	0/1/1/1
1	LLP	E	51	1	-	6/16/17/19	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	51	LLP	O3-C3	-5.85	1.23	1.36
1	A	51	LLP	O3-C3	-5.81	1.23	1.36
1	B	51	LLP	O3-C3	-5.55	1.24	1.36
1	G	51	LLP	O3-C3	-5.53	1.24	1.36
1	D	51	LLP	O3-C3	-5.42	1.24	1.36
1	H	51	LLP	O3-C3	-5.34	1.24	1.36
1	E	51	LLP	O3-C3	-5.32	1.24	1.36
1	F	51	LLP	O3-C3	-5.29	1.24	1.36
1	H	51	LLP	C4-C4'	3.21	1.53	1.46
1	F	51	LLP	C2-N1	3.15	1.39	1.33
1	E	51	LLP	C2-N1	3.13	1.39	1.33
1	B	51	LLP	C2-N1	3.13	1.39	1.33
1	D	51	LLP	C4-C4'	3.11	1.53	1.46
1	H	51	LLP	C2-N1	3.08	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	51	LLP	C2-N1	2.89	1.39	1.33
1	F	51	LLP	C4-C4'	2.82	1.52	1.46
1	D	51	LLP	C2-N1	2.75	1.38	1.33
1	E	51	LLP	C4-C4'	2.74	1.52	1.46
1	F	51	LLP	C4'-NZ	2.72	1.36	1.27
1	A	51	LLP	C3-C2	-2.64	1.38	1.41
1	G	51	LLP	C4-C4'	2.61	1.52	1.46
1	C	51	LLP	C4'-NZ	2.59	1.35	1.27
1	G	51	LLP	C4'-NZ	2.58	1.35	1.27
1	D	51	LLP	C4'-NZ	2.56	1.35	1.27
1	H	51	LLP	C4'-NZ	2.54	1.35	1.27
1	A	51	LLP	C4-C4'	2.48	1.51	1.46
1	B	51	LLP	C4'-NZ	2.45	1.35	1.27
1	B	51	LLP	C4-C4'	2.45	1.51	1.46
1	E	51	LLP	C4'-NZ	2.40	1.35	1.27
1	A	51	LLP	P-OP2	-2.37	1.46	1.54
1	C	51	LLP	C4-C4'	2.32	1.51	1.46
1	A	51	LLP	C2-N1	2.30	1.38	1.33
1	F	51	LLP	CE-NZ	2.27	1.51	1.46
1	E	51	LLP	P-OP2	-2.23	1.46	1.54
1	A	51	LLP	C4'-NZ	2.20	1.34	1.27
1	B	51	LLP	C6-N1	2.20	1.38	1.34
1	C	51	LLP	C2-N1	2.18	1.37	1.33
1	D	51	LLP	P-OP2	-2.14	1.46	1.54
1	F	51	LLP	C6-N1	2.13	1.38	1.34
1	H	51	LLP	P-OP2	-2.06	1.47	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	51	LLP	C5-C6-N1	-2.94	119.05	123.83
1	D	51	LLP	C5-C4-C4'	2.84	125.86	121.47
1	H	51	LLP	C5-C4-C4'	2.81	125.81	121.47
1	G	51	LLP	C5-C6-N1	-2.77	119.32	123.83
1	H	51	LLP	C5-C6-N1	-2.75	119.36	123.83
1	F	51	LLP	OP3-P-OP2	2.70	117.92	107.80
1	G	51	LLP	OP3-P-OP2	2.65	117.73	107.80
1	D	51	LLP	C3-C4-C4'	-2.62	115.67	120.40
1	C	51	LLP	OP3-P-OP2	2.61	117.60	107.80
1	D	51	LLP	C5-C6-N1	-2.60	119.61	123.83
1	A	51	LLP	C5-C6-N1	-2.57	119.66	123.83
1	E	51	LLP	C2'-C2-C3	-2.53	117.84	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	51	LLP	C3-C4-C4'	-2.52	115.86	120.40
1	H	51	LLP	C2'-C2-C3	-2.50	117.87	120.80
