Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 08:14 PM EDT

PDB ID	:	1USY
Title	:	ATP phosphoribosyl transferase (HisG:HisZ) complex from Thermotoga maritima
Authors	:	Vega, M.C.; Fernandez, F.J.; Murphy, G.E.; Zou, P.; Popov, A.; Wilmanns, M.
Deposited on	:	2003-12-01
Resolution	:	2.52 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 (i) 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 (i)) were used in the production of this report:

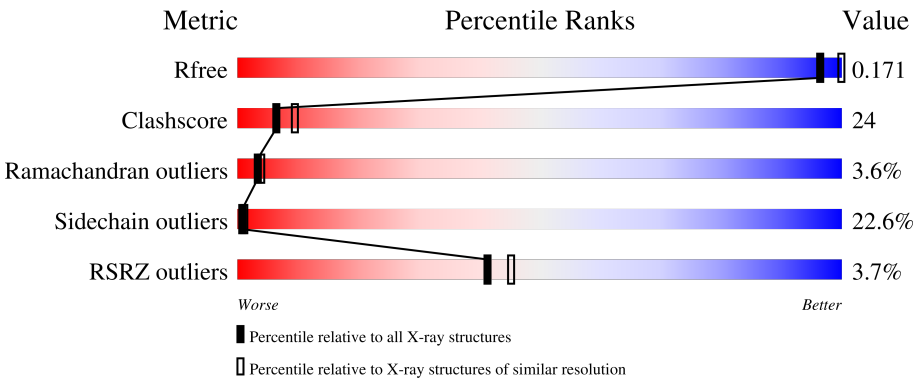
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.52 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}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 <=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	275	2% 54% 32% 12% •
1	B	275	4% 52% 35% 12% •
1	D	275	5% 45% 42% 12% •
2	C	275	5% 56% 28% 13% •
3	E	208	5% 45% 40% 11% •

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Mol	Chain	Length	Quality of chain
3	F	208	2% 53% 32% 11%
3	G	208	5% 50% 36% 12%
4	H	208	% 48% 41% 8%

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
5	HIS	C	1275	-	-	X	-
5	HIS	E	1204	-	-	X	-
5	HIS	E	1205	-	-	X	-
5	HIS	F	1204	-	-	X	X
5	HIS	G	1206	-	-	X	-
5	HIS	H	1203	-	-	X	-
5	HIS	H	1204	-	-	X	-
6	PO4	E	1202	-	-	X	-
6	PO4	H	1202	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15636 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 ATP PHOSPHORIBOSYLTRANSFERASE REGULATORY SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	2210	1423	353	429	5	14	0	0
1	B	275	2210	1423	353	429	5	17	0	0
1	D	274	2202	1418	352	428	4	11	0	0

- Molecule 2 is a protein called ATP PHOSPHORIBOSYLTRANSFERASE REGULATORY SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	275	2206	1422	353	427	4	23	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	68	GLU	ASP	conflict	UNP Q9X0D3
C	134	LEU	VAL	conflict	UNP Q9X0D3

- Molecule 3 is a protein called ATP PHOSPHORIBOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	202	1599	1027	273	291	8	7	0	1
3	F	203	1605	1030	274	293	8	2	0	1
3	G	204	1613	1034	276	295	8	0	0	1

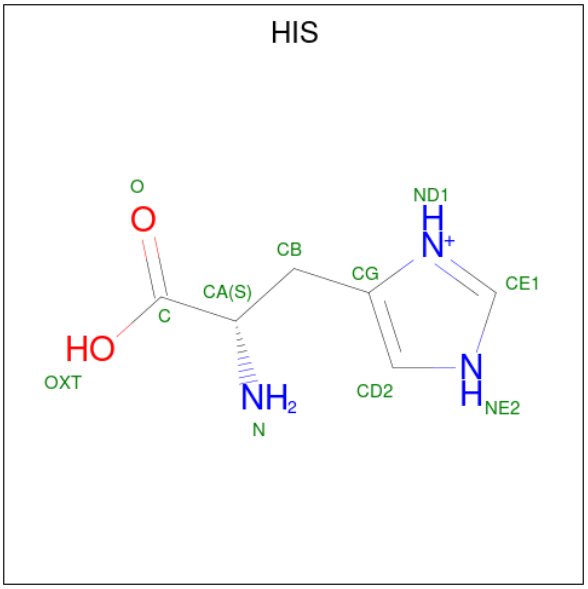
- Molecule 4 is a protein called ATP PHOSPHORIBOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	202	1599	1028	274	289	8	5	0	1

There is a discrepancy between the modelled and reference sequences:

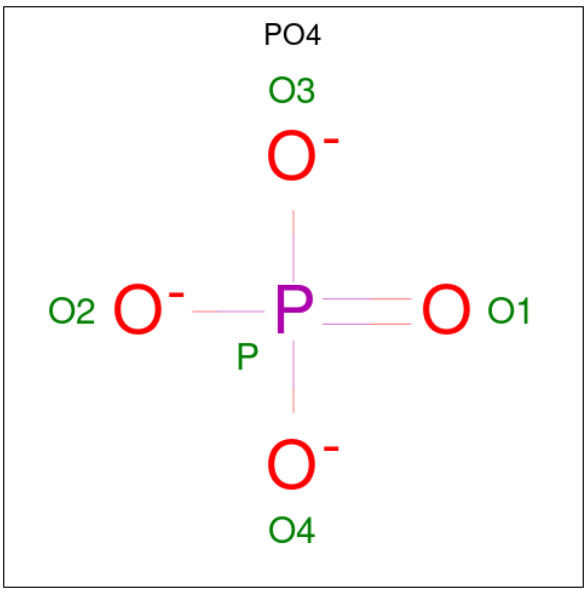
Chain	Residue	Modelled	Actual	Comment	Reference
H	186	LYS	GLU	conflict	UNP Q9X0D2

- Molecule 5 is HISTIDINE (three-letter code: HIS) (formula: $C_6H_{10}N_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	1	11	6	3	2	0	0
5	D	1	11	6	3	2	5	0
5	E	1	11	6	3	2	3	0
5	E	1	11	6	3	2	2	0
5	F	1	11	6	3	2	2	0
5	G	1	11	6	3	2	0	0
5	H	1	11	6	3	2	0	0
5	H	1	11	6	3	2	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	41	Total O 41 41	0	0
7	B	40	Total O 40 40	0	0
7	C	50	Total O 50 50	0	0
7	D	42	Total O 42 42	0	0
7	E	20	Total O 20 20	0	0

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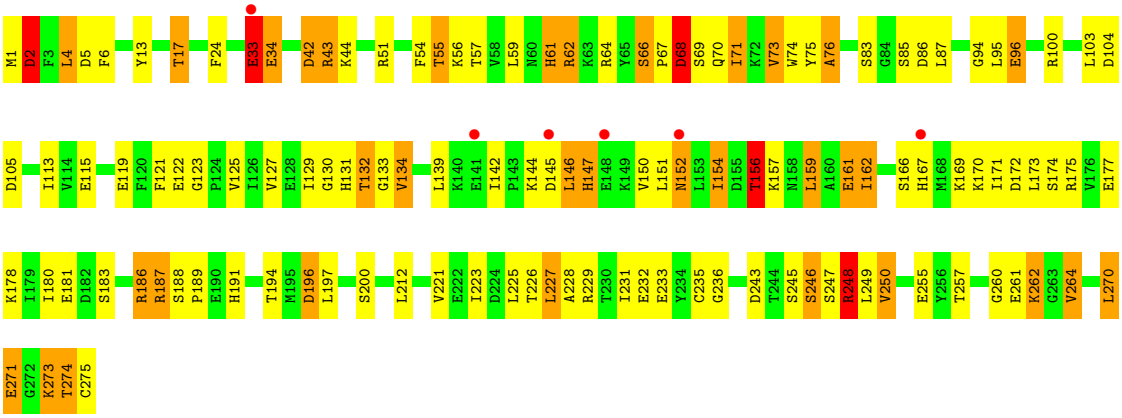
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	F	31	31	31	0	0
			Total	O		
7	G	27	27	27	0	0
			Total	O		
7	H	23	23	23	0	0

3 Residue-property plots (i)

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.

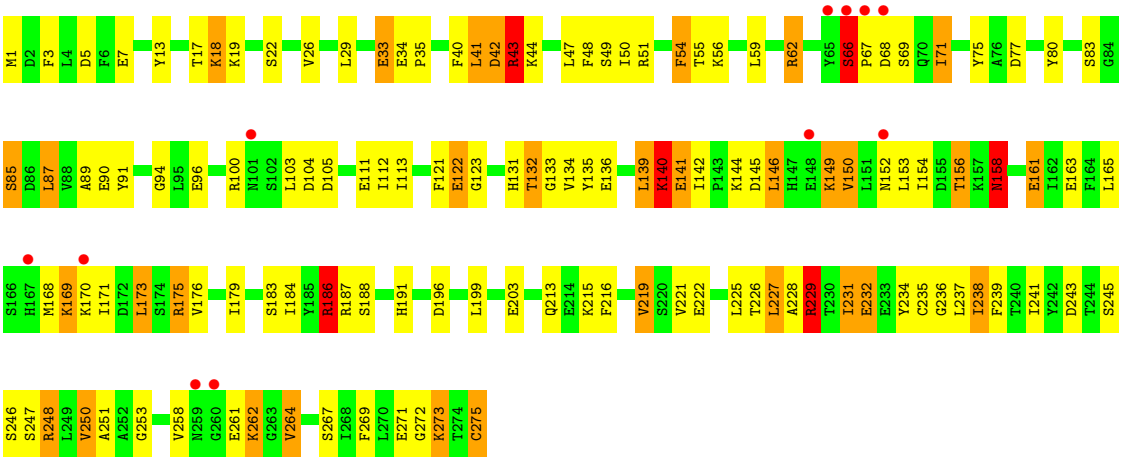
• Molecule 1: ATP PHOSPHORIBOSYLTRANSFERASE REGULATORY SUBUNIT

Chain A:



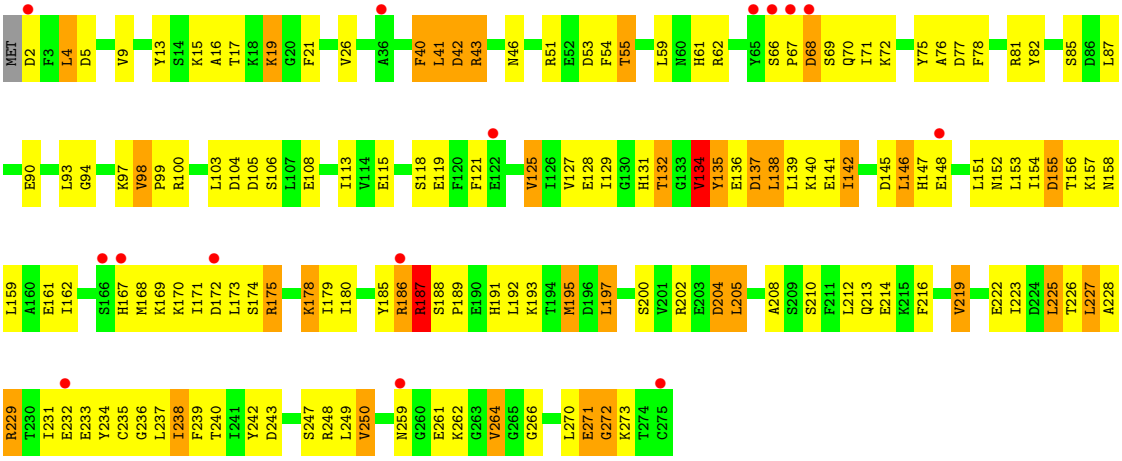
• Molecule 1: ATP PHOSPHORIBOSYLTRANSFERASE REGULATORY SUBUNIT