1	B	51	LLP	OP3-P-OP4	-2.41	100.39	106.67
1	B	51	LLP	OP3-P-OP2	2.36	116.64	107.80
1	B	51	LLP	C5'-C5-C6	-2.35	115.54	119.36
1	H	51	LLP	C4-C3-C2	-2.34	118.83	120.14
1	B	51	LLP	C5-C6-N1	-2.31	120.08	123.83
1	F	51	LLP	C5-C6-N1	-2.31	120.08	123.83
1	B	51	LLP	OP4-P-OP1	-2.27	100.31	106.44
1	C	51	LLP	C5-C6-N1	-2.26	120.16	123.83
1	G	51	LLP	OP2-P-OP4	-2.26	100.78	106.67
1	C	51	LLP	OP3-P-OP4	-2.26	100.79	106.67
1	A	51	LLP	OP4-P-OP1	-2.21	100.46	106.44
1	E	51	LLP	C4-C3-C2	-2.20	118.91	120.14
1	D	51	LLP	OP3-P-OP4	-2.19	100.97	106.67
1	H	51	LLP	OP3-P-OP2	2.16	115.91	107.80
1	F	51	LLP	OP3-P-OP4	-2.15	101.05	106.67
1	C	51	LLP	OP3-P-OP1	2.14	119.19	110.83
1	H	51	LLP	O3-C3-C2	2.03	121.78	117.58
1	A	51	LLP	C3-C4-C4'	-2.02	116.75	120.40
1	H	51	LLP	C6-C5-C4	2.01	121.66	118.21

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	51	LLP	C4-C4'-NZ-CE
1	A	51	LLP	C5'-OP4-P-OP2
1	A	51	LLP	C5'-OP4-P-OP3
1	B	51	LLP	C4-C4'-NZ-CE
1	B	51	LLP	C5'-OP4-P-OP1
1	B	51	LLP	C5'-OP4-P-OP2
1	B	51	LLP	C5'-OP4-P-OP3
1	C	51	LLP	C4-C4'-NZ-CE
1	C	51	LLP	C5'-OP4-P-OP3
1	D	51	LLP	C4-C4'-NZ-CE
1	D	51	LLP	C5'-OP4-P-OP2
1	D	51	LLP	C5'-OP4-P-OP3
1	E	51	LLP	C4-C4'-NZ-CE
1	E	51	LLP	C5'-OP4-P-OP2
1	E	51	LLP	C5'-OP4-P-OP3
1	F	51	LLP	C4-C4'-NZ-CE

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Mol	Chain	Res	Type	Atoms
1	F	51	LLP	C5'-OP4-P-OP1
1	F	51	LLP	C5'-OP4-P-OP2
1	F	51	LLP	C5'-OP4-P-OP3
1	G	51	LLP	C4-C4'-NZ-CE
1	G	51	LLP	C5'-OP4-P-OP2
1	G	51	LLP	C5'-OP4-P-OP3
1	H	51	LLP	C4-C4'-NZ-CE
1	H	51	LLP	C5'-OP4-P-OP2
1	H	51	LLP	C5'-OP4-P-OP3
1	H	51	LLP	C5'-OP4-P-OP1
1	A	51	LLP	CA-CB-CG-CD
1	B	51	LLP	CA-CB-CG-CD
1	E	51	LLP	CA-CB-CG-CD
1	F	51	LLP	CA-CB-CG-CD
1	G	51	LLP	CA-CB-CG-CD
1	A	51	LLP	CE-CD-CG-CB
1	C	51	LLP	CA-CB-CG-CD
1	E	51	LLP	CE-CD-CG-CB
1	B	51	LLP	CE-CD-CG-CB
1	D	51	LLP	CE-CD-CG-CB
1	C	51	LLP	C5'-OP4-P-OP2
1	D	51	LLP	CA-CB-CG-CD
1	H	51	LLP	CE-CD-CG-CB
1	H	51	LLP	CA-CB-CG-CD
1	F	51	LLP	CE-CD-CG-CB
1	C	51	LLP	CE-CD-CG-CB
1	G	51	LLP	CE-CD-CG-CB
1	B	51	LLP	C6-C5-C5'-OP4
1	A	51	LLP	C5'-OP4-P-OP1
1	E	51	LLP	C5'-OP4-P-OP1
1	B	51	LLP	C4-C5-C5'-OP4
1	F	51	LLP	C4-C5-C5'-OP4
1	F	51	LLP	C3-C4-C4'-NZ

There are no ring outliers.