Chain B:



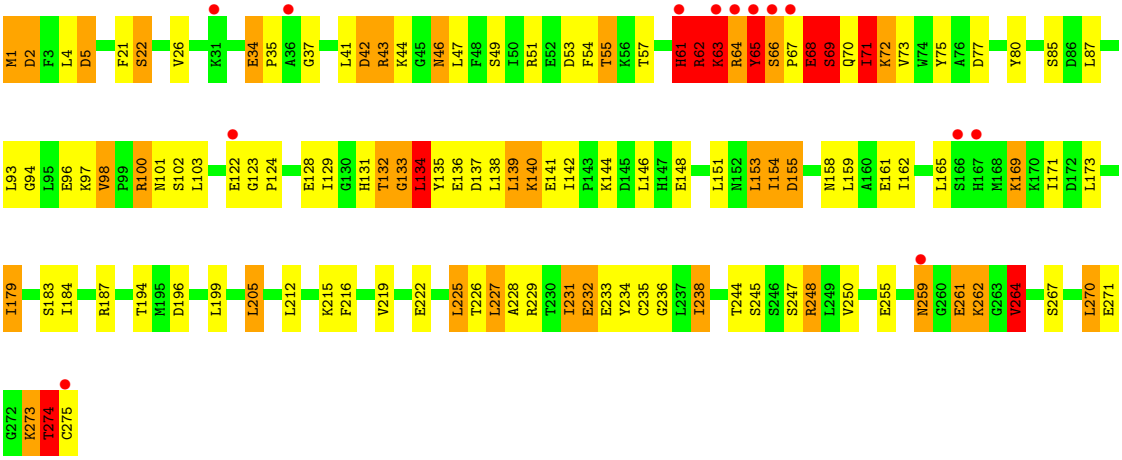
• Molecule 1: ATP PHOSPHORIBOSYLTRANSFERASE REGULATORY SUBUNIT

Chain D:



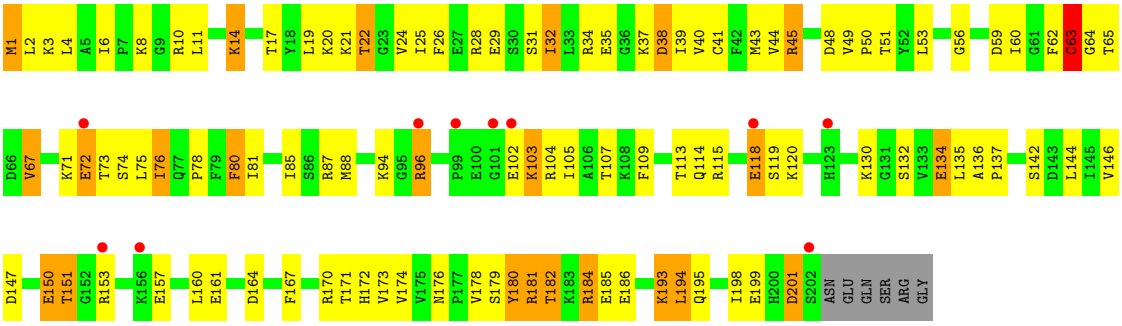
- Molecule 2: ATP PHOSPHORIBOSYLTRANSFERASE REGULATORY SUBUNIT

Chain C:



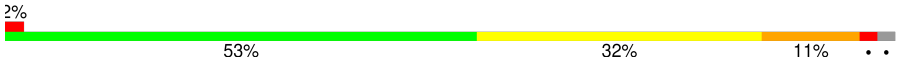
- Molecule 3: ATP PHOSPHORIBOSYLTRANSFERASE

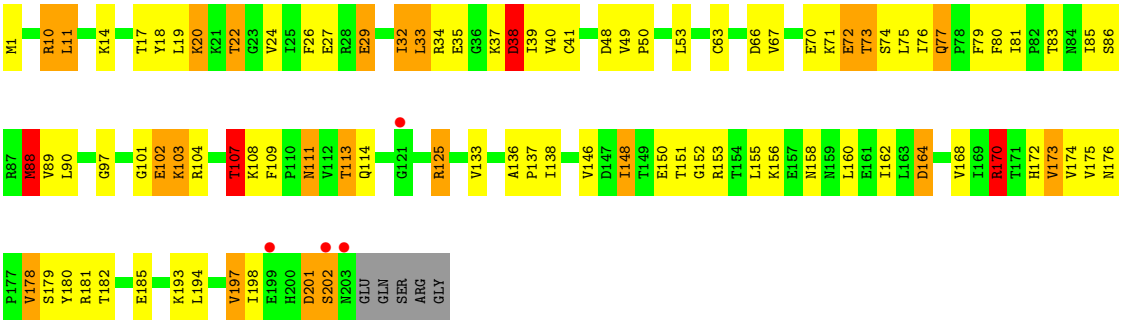
Chain E:



- Molecule 3: ATP PHOSPHORIBOSYLTRANSFERASE

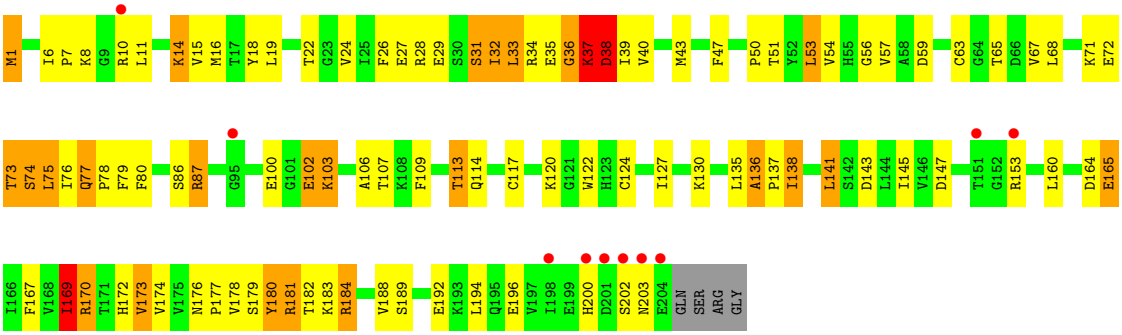
Chain F:





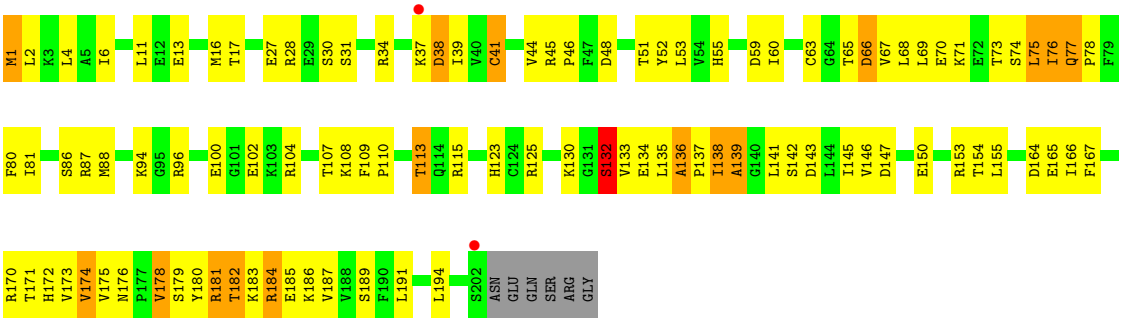
• Molecule 3: ATP PHOSPHORIBOSYLTRANSFERASE

Chain G:



• Molecule 4: ATP PHOSPHORIBOSYLTRANSFERASE

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	101.58Å 134.40Å 154.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.52 12.00 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.1 (12.00-2.52) 98.4 (12.00-2.53)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.70 (at 2.52Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.203 , 0.287 0.209 , 0.171	Depositor DCC
R_{free} test set	518 reflections (0.75%)	wwPDB-VP
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 59.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15636	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.93	3/2256 (0.1%)	1.11	16/3043 (0.5%)
1	B	1.34	2/2256 (0.1%)	1.02	12/3043 (0.4%)
1	D	0.78	0/2248	1.01	13/3033 (0.4%)
2	C	0.83	1/2252 (0.0%)	1.08	16/3039 (0.5%)
3	E	0.79	2/1628 (0.1%)	1.01	7/2200 (0.3%)
3	F	1.14	4/1634 (0.2%)	1.09	9/2208 (0.4%)
3	G	0.72	2/1642 (0.1%)	0.97	8/2219 (0.4%)
4	H	0.91	2/1628 (0.1%)	1.01	7/2199 (0.3%)
All	All	0.96	16/15544 (0.1%)	1.04	88/20984 (0.4%)

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	A	0	2
1	B	0	1
2	C	0	2
3	F	0	1
All	All	0	6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	CYS	CB-SG	-51.19	0.95	1.82
3	F	125	ARG	NE-CZ	33.64	1.76	1.33
4	H	100	GLU	CD-OE1	19.19	1.46	1.25
1	A	33	GLU	C-N	-17.25	0.94	1.34
1	A	34	GLU	CG-CD	-13.40	1.31	1.51
1	B	33	GLU	CB-CG	12.90	1.76	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	125	ARG	CG-CD	-9.63	1.27	1.51
3	G	63	CYS	CB-SG	-7.15	1.70	1.82
3	F	88	MET	SD-CE	-5.93	1.44	1.77
2	C	274	THR	C-N	-5.71	1.21	1.34
3	E	103	LYS	CA-CB	-5.66	1.41	1.53
4	H	100	GLU	CA-CB	-5.59	1.41	1.53
1	A	260	GLY	C-N	5.54	1.46	1.34
3	F	202	SER	C-N	-5.53	1.21	1.34
3	E	63	CYS	CB-SG	-5.38	1.73	1.81
3	G	43	MET	SD-CE	-5.05	1.49	1.77

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	125	ARG	NE-CZ-NH2	-18.39	111.10	120.30
1	A	34	GLU	CG-CD-OE1	-17.38	83.55	118.30
1	A	34	GLU	CG-CD-OE2	13.97	146.24	118.30
3	F	125	ARG	NE-CZ-NH1	13.03	126.81	120.30
4	H	181	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	D	204	ASP	CB-CG-OD2	9.12	126.51	118.30
1	B	77	ASP	CB-CG-OD2	8.93	126.34	118.30
1	D	53	ASP	CB-CG-OD2	8.78	126.20	118.30
2	C	42	ASP	CB-CG-OD2	8.74	126.17	118.30
1	B	186	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	B	186	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	A	248	ARG	NE-CZ-NH2	7.48	124.04	120.30
3	F	66	ASP	CB-CG-OD2	7.18	124.77	118.30
3	G	181	ARG	NE-CZ-NH1	7.09	123.85	120.30
3	G	164	ASP	CB-CG-OD2	7.09	124.68	118.30
1	A	42	ASP	CB-CG-OD2	7.05	124.65	118.30
2	C	77	ASP	CB-CG-OD2	7.03	124.63	118.30
2	C	2	ASP	CB-CG-OD2	6.97	124.58	118.30
1	B	196	ASP	CB-CG-OD2	6.92	124.52	118.30
1	A	104	ASP	CB-CG-OD2	6.92	124.52	118.30
2	C	155	ASP	CB-CG-OD2	6.88	124.49	118.30
1	B	229	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	A	51	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	140	LYS	O-C-N	6.85	133.66	122.70
1	D	105	ASP	CB-CG-OD2	6.85	124.46	118.30
4	H	147	ASP	CB-CG-OD2	6.79	124.41	118.30
3	F	48	ASP	CB-CG-OD2	6.78	124.41	118.30
2	C	64	ARG	NE-CZ-NH2	6.66	123.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	181	ARG	NE-CZ-NH1	6.56	123.58	120.30
2	C	62	ARG	NE-CZ-NH2	6.52	123.56	120.30
4	H	48	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	196	ASP	CB-CG-OD2	6.36	124.02	118.30
1	D	155	ASP	CB-CG-OD2	6.33	123.99	118.30
3	F	164	ASP	CB-CG-OD2	6.28	123.95	118.30
2	C	69	SER	N-CA-C	6.18	127.70	111.00
3	E	181	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	243	ASP	CB-CG-OD2	6.10	123.79	118.30
2	C	248	ARG	NE-CZ-NH2	6.08	123.34	120.30
4	H	59	ASP	CB-CG-OD2	6.01	123.71	118.30
1	D	77	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	140	LYS	CA-C-N	-5.97	104.07	117.20
1	B	5	ASP	CB-CG-OD2	5.94	123.64	118.30
1	B	104	ASP	CB-CG-OD2	5.93	123.64	118.30
2	C	5	ASP	CB-CG-OD2	5.93	123.63	118.30
3	F	63	CYS	CB-CA-C	-5.91	98.58	110.40
2	C	274	THR	O-C-N	5.84	132.04	122.70
3	G	59	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	264	VAL	CB-CA-C	-5.83	100.33	111.40
4	H	66	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	51	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	D	243	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	105	ASP	CB-CG-OD2	5.63	123.37	118.30
3	G	143	ASP	CB-CG-OD2	5.62	123.36	118.30
4	H	164	ASP	CB-CG-OD2	5.59	123.34	118.30
3	E	201	ASP	CB-CG-OD2	5.58	123.32	118.30
1	D	172	ASP	CB-CG-OD2	5.51	123.26	118.30
1	D	187	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	B	275	CYS	CA-CB-SG	-5.48	104.13	114.00
1	A	156	THR	OG1-CB-CG2	-5.46	97.44	110.00
1	A	186	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	137	ASP	CB-CG-OD2	5.40	123.16	118.30
3	F	170	ARG	NE-CZ-NH1	5.40	123.00	120.30
3	G	181	ARG	NE-CZ-NH2	-5.34	117.63	120.30
3	E	164	ASP	CB-CG-OD2	5.32	123.09	118.30
3	F	33	LEU	CA-CB-CG	5.32	127.54	115.30
2	C	69	SER	N-CA-CB	-5.31	102.54	110.50
1	A	2	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	264	VAL	CB-CA-C	-5.27	101.39	111.40
2	C	68	GLU	O-C-N	5.26	131.11	122.70
3	E	181	ARG	NE-CZ-NH1	5.24	122.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	48	ASP	CB-CG-OD2	5.22	123.00	118.30
3	G	38	ASP	CB-CG-OD2	5.21	122.99	118.30
3	F	38	ASP	CB-CG-OD2	5.18	122.96	118.30
2	C	274	THR	CA-C-N	-5.18	105.81	117.20
1	D	2	ASP	CB-CG-OD2	5.17	122.95	118.30
1	D	195	MET	CG-SD-CE	5.17	108.47	100.20
1	D	104	ASP	CB-CG-OD2	5.16	122.94	118.30
1	D	42	ASP	CB-CG-OD2	5.16	122.94	118.30
2	C	196	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	86	ASP	CB-CG-OD2	5.13	122.92	118.30
3	G	147	ASP	CB-CG-OD2	5.12	122.91	118.30
3	E	147	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	105	ASP	CB-CG-OD2	5.10	122.89	118.30
2	C	53	ASP	CB-CG-OD2	5.09	122.88	118.30
2	C	264	VAL	CB-CA-C	-5.07	101.77	111.40
1	A	261	GLU	O-C-N	5.05	130.79	122.70
3	G	169	ILE	CG1-CB-CG2	-5.05	100.29	111.40
3	E	59	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	33	GLU	Mainchain
1	A	34	GLU	Sidechain
1	B	122	GLU	Peptide
2	C	71	ILE	Mainchain
2	C	98	VAL	Mainchain
3	F	107	THR	Mainchain

5.2 Too-close contacts (i)

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	2210	0	2196	90	0
1	B	2210	0	2197	103	0
1	D	2202	0	2185	108	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2206	0	2196	106	0
3	E	1599	0	1664	92	0
3	F	1605	0	1669	73	0
3	G	1613	0	1675	90	1
4	H	1599	0	1671	102	0
5	C	11	0	6	7	0
5	D	11	0	6	0	0
5	E	22	0	12	15	0
5	F	11	0	6	8	0
5	G	11	0	6	6	0
5	H	22	0	12	23	0
6	E	10	0	0	2	0
6	F	5	0	0	0	0
6	G	10	0	0	0	0
6	H	5	0	0	2	0
7	A	41	0	0	4	0
7	B	40	0	0	0	0
7	C	50	0	0	5	0
7	D	42	0	0	2	0
7	E	20	0	0	2	0
7	F	31	0	0	1	0
7	G	27	0	0	3	0
7	H	23	0	0	3	0
All	All	15636	0	15501	735	1

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 24.