8 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	51	LLP	6	0
1	F	51	LLP	4	0
1	C	51	LLP	4	0
1	D	51	LLP	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	51	LLP	5	0
1	H	51	LLP	5	0
1	G	51	LLP	4	0
1	E	51	LLP	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	401	-	4,4,4	0.84	0	6,6,6	0.83	0
2	PO4	A	401	-	4,4,4	1.26	0	6,6,6	0.99	0
2	PO4	B	401	-	4,4,4	0.86	0	6,6,6	0.71	0
2	PO4	E	401	-	4,4,4	1.07	0	6,6,6	1.26	1 (16%)
2	PO4	F	401	-	4,4,4	0.97	0	6,6,6	0.51	0
2	PO4	G	401	-	4,4,4	0.87	0	6,6,6	0.83	0
2	PO4	D	401	-	4,4,4	0.66	0	6,6,6	1.02	0
2	PO4	H	401	-	4,4,4	0.88	0	6,6,6	0.75	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	PO4	O4-P-O1	-2.77	101.17	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	PO4	2	0
2	A	401	PO4	2	0
2	E	401	PO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	329/342 (96%)	0.25	7 (2%) 63 44	53, 68, 80, 87	0
1	B	322/342 (94%)	0.32	12 (3%) 45 31	55, 68, 81, 86	1 (0%)
1	C	322/342 (94%)	0.25	9 (2%) 55 36	55, 68, 81, 87	0
1	D	328/342 (95%)	0.27	6 (1%) 67 49	53, 68, 80, 86	0
1	E	329/342 (96%)	0.25	6 (1%) 67 49	53, 68, 80, 86	0
1	F	317/342 (92%)	0.65	19 (5%) 27 19	55, 68, 80, 88	0
1	G	323/342 (94%)	0.45	5 (1%) 72 53	55, 68, 81, 86	0
1	H	330/342 (96%)	0.29	5 (1%) 72 53	54, 68, 81, 87	0
All	All	2600/2736 (95%)	0.34	69 (2%) 56 37	53, 68, 80, 88	1 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	208	HIS	5.6
1	C	6	LEU	4.6
1	B	9	PHE	3.9
1	F	193	SER	3.4
1	B	7	THR	3.3
1	G	226	GLU	3.3
1	B	182	GLU	3.2
1	A	182	GLU	3.1
1	A	-1	ALA	3.1
1	B	6	LEU	3.0
1	F	14	PHE	3.0
1	D	16	GLY	3.0
1	A	6	LEU	3.0
1	A	269	MET	3.0
1	F	212	ASP	2.8
1	H	182	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	182	GLU	2.8
1	F	164	LEU	2.8
1	F	247	THR	2.8
1	E	269	MET	2.7
1	G	5	HIS	2.7
1	F	8	ARG	2.7
1	C	245	THR	2.6
1	B	226	GLU	2.6
1	C	328	VAL	2.6
1	D	6	LEU	2.6
1	E	-1	ALA	2.6
1	D	7	THR	2.6
1	B	10	PRO	2.5
1	C	7	THR	2.5
1	H	104	GLY	2.5
1	F	64	ARG	2.5
1	D	239	ALA	2.5
1	F	157	PRO	2.5
1	B	328	VAL	2.5
1	E	178	GLN	2.4
1	B	207	GLU	2.4
1	A	30	TYR	2.4
1	B	206	LEU	2.3
1	F	70	LEU	2.3
1	H	107	ALA	2.3
1	C	215	LEU	2.3
1	F	5	HIS	2.3
1	D	30	TYR	2.3
1	G	182	GLU	2.3
1	A	325	HIS	2.3
1	F	192	ALA	2.2
1	F	95	CYS	2.2
1	C	212	ASP	2.2
1	G	328	VAL	2.2
1	A	13	GLU	2.2
1	C	249	ASP	2.2
1	H	7	THR	2.2
1	H	1	MET	2.2
1	C	243	ALA	2.2
1	F	158	VAL	2.1
1	B	179	GLN	2.1
1	F	328	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	280	GLY	2.1
1	E	23	TYR	2.1
1	D	327	HIS	2.1
1	F	206	LEU	2.1
1	F	147	GLU	2.1
1	F	94	HIS	2.1
1	B	173	ALA	2.1
1	F	220	VAL	2.0
1	F	154	TYR	2.0
1	B	227	GLN	2.0
1	G	7	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	LLP	B	51	24/25	0.93	0.11	55,56,57,58	0
1	LLP	G	51	24/25	0.94	0.11	55,56,57,58	0
1	LLP	H	51	24/25	0.94	0.10	55,56,57,58	0
1	LLP	F	51	24/25	0.95	0.10	55,57,57,58	0
1	LLP	C	51	24/25	0.95	0.08	55,56,57,58	0
1	LLP	E	51	24/25	0.95	0.08	55,56,57,58	0
1	LLP	A	51	24/25	0.97	0.09	55,56,57,58	0
1	LLP	D	51	24/25	0.97	0.09	55,56,57,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	A	401	5/5	0.91	0.14	81,81,82,83	0
2	PO4	G	401	5/5	0.91	0.14	108,108,109,109	0
2	PO4	B	401	5/5	0.92	0.17	123,123,124,124	0
2	PO4	F	401	5/5	0.93	0.15	154,154,155,155	0
2	PO4	D	401	5/5	0.93	0.10	83,85,85,85	0
2	PO4	E	401	5/5	0.95	0.11	75,76,76,77	0
2	PO4	C	401	5/5	0.96	0.10	97,98,98,98	0
2	PO4	H	401	5/5	0.96	0.12	112,113,113,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.