All (735) 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)
4:H:78:PRO:CB	5:H:1203:HIS:O	1.77	1.30
3:E:65:THR:HG1	5:E:1205:HIS:CE1	1.53	1.26
2:C:72:LYS:O	2:C:73:VAL:HG13	1.42	1.19
5:E:1205:HIS:O	5:E:1205:HIS:CD2	1.94	1.19
5:E:1205:HIS:O	5:E:1205:HIS:HD2	1.24	1.16
3:G:65:THR:HB	3:G:169:ILE:HG22	1.20	1.16
4:H:78:PRO:HB3	5:H:1203:HIS:O	1.00	1.16
3:F:172:HIS:CE1	5:F:1204:HIS:HB3	1.82	1.15
2:C:138:LEU:O	2:C:139:LEU:HB2	1.47	1.14
3:E:107:THR:HG21	3:E:113:THR:HG21	1.18	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:172:HIS:HE1	5:F:1204:HIS:HB3	1.14	1.11
1:B:269:PHE:HB3	1:B:271:GLU:HG3	1.23	1.11
2:C:274:THR:CG2	2:C:275:CYS:N	2.10	1.11
4:H:180:TYR:O	4:H:184:ARG:HB3	1.52	1.09
1:A:248:ARG:HD2	1:A:249:LEU:H	1.13	1.08
3:F:172:HIS:CE1	5:F:1204:HIS:CB	2.36	1.08
4:H:180:TYR:OH	5:H:1203:HIS:N	1.89	1.05
3:E:172:HIS:NE2	5:E:1205:HIS:CE1	2.24	1.05
3:F:175:VAL:HG11	3:F:180:TYR:HD2	1.22	1.05
1:B:226:THR:O	1:B:227:LEU:HD23	1.55	1.05
3:G:107:THR:HG21	3:G:113:THR:HG21	1.39	1.05
3:E:65:THR:OG1	5:E:1205:HIS:CE1	2.10	1.04
3:E:78:PRO:HB3	5:E:1204:HIS:HB3	1.36	1.03
2:C:66:SER:HB3	2:C:67:PRO:CD	1.88	1.02
4:H:180:TYR:CE1	5:H:1203:HIS:N	2.28	1.01
2:C:226:THR:O	2:C:227:LEU:HB2	1.58	1.00
3:F:170:ARG:HH11	3:F:170:ARG:HG2	1.28	0.98
4:H:78:PRO:HB3	5:H:1203:HIS:C	1.84	0.98
2:C:1:MET:HE1	1:D:62:ARG:HA	1.45	0.97
2:C:137:ASP:O	2:C:140:LYS:HB2	1.64	0.97
3:F:107:THR:HB	3:F:109:PHE:H	1.28	0.97
1:D:62:ARG:HG2	1:D:62:ARG:HH11	1.32	0.94
3:G:29:GLU:HG2	3:G:34:ARG:HG3	1.46	0.94
1:B:226:THR:O	1:B:227:LEU:CD2	2.16	0.94
3:E:41:CYS:HB3	3:E:43:MET:HE1	1.50	0.93
4:H:170:ARG:NH1	5:H:1204:HIS:CE1	2.37	0.93
1:D:270:LEU:O	1:D:271:GLU:HB2	1.65	0.93
3:F:107:THR:HG22	3:F:146:VAL:O	1.69	0.93
2:C:228:ALA:O	2:C:231:ILE:HG23	1.68	0.92
2:C:274:THR:HG23	2:C:275:CYS:N	1.83	0.92
3:G:32:ILE:HG23	4:H:135:LEU:HD21	1.50	0.91
1:B:62:ARG:HG3	1:B:71:ILE:HD13	1.53	0.91
2:C:66:SER:HB3	2:C:67:PRO:HD2	1.52	0.91
1:A:131:HIS:HD2	1:A:133:GLY:H	1.00	0.91
3:G:135:LEU:O	3:G:136:ALA:CB	2.18	0.91
3:E:107:THR:HG21	3:E:113:THR:CG2	2.01	0.90
3:G:130:LYS:NZ	3:G:130:LYS:HB3	1.87	0.89
1:D:132:THR:HG22	7:D:2026:HOH:O	1.72	0.89
1:D:145:ASP:O	1:D:146:LEU:HB2	1.70	0.88
2:C:274:THR:HG22	2:C:275:CYS:N	1.89	0.87
1:A:226:THR:O	1:A:227:LEU:HB2	1.71	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:NH2	1:A:194:THR:OG1	2.08	0.86
4:H:180:TYR:HE1	5:H:1203:HIS:N	1.68	0.86
1:A:154:ILE:HD11	1:A:226:THR:HA	1.55	0.86
1:A:248:ARG:HD2	1:A:249:LEU:N	1.91	0.85
2:C:72:LYS:O	2:C:73:VAL:CG1	2.24	0.85
4:H:170:ARG:NH1	5:H:1204:HIS:HE1	1.72	0.85
1:A:115:GLU:O	1:A:119:GLU:HG3	1.75	0.85
4:H:37:LYS:O	4:H:38:ASP:HB3	1.76	0.85
4:H:180:TYR:CZ	5:H:1203:HIS:N	2.45	0.84
3:G:135:LEU:O	3:G:136:ALA:HB3	1.75	0.84
5:C:1275:HIS:HB3	3:G:78:PRO:HB3	1.59	0.84
1:B:43:ARG:HG3	1:B:43:ARG:HH11	1.41	0.83
2:C:62:ARG:HG3	2:C:63:LYS:H	1.43	0.83
1:A:131:HIS:CD2	1:A:133:GLY:H	1.91	0.83
1:A:74:TRP:CE3	1:A:75:TYR:O	2.31	0.83
3:E:1:MET:CE	3:E:40:VAL:HG13	2.09	0.82
2:C:123:GLY:HA3	2:C:245:SER:HB2	1.59	0.82
1:B:150:VAL:O	1:B:154:ILE:HG12	1.79	0.82
1:A:139:LEU:HB3	1:A:147:HIS:CE1	2.15	0.82
1:D:195:MET:HB3	1:D:197:LEU:CD2	2.09	0.82
2:C:135:TYR:O	2:C:138:LEU:O	1.97	0.82
3:F:175:VAL:HG11	3:F:180:TYR:CD2	2.13	0.82
1:D:99:PRO:HA	1:D:262:LYS:O	1.80	0.81
3:G:107:THR:HG21	3:G:113:THR:CG2	2.10	0.81
1:B:132:THR:HG21	1:B:235:CYS:HA	1.61	0.81
2:C:184:ILE:CD1	5:C:1275:HIS:HA	2.11	0.81
1:B:41:LEU:HD13	1:D:41:LEU:CD1	2.10	0.80
3:F:194:LEU:HD23	3:F:198:ILE:CD1	2.10	0.80
3:E:94:LYS:HA	3:E:161:GLU:HG3	1.64	0.79
3:E:180:TYR:O	3:E:184:ARG:HB3	1.82	0.79
4:H:135:LEU:O	4:H:136:ALA:CB	2.29	0.79
2:C:1:MET:CE	1:D:62:ARG:HA	2.11	0.79
4:H:180:TYR:OH	5:H:1203:HIS:CA	2.31	0.79
2:C:93:LEU:HG	2:C:270:LEU:HD21	1.64	0.79
3:F:19:LEU:O	3:F:22:THR:HG22	1.83	0.79
3:G:136:ALA:HB3	3:G:137:PRO:HD3	1.65	0.79
1:D:129:ILE:HD11	1:D:212:LEU:HD12	1.63	0.79
1:D:98:VAL:O	1:D:98:VAL:CG1	2.31	0.78
4:H:170:ARG:HH11	5:H:1204:HIS:CE1	2.00	0.78
3:E:76:ILE:HD11	3:E:78:PRO:HG3	1.63	0.78
5:E:1205:HIS:CD2	5:E:1205:HIS:C	2.57	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:100:ARG:HG2	2:C:264:VAL:HG22	1.63	0.78
3:G:53:LEU:CD2	3:G:174:VAL:HG23	2.12	0.78
3:E:88:MET:CE	3:E:146:VAL:HG23	2.14	0.77
1:B:269:PHE:HB3	1:B:271:GLU:CG	2.09	0.77
4:H:138:ILE:O	4:H:139:ALA:CB	2.33	0.77
1:B:246:SER:HB3	1:B:248:ARG:HG3	1.66	0.77
1:A:132:THR:HG22	7:A:2022:HOH:O	1.82	0.77
3:F:172:HIS:CE1	5:F:1204:HIS:HB2	2.19	0.77
4:H:53:LEU:HD13	4:H:174:VAL:CG2	2.15	0.77
1:B:55:THR:HG22	1:B:96:GLU:OE2	1.84	0.77
3:G:73:THR:HG22	3:G:73:THR:O	1.84	0.77
1:A:75:TYR:CZ	1:A:94:GLY:HA3	2.20	0.76
3:E:22:THR:HG23	3:E:193:LYS:HE3	1.65	0.76
3:E:41:CYS:HB3	3:E:43:MET:CE	2.14	0.76
1:D:134:VAL:HG12	1:D:138:LEU:CD2	2.14	0.76
2:C:66:SER:CB	2:C:67:PRO:CD	2.63	0.76
1:A:71:ILE:HD11	1:B:1:MET:SD	2.25	0.76
1:B:132:THR:HG22	1:B:236:GLY:H	1.51	0.76
4:H:65:THR:HG23	5:H:1204:HIS:HB3	1.66	0.75
1:B:156:THR:HG22	1:B:158:ASN:HB2	1.68	0.75
1:B:132:THR:CG2	1:B:236:GLY:H	1.98	0.75
3:E:8:LYS:HD2	3:E:45:ARG:NH2	2.02	0.75
1:B:258:VAL:O	1:B:261:GLU:HB2	1.86	0.75
2:C:128:GLU:OE2	3:G:181:ARG:HD3	1.86	0.75
3:E:107:THR:CG2	3:E:113:THR:HG21	2.07	0.75
2:C:134:LEU:HD12	2:C:134:LEU:O	1.87	0.74
2:C:1:MET:HE1	1:D:62:ARG:CA	2.18	0.74
1:B:90:GLU:HB2	1:B:271:GLU:OE1	1.87	0.74
1:D:132:THR:HG21	1:D:235:CYS:HA	1.68	0.74
3:E:135:LEU:HD13	3:F:32:ILE:HG22	1.70	0.74
4:H:78:PRO:CG	5:H:1203:HIS:O	2.35	0.73
3:E:26:PHE:O	3:E:35:GLU:O	2.05	0.73
2:C:66:SER:CB	2:C:67:PRO:HD2	2.17	0.73
3:G:71:LYS:O	3:G:73:THR:N	2.21	0.73
1:A:156:THR:HG22	4:H:75:LEU:O	1.89	0.73
3:E:8:LYS:HD2	3:E:45:ARG:HH21	1.53	0.73
3:F:194:LEU:HD23	3:F:198:ILE:HD12	1.70	0.72
3:G:130:LYS:HB3	3:G:130:LYS:HZ3	1.53	0.72
3:F:136:ALA:HB3	3:F:137:PRO:HD3	1.72	0.72
1:D:189:PRO:HA	1:D:223:ILE:HD12	1.72	0.71
1:D:208:ALA:HB2	1:D:237:LEU:HD21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:66:SER:HB3	2:C:67:PRO:HD3	1.71	0.71
1:A:66:SER:OG	1:A:67:PRO:HD3	1.90	0.71
3:E:56:GLY:HA2	3:E:176:ASN:HD21	1.54	0.71
2:C:184:ILE:HD11	5:C:1275:HIS:HA	1.71	0.71
2:C:62:ARG:HG3	2:C:63:LYS:N	2.05	0.70
3:E:63:CYS:HB3	3:E:67:VAL:HG22	1.73	0.70
3:F:14:LYS:O	3:F:17:THR:HG22	1.90	0.70
1:B:269:PHE:CB	1:B:271:GLU:HG3	2.13	0.70
2:C:1:MET:HE2	1:D:61:HIS:O	1.90	0.70
3:G:65:THR:CB	3:G:169:ILE:HG22	2.12	0.70
1:A:161:GLU:HG3	7:A:2023:HOH:O	1.91	0.70
4:H:75:LEU:HD22	4:H:75:LEU:H	1.56	0.70
1:A:13:TYR:O	1:A:17:THR:HG23	1.92	0.70
4:H:107:THR:HG21	4:H:113:THR:HG21	1.74	0.70
4:H:88:MET:HE1	4:H:146:VAL:HG12	1.72	0.69
1:B:43:ARG:HG3	1:B:43:ARG:NH1	2.05	0.69
1:D:195:MET:HB3	1:D:197:LEU:HD21	1.72	0.69
3:G:32:ILE:HG23	4:H:135:LEU:CD2	2.23	0.69
2:C:132:THR:HG21	2:C:235:CYS:HA	1.73	0.69
3:E:78:PRO:CB	5:E:1204:HIS:HB3	2.20	0.69
3:F:170:ARG:HG2	3:F:170:ARG:NH1	2.00	0.69
1:D:195:MET:CB	1:D:197:LEU:HD21	2.23	0.69
2:C:26:VAL:O	2:C:51:ARG:NH2	2.26	0.68
3:E:19:LEU:HB3	3:E:24:VAL:HG11	1.76	0.68
1:A:270:LEU:O	1:A:271:GLU:HB3	1.91	0.68
2:C:57:THR:O	2:C:61:HIS:HB2	1.92	0.68
4:H:178:VAL:O	4:H:182:THR:HB	1.93	0.68
4:H:4:LEU:HD22	4:H:60:ILE:HB	1.76	0.68
4:H:135:LEU:O	4:H:136:ALA:HB3	1.92	0.68
2:C:234:TYR:CB	2:C:238:ILE:HD11	2.24	0.68
3:F:172:HIS:NE2	5:F:1204:HIS:HB2	2.08	0.68
3:E:135:LEU:HD13	3:F:32:ILE:CG2	2.24	0.68
3:E:1:MET:HE3	3:E:40:VAL:HG13	1.75	0.68
4:H:180:TYR:OH	5:H:1203:HIS:HA	1.93	0.68
1:B:80:TYR:HB3	1:B:87:LEU:HD21	1.74	0.67
3:E:180:TYR:OH	5:E:1204:HIS:CA	2.42	0.67
1:D:145:ASP:O	1:D:145:ASP:OD1	2.13	0.67
3:E:62:PHE:HD2	3:E:81:ILE:HD11	1.59	0.67
2:C:42:ASP:OD2	2:C:43:ARG:N	2.28	0.67
1:A:24:PHE:HB2	1:A:73:VAL:HG22	1.76	0.66
2:C:21:PHE:HA	2:C:72:LYS:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:GLU:O	1:D:272:GLY:O	2.14	0.66
3:G:6:ILE:HG23	3:G:7:PRO:HD2	1.76	0.66
4:H:75:LEU:HD22	4:H:75:LEU:N	2.10	0.66
1:A:121:PHE:CZ	1:A:250:VAL:HG22	2.31	0.66
1:B:146:LEU:O	1:B:150:VAL:HG13	1.95	0.66
2:C:133:GLY:O	2:C:135:TYR:N	2.28	0.66
3:E:14:LYS:O	3:E:17:THR:HG22	1.94	0.66
3:F:88:MET:HE1	3:F:109:PHE:CE1	2.31	0.66
3:F:107:THR:CG2	3:F:146:VAL:O	2.41	0.66
1:B:131:HIS:HD2	1:B:133:GLY:H	1.40	0.66
1:B:139:LEU:O	1:B:142:ILE:HB	1.94	0.66
2:C:129:ILE:HD11	2:C:212:LEU:HD12	1.77	0.66
1:D:98:VAL:O	1:D:98:VAL:HG12	1.96	0.66
3:F:22:THR:HG22	3:F:24:VAL:HG23	1.77	0.66
3:E:71:LYS:O	3:E:73:THR:N	2.29	0.65
4:H:27:GLU:OE1	4:H:37:LYS:HG2	1.95	0.65
1:B:152:ASN:O	1:B:156:THR:HB	1.97	0.65
3:F:107:THR:HB	3:F:109:PHE:N	2.06	0.65
3:G:130:LYS:HB3	3:G:130:LYS:HZ2	1.60	0.65
1:B:229:ARG:HG2	1:B:229:ARG:HH11	1.61	0.65
1:D:248:ARG:HB2	1:D:273:LYS:O	1.97	0.65
1:B:123:GLY:HA3	1:B:245:SER:HB2	1.78	0.65
1:D:75:TYR:CZ	1:D:94:GLY:HA3	2.32	0.65
3:E:178:VAL:HG23	3:E:179:SER:N	2.12	0.65
3:G:179:SER:HA	3:G:182:THR:OG1	1.96	0.65
2:C:261:GLU:O	2:C:262:LYS:HB2	1.95	0.64
1:D:138:LEU:HD11	1:D:179:ILE:CD1	2.26	0.64
3:F:22:THR:CG2	3:F:24:VAL:HG23	2.28	0.64
3:F:53:LEU:HD11	3:F:174:VAL:HG23	1.79	0.64
3:F:179:SER:HA	3:F:182:THR:OG1	1.98	0.64
1:D:187:ARG:NH2	1:D:222:GLU:OE2	2.29	0.64
1:A:274:THR:O	1:A:275:CYS:HB2	1.98	0.64
3:G:53:LEU:HD21	3:G:174:VAL:HG23	1.79	0.64
1:D:62:ARG:HG2	1:D:62:ARG:NH1	2.05	0.64
3:E:88:MET:HE1	3:E:146:VAL:HG23	1.79	0.64
3:E:88:MET:CE	3:E:146:VAL:CG2	2.76	0.64
4:H:172:HIS:CE1	5:H:1204:HIS:HB2	2.32	0.64
2:C:136:GLU:CD	2:C:136:GLU:H	2.02	0.64
3:G:184:ARG:NH1	3:G:184:ARG:HG2	2.10	0.64
1:A:183:SER:O	1:A:187:ARG:HD2	1.98	0.64
2:C:62:ARG:HB2	2:C:62:ARG:CZ	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:138:ILE:HD13	3:G:138:ILE:N	2.13	0.64
3:G:37:LYS:O	3:G:38:ASP:HB3	1.98	0.63
2:C:274:THR:HG23	7:C:2050:HOH:O	1.99	0.63
3:E:88:MET:HE3	3:E:146:VAL:HG23	1.78	0.63
2:C:138:LEU:O	2:C:139:LEU:CB	2.31	0.63
3:E:180:TYR:OH	5:E:1204:HIS:HB2	1.98	0.63
2:C:234:TYR:HB2	2:C:238:ILE:HD11	1.81	0.63
1:B:228:ALA:O	1:B:231:ILE:HB	1.99	0.62
3:E:71:LYS:C	3:E:73:THR:H	2.02	0.62
3:E:88:MET:HE1	3:E:146:VAL:CG2	2.28	0.62
1:A:74:TRP:HE3	1:A:75:TYR:O	1.81	0.62
1:B:100:ARG:NH2	1:B:262:LYS:HG2	2.14	0.62
1:B:123:GLY:CA	1:B:245:SER:HB2	2.30	0.62
1:D:138:LEU:HD11	1:D:179:ILE:HD11	1.80	0.62
1:B:42:ASP:OD1	1:B:44:LYS:N	2.32	0.62
1:D:129:ILE:HD11	1:D:212:LEU:CD1	2.30	0.62
2:C:183:SER:O	2:C:187:ARG:HD2	1.98	0.62
3:G:26:PHE:O	3:G:27:GLU:HG2	1.99	0.62
2:C:184:ILE:HD13	5:C:1275:HIS:HA	1.81	0.62
4:H:175:VAL:HG11	4:H:180:TYR:HD1	1.65	0.62
3:G:76:ILE:HD13	3:G:180:TYR:CD2	2.34	0.62
1:B:51:ARG:HD3	1:B:54:PHE:CE1	2.35	0.62
3:E:22:THR:HG23	3:E:193:LYS:CE	2.29	0.62
3:G:170:ARG:HG3	5:G:1206:HIS:HE1	1.64	0.61
3:G:29:GLU:HG2	3:G:34:ARG:CG	2.24	0.61
3:F:194:LEU:CD2	3:F:198:ILE:CD1	2.78	0.61
3:G:109:PHE:O	3:G:113:THR:HG23	2.00	0.61
2:C:274:THR:HG21	7:C:2023:HOH:O	1.98	0.61
4:H:180:TYR:O	4:H:184:ARG:CB	2.38	0.61
1:A:13:TYR:HD1	1:A:74:TRP:CZ2	2.19	0.61
1:B:213:GLN:HG3	1:B:221:VAL:CG2	2.31	0.61
4:H:136:ALA:HB3	4:H:137:PRO:HD3	1.82	0.61
3:E:17:THR:O	3:E:21:LYS:HG3	2.01	0.61
3:E:63:CYS:HB3	3:E:67:VAL:CG2	2.29	0.61
3:F:89:VAL:HG11	3:F:162:ILE:HG12	1.83	0.61
3:G:65:THR:HG23	5:G:1206:HIS:CB	2.30	0.61
1:B:123:GLY:HA3	1:B:243:ASP:OD1	2.01	0.61
4:H:44:VAL:HG21	4:H:52:TYR:CE1	2.36	0.61
1:A:24:PHE:HB2	1:A:73:VAL:CG2	2.31	0.61
2:C:232:GLU:O	2:C:232:GLU:HG2	2.00	0.61
1:D:145:ASP:O	1:D:146:LEU:CB	2.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ARG:HG3	1:B:71:ILE:CD1	2.29	0.60
1:D:13:TYR:O	1:D:17:THR:HG23	2.01	0.60
4:H:88:MET:CE	4:H:146:VAL:HG12	2.30	0.60
3:E:178:VAL:HG23	3:E:179:SER:H	1.65	0.60
3:G:73:THR:O	3:G:73:THR:CG2	2.49	0.60
4:H:44:VAL:HG22	7:H:2008:HOH:O	2.02	0.60
3:G:184:ARG:HG2	3:G:184:ARG:HH11	1.65	0.60
1:B:156:THR:HG21	7:E:2012:HOH:O	2.00	0.60
1:B:41:LEU:HD13	1:D:41:LEU:HD11	1.83	0.60
1:B:90:GLU:CB	1:B:271:GLU:OE1	2.49	0.60
1:D:189:PRO:HG2	1:D:213:GLN:OE1	2.01	0.60
3:E:22:THR:CG2	3:E:193:LYS:HE3	2.31	0.60
4:H:109:PHE:O	4:H:113:THR:HG23	2.01	0.60
1:D:153:LEU:CD2	1:D:161:GLU:HB3	2.32	0.59
3:E:19:LEU:O	3:E:24:VAL:HG12	2.02	0.59
3:F:86:SER:HB3	3:F:150:GLU:HG3	1.83	0.59
3:F:170:ARG:HH11	3:F:170:ARG:CG	2.10	0.59
1:D:72:LYS:HG3	1:D:97:LYS:HD2	1.85	0.59
3:E:80:PHE:HB3	3:E:171:THR:O	2.02	0.59
4:H:170:ARG:HH12	5:H:1204:HIS:CE1	2.19	0.59
3:F:172:HIS:NE2	5:F:1204:HIS:CB	2.65	0.59
4:H:53:LEU:HD13	4:H:174:VAL:HG23	1.82	0.59
4:H:102:GLU:HA	4:H:102:GLU:OE2	2.03	0.59
1:B:131:HIS:CD2	1:B:133:GLY:H	2.20	0.59
1:B:246:SER:HB3	1:B:248:ARG:CG	2.32	0.59
1:D:55:THR:O	1:D:59:LEU:HG	2.02	0.59
1:D:132:THR:HB	1:D:236:GLY:H	1.67	0.59
4:H:138:ILE:O	4:H:139:ALA:HB3	2.02	0.59
3:E:115:ARG:NH2	7:E:2013:HOH:O	2.35	0.58
1:B:47:LEU:HD11	1:D:43:ARG:HE	1.68	0.58
3:E:195:GLN:O	3:E:199:GLU:HB2	2.04	0.58
3:G:53:LEU:HD23	3:G:174:VAL:HG23	1.84	0.58
1:D:175:ARG:O	1:D:179:ILE:HD12	2.02	0.58
1:A:150:VAL:O	1:A:154:ILE:HG22	2.02	0.58
2:C:71:ILE:CD1	2:C:98:VAL:HG12	2.33	0.58
4:H:68:LEU:O	4:H:71:LYS:O	2.21	0.58
1:B:62:ARG:CG	1:B:71:ILE:HD13	2.32	0.58
1:D:204:ASP:HB3	1:D:237:LEU:HD13	1.86	0.58
4:H:109:PHE:O	4:H:113:THR:CG2	2.52	0.58
4:H:133:VAL:O	4:H:135:LEU:O	2.21	0.58
1:B:29:LEU:HD22	1:B:48:PHE:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:138:ILE:HD11	3:F:158:ASN:HB3	1.86	0.58
1:B:241:ILE:HB	1:B:251:ALA:HB3	1.85	0.58
4:H:46:PRO:HG2	7:H:2007:HOH:O	2.04	0.57
1:A:100:ARG:HB3	1:A:262:LYS:HB2	1.87	0.57
1:D:134:VAL:HG12	1:D:138:LEU:HD22	1.86	0.57
3:E:151:THR:OG1	6:E:1202:PO4:O4	2.22	0.57
3:F:107:THR:HG23	3:F:146:VAL:HB	1.85	0.57
1:A:67:PRO:O	1:A:68:ASP:HB2	2.02	0.57
1:B:156:THR:CG2	1:B:158:ASN:HB2	2.35	0.57
1:A:173:LEU:O	1:A:175:ARG:N	2.38	0.57
1:D:66:SER:HB3	1:D:67:PRO:HD2	1.87	0.57
3:F:194:LEU:CD2	3:F:198:ILE:HD11	2.34	0.57
2:C:137:ASP:OD1	2:C:140:LYS:HE3	2.05	0.56
1:B:47:LEU:CD1	1:D:43:ARG:HE	2.18	0.56
4:H:88:MET:CE	4:H:146:VAL:CG1	2.84	0.56
1:A:68:ASP:O	1:A:69:SER:HB2	2.05	0.56
2:C:42:ASP:OD1	2:C:46:ASN:ND2	2.39	0.56
4:H:88:MET:HE3	4:H:146:VAL:CG1	2.36	0.56
1:A:44:LYS:HD3	1:B:85:SER:HA	1.88	0.56
1:D:135:TYR:H	1:D:138:LEU:HD23	1.70	0.56
1:D:153:LEU:HD21	1:D:161:GLU:HB3	1.88	0.56
3:G:76:ILE:HD13	3:G:180:TYR:HD2	1.70	0.56
1:B:183:SER:O	1:B:187:ARG:HD2	2.05	0.56
3:G:65:THR:HG23	5:G:1206:HIS:HB3	1.87	0.56
3:G:136:ALA:HB3	3:G:137:PRO:CD	2.33	0.56
1:D:192:LEU:HD21	1:D:223:ILE:HD13	1.88	0.56
1:B:90:GLU:HB2	1:B:271:GLU:CD	2.25	0.56
1:A:123:GLY:CA	1:A:245:SER:HB2	2.37	0.55
1:B:184:ILE:CD1	5:E:1204:HIS:HA	2.36	0.55
1:D:98:VAL:O	1:D:98:VAL:HG13	2.06	0.55
3:F:49:VAL:HB	3:F:50:PRO:HD3	1.87	0.55
1:B:19:LYS:HG3	1:B:112:ILE:HD11	1.87	0.55
1:B:213:GLN:HG3	1:B:221:VAL:HG21	1.88	0.55
4:H:176:ASN:HD22	4:H:179:SER:H	1.54	0.55
1:D:40:PHE:N	1:D:40:PHE:CD1	2.74	0.55
3:F:50:PRO:HB3	3:F:73:THR:HG21	1.89	0.55
3:E:34:ARG:HB2	3:E:41:CYS:HB2	1.89	0.55
3:G:32:ILE:HG12	4:H:132:SER:HB3	1.89	0.55
1:A:2:ASP:OD2	1:A:273:LYS:NZ	2.40	0.55
1:B:131:HIS:O	1:B:134:VAL:HG12	2.07	0.55
1:B:239:PHE:CE2	1:B:253:GLY:HA3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:8:LYS:NZ	3:G:31:SER:O	2.39	0.55
1:A:74:TRP:CZ3	1:A:75:TYR:O	2.60	0.55
1:B:154:ILE:CD1	1:B:176:VAL:HG13	2.37	0.55
1:B:226:THR:O	1:B:227:LEU:HD22	2.05	0.55
3:E:1:MET:HE1	3:E:40:VAL:HG13	1.86	0.55
3:F:89:VAL:HG12	3:F:90:LEU:O	2.06	0.55
1:B:90:GLU:HB2	1:B:271:GLU:HG2	1.89	0.54
1:D:157:LYS:HD2	3:F:76:ILE:HD13	1.89	0.54
4:H:107:THR:HG21	4:H:113:THR:CG2	2.37	0.54
1:D:227:LEU:HB2	7:D:2039:HOH:O	2.06	0.54
1:D:13:TYR:CE1	1:D:17:THR:HG21	2.42	0.54
4:H:191:LEU:HD13	5:H:1203:HIS:HB3	1.89	0.54
2:C:131:HIS:HB2	2:C:205:LEU:HD11	1.88	0.54
1:A:139:LEU:HA	1:A:142:ILE:HD12	1.90	0.54
1:A:274:THR:HG21	3:G:102:GLU:OE1	2.08	0.54
3:E:62:PHE:CD2	3:E:81:ILE:HD11	2.40	0.54
1:A:162:ILE:HD13	1:A:180:ILE:CD1	2.37	0.54
1:A:162:ILE:HG21	1:A:177:GLU:HG2	1.89	0.54
1:B:62:ARG:NH2	1:B:68:ASP:OD1	2.41	0.54
2:C:2:ASP:OD1	2:C:273:LYS:NZ	2.40	0.54
4:H:176:ASN:HD21	4:H:178:VAL:HG13	1.73	0.54
1:D:134:VAL:HG12	1:D:138:LEU:HD21	1.89	0.54
3:G:54:VAL:HG21	3:G:73:THR:OG1	2.08	0.53
4:H:1:MET:H2	4:H:186:LYS:HZ2	1.54	0.53
1:B:247:SER:OG	3:E:182:THR:HG21	2.08	0.53
1:D:125:VAL:HG12	1:D:219:VAL:HB	1.89	0.53
1:B:199:LEU:O	1:B:203:GLU:HG2	2.09	0.53
1:A:131:HIS:HD2	1:A:133:GLY:N	1.85	0.53
2:C:153:LEU:HB3	2:C:162:ILE:HD11	1.90	0.53
4:H:6:ILE:HD12	4:H:41:CYS:SG	2.48	0.53
3:G:73:THR:HG23	3:G:75:LEU:HD13	1.91	0.53
2:C:151:LEU:O	2:C:154:ILE:HG22	2.08	0.53
3:E:107:THR:HB	3:E:109:PHE:H	1.72	0.53
3:F:88:MET:HE3	3:F:109:PHE:CD1	2.44	0.53
4:H:75:LEU:N	4:H:75:LEU:CD2	2.71	0.53
1:A:152:ASN:OD1	1:A:152:ASN:C	2.47	0.53
1:D:134:VAL:O	1:D:136:GLU:N	2.41	0.53
3:F:71:LYS:O	3:F:72:GLU:HG3	2.08	0.53
3:F:77:GLN:OE1	5:F:1204:HIS:O	2.25	0.53
1:A:154:ILE:CD1	1:A:226:THR:HA	2.36	0.53
3:E:180:TYR:OH	5:E:1204:HIS:CB	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:76:ILE:HG21	3:G:180:TYR:CE2	2.44	0.53
1:B:229:ARG:HG2	1:B:229:ARG:NH1	2.25	0.52
1:D:62:ARG:HG3	1:D:71:ILE:HD12	1.91	0.52
3:G:76:ILE:HD12	3:G:177:PRO:HA	1.91	0.52
1:A:66:SER:OG	1:A:67:PRO:CD	2.56	0.52
3:F:10:ARG:NH2	3:F:11:LEU:HD21	2.24	0.52
4:H:63:CYS:HB2	4:H:67:VAL:CG2	2.38	0.52
5:H:1203:HIS:C	5:H:1203:HIS:CD2	2.83	0.52
2:C:244:THR:HA	3:G:182:THR:HG22	1.92	0.52
1:B:246:SER:CB	1:B:248:ARG:HG3	2.38	0.52
2:C:138:LEU:HD11	2:C:179:ILE:HD13	1.91	0.52
3:G:107:THR:CG2	3:G:113:THR:HG21	2.27	0.52
4:H:65:THR:CG2	5:H:1204:HIS:HB3	2.37	0.52
1:A:55:THR:HB	1:A:96:GLU:CD	2.30	0.52
3:F:26:PHE:O	3:F:35:GLU:O	2.26	0.52
1:A:123:GLY:HA3	1:A:245:SER:HB2	1.92	0.52
2:C:22:SER:O	2:C:73:VAL:HA	2.09	0.52
3:G:135:LEU:HA	3:G:138:ILE:HG12	1.92	0.52
3:G:172:HIS:NE2	5:G:1206:HIS:ND1	2.52	0.52
5:C:1275:HIS:CB	3:G:78:PRO:HB3	2.37	0.52
2:C:98:VAL:HG13	2:C:98:VAL:O	2.08	0.52
3:F:88:MET:CE	3:F:109:PHE:CD1	2.93	0.52
3:G:184:ARG:HH11	3:G:184:ARG:CG	2.23	0.52
2:C:138:LEU:HD11	2:C:179:ILE:CD1	2.40	0.51
4:H:6:ILE:HD13	4:H:16:MET:SD	2.49	0.51
1:A:247:SER:OG	4:H:182:THR:HG21	2.11	0.51
4:H:75:LEU:H	4:H:75:LEU:CD2	2.23	0.51
1:B:186:ARG:HB3	1:B:191:HIS:CD2	2.46	0.51
3:E:6:ILE:CD1	3:E:41:CYS:SG	2.98	0.51
3:F:89:VAL:O	3:F:146:VAL:HA	2.10	0.51
1:B:184:ILE:HD11	5:E:1204:HIS:HA	1.92	0.51
4:H:60:ILE:HD11	4:H:187:VAL:HG13	1.91	0.51
3:E:19:LEU:C	3:E:24:VAL:HG12	2.31	0.51
3:E:56:GLY:HA2	3:E:176:ASN:ND2	2.24	0.51
4:H:88:MET:HE3	4:H:146:VAL:HG13	1.91	0.51
1:B:121:PHE:CE1	1:B:250:VAL:HG13	2.45	0.51
3:F:172:HIS:HE1	5:F:1204:HIS:CB	1.89	0.51
3:F:70:GLU:CD	3:F:111:ASN:HB2	2.31	0.51
3:F:107:THR:OG1	3:F:113:THR:HG21	2.10	0.51
3:E:180:TYR:OH	5:E:1204:HIS:HA	2.11	0.51
1:A:2:ASP:HB3	1:A:273:LYS:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:O	1:A:271:GLU:CB	2.57	0.50
3:E:29:GLU:HG2	3:E:34:ARG:HG3	1.91	0.50
2:C:261:GLU:O	2:C:262:LYS:CB	2.59	0.50
3:E:136:ALA:N	3:E:137:PRO:HD2	2.26	0.50
3:E:105:ILE:HA	3:E:144:LEU:O	2.11	0.50
1:A:57:THR:O	1:A:61:HIS:HB2	2.11	0.50
1:A:127:VAL:HG23	1:A:127:VAL:O	2.12	0.50
3:F:109:PHE:CZ	3:F:148:ILE:HD11	2.46	0.50
1:A:226:THR:O	1:A:227:LEU:CB	2.50	0.50
1:A:127:VAL:O	1:A:127:VAL:CG2	2.60	0.50
1:B:91:TYR:H	1:B:271:GLU:HA	1.76	0.50
5:C:1275:HIS:C	5:C:1275:HIS:CD2	2.84	0.50
3:E:88:MET:HE3	3:E:146:VAL:CG2	2.40	0.50
2:C:134:LEU:CD2	2:C:225:LEU:HG	2.41	0.50
4:H:138:ILE:O	4:H:139:ALA:HB2	2.10	0.50
1:B:75:TYR:CZ	1:B:94:GLY:HA3	2.46	0.49
1:D:192:LEU:O	1:D:202:ARG:NH2	2.45	0.49
1:D:197:LEU:N	1:D:197:LEU:HD23	2.27	0.49
1:B:234:TYR:HB3	1:B:238:ILE:HD11	1.93	0.49
3:E:19:LEU:HB3	3:E:24:VAL:CG1	2.42	0.49
3:E:49:VAL:N	3:E:50:PRO:HD2	2.28	0.49
4:H:74:SER:O	4:H:74:SER:OG	2.28	0.49
2:C:2:ASP:OD2	1:D:61:HIS:ND1	2.44	0.49
2:C:155:ASP:OD1	2:C:229:ARG:NE	2.46	0.49
4:H:13:GLU:O	4:H:17:THR:HG22	2.13	0.49
1:B:90:GLU:HB2	1:B:271:GLU:CG	2.42	0.49
2:C:69:SER:CB	7:C:2016:HOH:O	2.60	0.49
1:D:155:ASP:OD1	1:D:229:ARG:NH1	2.41	0.49
2:C:234:TYR:HB3	2:C:238:ILE:HD11	1.95	0.49
3:E:132:SER:HB3	3:E:135:LEU:HD22	1.95	0.49
3:F:29:GLU:HA	3:F:34:ARG:HG3	1.94	0.49
1:A:100:ARG:HD2	1:A:255:GLU:HG2	1.95	0.48
2:C:155:ASP:OD1	2:C:229:ARG:CZ	2.61	0.48
2:C:67:PRO:O	2:C:68:GLU:HB2	2.13	0.48
1:D:240:THR:HG22	1:D:249:LEU:CD1	2.43	0.48
3:E:4:LEU:HD22	3:E:60:ILE:HB	1.94	0.48
7:A:2023:HOH:O	5:H:1204:HIS:CD2	2.65	0.48
3:F:53:LEU:HD11	3:F:174:VAL:CG2	2.44	0.48
2:C:68:GLU:HA	2:C:68:GLU:OE1	2.12	0.48
1:B:135:TYR:CD1	1:B:231:ILE:HG13	2.48	0.48
1:B:170:LYS:O	1:B:171:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:VAL:HG22	1:A:221:VAL:HA	1.96	0.48
1:B:100:ARG:HH22	1:B:262:LYS:HG2	1.79	0.48
1:B:132:THR:HG22	1:B:236:GLY:N	2.25	0.48
1:D:142:ILE:HG22	1:D:147:HIS:CD2	2.48	0.48
1:D:234:TYR:CB	1:D:238:ILE:HD11	2.44	0.48
3:F:107:THR:CG2	3:F:146:VAL:HB	2.43	0.48
4:H:37:LYS:O	4:H:38:ASP:CB	2.54	0.48
1:A:129:ILE:HG22	1:A:130:GLY:N	2.28	0.48
1:B:66:SER:N	1:B:67:PRO:HD3	2.28	0.48
1:D:185:TYR:O	1:D:186:ARG:HD3	2.14	0.48
4:H:1:MET:N	4:H:186:LYS:NZ	2.61	0.48
2:C:70:GLN:HE22	2:C:101:ASN:HD21	1.61	0.48
4:H:166:ILE:HG22	4:H:167:PHE:CD2	2.49	0.48
3:F:18:TYR:HE1	3:F:81:ILE:HG23	1.78	0.47
3:F:109:PHE:O	3:F:113:THR:HG22	2.14	0.47
4:H:135:LEU:HA	4:H:138:ILE:HD12	1.96	0.47
1:A:186:ARG:HH21	1:A:191:HIS:CD2	2.32	0.47
3:E:78:PRO:HB3	5:E:1204:HIS:CB	2.25	0.47
4:H:183:LYS:O	4:H:187:VAL:HG23	2.13	0.47
1:A:127:VAL:HG21	1:A:212:LEU:HD13	1.96	0.47
2:C:42:ASP:OD1	1:D:82:TYR:OH	2.28	0.47
1:A:75:TYR:O	1:A:76:ALA:CB	2.62	0.47
2:C:55:THR:HB	2:C:96:GLU:OE1	2.14	0.47
1:D:216:PHE:HB3	1:D:219:VAL:HG13	1.97	0.47
2:C:62:ARG:CG	2:C:63:LYS:N	2.75	0.47
1:A:62:ARG:HB2	1:A:71:ILE:HD13	1.95	0.47
3:E:71:LYS:C	3:E:73:THR:N	2.68	0.47
3:F:89:VAL:HG13	3:F:164:ASP:O	2.15	0.47
3:G:1:MET:SD	3:G:40:VAL:HG23	2.55	0.47
1:D:16:ALA:HB1	1:D:21:PHE:HB2	1.96	0.47
1:D:186:ARG:HB3	1:D:191:HIS:CG	2.49	0.47
1:D:234:TYR:HB2	1:D:238:ILE:HD11	1.96	0.47
3:F:53:LEU:CD1	3:F:174:VAL:HG23	2.44	0.47
3:F:79:PHE:O	3:F:173:VAL:HG12	2.15	0.47
5:G:1206:HIS:C	5:G:1206:HIS:CD2	2.87	0.47
4:H:69:LEU:O	4:H:115:ARG:NH2	2.47	0.47
5:C:1275:HIS:HB3	3:G:78:PRO:CB	2.38	0.47
3:F:152:GLY:O	3:F:156:LYS:HG3	2.15	0.47
3:G:87:ARG:HH11	3:G:165:GLU:HG3	1.80	0.47
3:E:118:GLU:C	3:E:120:LYS:H	2.18	0.47
4:H:150:GLU:HG3	6:H:1202:PO4:O3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PHE:CZ	1:A:250:VAL:CG2	2.98	0.47
3:E:64:GLY:HA2	3:E:171:THR:HA	1.97	0.47
1:B:154:ILE:HD13	1:B:176:VAL:HG13	1.97	0.46
2:C:61:HIS:HB3	2:C:62:ARG:H	1.50	0.46
3:E:194:LEU:O	3:E:198:ILE:HG13	2.15	0.46
3:G:167:PHE:HE1	3:G:169:ILE:CG2	2.28	0.46
1:A:173:LEU:HD23	1:A:173:LEU:HA	1.76	0.46
1:D:242:TYR:CZ	3:F:181:ARG:HD3	2.49	0.46
3:E:4:LEU:HA	3:E:60:ILE:O	2.15	0.46
4:H:63:CYS:HB2	4:H:67:VAL:HG21	1.97	0.46
3:F:17:THR:HG21	7:F:2002:HOH:O	2.15	0.46
3:F:201:ASP:OD1	3:F:201:ASP:N	2.47	0.46
3:G:76:ILE:HG21	3:G:180:TYR:HE2	1.80	0.46
1:A:245:SER:C	1:A:246:SER:O	2.52	0.46
1:D:248:ARG:HA	3:F:178:VAL:HG21	1.98	0.46
3:E:1:MET:HE3	3:E:40:VAL:CG1	2.43	0.46
3:E:53:LEU:CD1	3:E:174:VAL:HG23	2.46	0.46
3:E:150:GLU:HG3	6:E:1202:PO4:O4	2.16	0.46
3:E:178:VAL:O	3:E:182:THR:HB	2.15	0.46
1:D:162:ILE:HD13	1:D:180:ILE:HD12	1.98	0.46
4:H:81:ILE:HD11	4:H:173:VAL:HG12	1.96	0.46
1:A:13:TYR:CE1	1:A:17:THR:HG21	2.51	0.46
1:D:231:ILE:CG2	1:D:232:GLU:N	2.79	0.46
1:D:240:THR:CG2	1:D:249:LEU:HD11	2.45	0.46
1:A:186:ARG:NH2	1:A:191:HIS:HB3	2.30	0.46
1:B:62:ARG:NH1	1:B:69:SER:O	2.49	0.46
1:B:141:GLU:OE2	1:B:175:ARG:HD3	2.15	0.46
2:C:134:LEU:O	2:C:134:LEU:CD1	2.61	0.46
1:D:195:MET:HB2	1:D:197:LEU:HD21	1.95	0.46
1:D:153:LEU:HD23	1:D:161:GLU:HB3	1.98	0.46
3:E:53:LEU:HD13	3:E:174:VAL:HG23	1.98	0.46
3:G:26:PHE:O	3:G:35:GLU:O	2.34	0.46
3:G:37:LYS:O	3:G:38:ASP:CB	2.63	0.46
1:A:123:GLY:H	1:A:245:SER:CB	2.29	0.46
1:D:51:ARG:NH1	1:D:78:PHE:O	2.45	0.46
1:B:161:GLU:OE2	3:E:170:ARG:NH2	2.49	0.45
2:C:138:LEU:HD21	2:C:179:ILE:HD12	1.97	0.45
2:C:216:PHE:HB3	2:C:219:VAL:HG13	1.97	0.45
4:H:154:THR:OG1	6:H:1202:PO4:O4	2.34	0.45
4:H:166:ILE:HG22	4:H:167:PHE:HD2	1.80	0.45
2:C:124:PRO:HD2	2:C:244:THR:OG1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:184:ARG:HD2	7:G:2017:HOH:O	2.16	0.45
1:D:71:ILE:HB	1:D:98:VAL:HG12	1.98	0.45
3:G:135:LEU:O	3:G:136:ALA:HB2	2.13	0.45
1:B:186:ARG:HB3	1:B:191:HIS:NE2	2.31	0.45
1:A:146:LEU:HD22	1:A:169:LYS:HZ3	1.81	0.45
2:C:69:SER:HB3	7:C:2016:HOH:O	2.17	0.45
4:H:71:LYS:HB2	4:H:73:THR:HG23	1.98	0.45
4:H:88:MET:HG3	4:H:167:PHE:CZ	2.51	0.45
1:D:26:VAL:O	1:D:51:ARG:NH2	2.49	0.45
1:A:257:THR:HG22	7:A:2038:HOH:O	2.16	0.45
1:B:26:VAL:O	1:B:51:ARG:NH2	2.48	0.45
1:B:40:PHE:CE1	1:B:50:ILE:HB	2.52	0.45
2:C:228:ALA:O	2:C:231:ILE:CG2	2.52	0.45
3:G:36:GLY:O	3:G:38:ASP:OD1	2.34	0.45
4:H:6:ILE:CD1	4:H:41:CYS:SG	3.05	0.45
4:H:53:LEU:CD1	4:H:174:VAL:CG2	2.91	0.45
5:H:1204:HIS:CD2	5:H:1204:HIS:C	2.89	0.45
1:A:67:PRO:O	1:A:68:ASP:CB	2.64	0.45
1:B:42:ASP:OD1	1:B:42:ASP:C	2.54	0.45
1:B:140:LYS:NZ	1:B:144:LYS:HE3	2.32	0.45
2:C:69:SER:HB2	2:C:70:GLN:H	1.37	0.45
2:C:134:LEU:HD21	2:C:225:LEU:HG	1.98	0.45
1:D:158:ASN:O	1:D:162:ILE:HD12	2.17	0.45
1:D:240:THR:HG22	1:D:249:LEU:HD11	1.98	0.45
3:G:24:VAL:HG13	3:G:39:ILE:HG21	1.97	0.45
3:G:53:LEU:CD2	3:G:174:VAL:CG2	2.92	0.45
2:C:75:TYR:CZ	2:C:94:GLY:HA3	2.51	0.45
2:C:139:LEU:HA	2:C:142:ILE:HD12	1.99	0.45
1:D:127:VAL:HG11	1:D:212:LEU:HD13	1.98	0.45
4:H:1:MET:H3	4:H:186:LYS:HZ1	1.65	0.45
4:H:1:MET:H2	4:H:186:LYS:NZ	2.15	0.44
2:C:134:LEU:HD11	2:C:225:LEU:HB3	1.98	0.44
1:D:19:LYS:HG3	1:D:108:GLU:OE1	2.17	0.44
1:D:226:THR:O	1:D:228:ALA:N	2.48	0.44
3:F:108:LYS:HB2	3:F:108:LYS:HE2	1.74	0.44
3:G:106:ALA:HB3	3:G:145:ILE:HG22	1.99	0.44
1:B:140:LYS:HA	1:B:140:LYS:HD3	1.63	0.44
1:D:76:ALA:HB2	1:D:93:LEU:HD23	2.00	0.44
1:D:247:SER:HA	3:F:182:THR:HG21	1.98	0.44
3:G:103:LYS:H	3:G:103:LYS:HG2	1.54	0.44
1:D:9:VAL:HG22	1:D:93:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:MET:CB	1:D:197:LEU:CD2	2.84	0.44
1:A:123:GLY:N	1:A:245:SER:HB2	2.33	0.44
1:B:34:GLU:HA	1:B:35:PRO:HD3	1.89	0.44
1:B:132:THR:HG21	1:B:236:GLY:H	1.81	0.44
2:C:65:TYR:N	2:C:65:TYR:CD1	2.85	0.44
3:E:50:PRO:HB2	3:E:73:THR:HG21	2.00	0.44
3:G:14:LYS:HE3	7:G:2002:HOH:O	2.17	0.44
3:G:19:LEU:O	3:G:22:THR:HB	2.18	0.44
1:A:1:MET:CE	1:B:71:ILE:HG12	2.48	0.44
1:A:161:GLU:OE2	5:H:1204:HIS:NE2	2.51	0.44
3:F:20:LYS:C	3:F:22:THR:H	2.20	0.44
7:G:2011:HOH:O	4:H:45:ARG:HD2	2.17	0.44
1:A:257:THR:HG23	1:A:257:THR:O	2.18	0.44
3:G:15:VAL:O	3:G:18:TYR:HB2	2.17	0.44
3:G:50:PRO:HG2	3:G:71:LYS:HG3	1.99	0.44
1:B:231:ILE:HG22	1:B:232:GLU:HG3	1.99	0.44
2:C:71:ILE:HD12	2:C:98:VAL:HG12	2.00	0.44
2:C:71:ILE:HD13	2:C:71:ILE:O	2.17	0.44
2:C:146:LEU:HD11	2:C:169:LYS:HG2	2.00	0.44
3:G:65:THR:HB	3:G:169:ILE:CG2	2.15	0.44
3:G:86:SER:OG	3:G:169:ILE:HG13	2.17	0.44
4:H:108:LYS:C	4:H:110:PRO:HD3	2.37	0.44
3:F:194:LEU:HD21	3:F:198:ILE:HD11	2.00	0.43
1:B:231:ILE:HG22	1:B:232:GLU:N	2.33	0.43
1:B:43:ARG:HG3	1:B:43:ARG:O	2.18	0.43
2:C:226:THR:O	2:C:227:LEU:CB	2.39	0.43
2:C:244:THR:HA	3:G:182:THR:CG2	2.48	0.43
3:E:88:MET:HG3	3:E:167:PHE:CZ	2.53	0.43
3:G:127:ILE:HG21	3:G:141:LEU:HD13	2.00	0.43
1:D:121:PHE:CZ	1:D:250:VAL:HG22	2.52	0.43
1:A:4:LEU:O	1:A:6:PHE:N	2.52	0.43
2:C:154:ILE:CD1	2:C:226:THR:HA	2.48	0.43
1:A:156:THR:HG21	4:H:77:GLN:HE21	1.84	0.43
1:A:228:ALA:O	1:A:231:ILE:HB	2.19	0.43
1:B:142:ILE:HG12	1:B:173:LEU:HD23	2.01	0.43
3:E:176:ASN:OD1	3:E:178:VAL:HG22	2.19	0.43
3:F:175:VAL:CG1	3:F:180:TYR:HD2	2.09	0.43
1:A:123:GLY:H	1:A:245:SER:HB3	1.84	0.43
1:B:13:TYR:O	1:B:17:THR:OG1	2.31	0.43
1:B:186:ARG:HB3	1:B:191:HIS:CE1	2.53	0.43
3:F:107:THR:HG21	3:F:113:THR:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:118:GLU:O	3:E:120:LYS:N	2.51	0.43
1:B:149:LYS:HE3	1:B:153:LEU:HD11	2.01	0.43
1:B:158:ASN:ND2	1:B:161:GLU:H	2.17	0.43
2:C:171:ILE:HG22	2:C:173:LEU:CD2	2.49	0.43
1:D:195:MET:C	1:D:197:LEU:HD23	2.39	0.43
3:G:109:PHE:O	3:G:113:THR:CG2	2.66	0.43
2:C:51:ARG:HB2	7:C:2011:HOH:O	2.19	0.42
1:A:157:LYS:HB2	4:H:76:ILE:HD12	2.00	0.42
1:A:248:ARG:CD	1:A:249:LEU:H	2.05	0.42
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.90	0.42
3:G:79:PHE:O	3:G:173:VAL:HG13	2.20	0.42
4:H:134:GLU:OE2	4:H:154:THR:HG22	2.19	0.42
1:A:95:LEU:HD12	1:A:113:ILE:HD13	2.01	0.42
4:H:172:HIS:NE2	5:H:1204:HIS:HB2	2.34	0.42
1:A:13:TYR:O	1:A:17:THR:CG2	2.65	0.42
1:B:169:LYS:O	1:B:171:ILE:HD12	2.18	0.42
2:C:34:GLU:HA	2:C:35:PRO:HD3	1.91	0.42
1:D:100:ARG:HD3	1:D:264:VAL:HG22	2.01	0.42
1:D:271:GLU:HB3	1:D:272:GLY:H	1.47	0.42
4:H:4:LEU:HB2	4:H:41:CYS:HB3	2.02	0.42
1:A:59:LEU:C	1:A:61:HIS:H	2.22	0.42
1:B:66:SER:N	1:B:67:PRO:CD	2.83	0.42
2:C:153:LEU:HB3	2:C:162:ILE:CD1	2.49	0.42
2:C:229:ARG:NH2	3:G:74:SER:OG	2.53	0.42
1:D:178:LYS:HE2	1:D:195:MET:HA	2.01	0.42
3:E:1:MET:HE1	3:E:40:VAL:N	2.34	0.42
3:G:117:CYS:O	3:G:122:TRP:HB2	2.19	0.42
4:H:76:ILE:HG12	4:H:175:VAL:HB	2.02	0.42
1:A:62:ARG:NH1	1:A:69:SER:O	2.52	0.42
1:D:19:LYS:HE2	1:D:108:GLU:OE1	2.19	0.42
3:E:3:LYS:HG2	3:E:40:VAL:HG22	2.01	0.42
3:G:79:PHE:CE1	3:G:173:VAL:HG11	2.54	0.42
3:G:138:ILE:HD13	3:G:138:ILE:H	1.83	0.42
1:A:42:ASP:C	1:A:44:LYS:H	2.23	0.42
2:C:44:LYS:HG3	1:D:82:TYR:CE1	2.54	0.42
2:C:255:GLU:HG2	2:C:264:VAL:HG13	2.01	0.42
1:D:42:ASP:OD1	1:D:46:ASN:HB2	2.20	0.42
1:D:70:GLN:O	1:D:71:ILE:HG13	2.20	0.42
3:G:77:GLN:OE1	5:G:1206:HIS:HA	2.20	0.42
3:G:180:TYR:HD1	3:G:180:TYR:O	2.03	0.42
4:H:81:ILE:HB	4:H:171:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:MET:HE2	1:D:61:HIS:C	2.39	0.42
2:C:259:ASN:C	2:C:261:GLU:H	2.24	0.42
1:D:19:LYS:HG3	1:D:108:GLU:CD	2.40	0.42
3:E:37:LYS:O	3:E:38:ASP:HB2	2.18	0.42
3:F:136:ALA:N	3:F:137:PRO:CD	2.82	0.42
1:D:62:ARG:CD	1:D:71:ILE:HD12	2.50	0.41
3:E:134:GLU:H	3:E:134:GLU:HG2	1.49	0.41
1:D:225:LEU:CD1	1:D:225:LEU:N	2.83	0.41
3:E:32:ILE:HD13	3:E:32:ILE:HG21	1.77	0.41
3:G:53:LEU:HD12	3:G:53:LEU:HA	1.84	0.41
4:H:6:ILE:HD12	4:H:41:CYS:HB2	2.02	0.41
1:D:131:HIS:HB2	1:D:205:LEU:HD11	2.02	0.41
1:D:195:MET:HB3	1:D:197:LEU:HD22	1.95	0.41
3:G:33:LEU:HD22	3:G:35:GLU:HG2	2.01	0.41
1:B:216:PHE:HB3	1:B:219:VAL:HG13	2.01	0.41
3:E:50:PRO:HG3	3:E:71:LYS:HG3	2.03	0.41
3:F:193:LYS:O	3:F:197:VAL:HG13	2.20	0.41
3:G:57:VAL:HG21	4:H:141:LEU:HG	2.03	0.41
4:H:86:SER:HB3	4:H:150:GLU:HB3	2.03	0.41
1:D:115:GLU:O	1:D:119:GLU:HG3	2.21	0.41
3:E:53:LEU:CD1	3:E:174:VAL:CG2	2.98	0.41
4:H:55:HIS:HB2	7:H:2009:HOH:O	2.21	0.41
4:H:70:GLU:O	4:H:70:GLU:HG3	2.19	0.41
3:G:56:GLY:HA2	3:G:176:ASN:ND2	2.36	0.41
4:H:66:ASP:OD1	4:H:66:ASP:N	2.53	0.41
4:H:113:THR:HB	4:H:146:VAL:HG21	2.02	0.41
1:A:151:LEU:HA	1:A:154:ILE:CG2	2.51	0.41
1:A:262:LYS:H	1:A:262:LYS:HG2	1.35	0.41
1:B:123:GLY:CA	1:B:243:ASP:OD1	2.67	0.41
3:G:188:VAL:O	3:G:192:GLU:HB2	2.19	0.41
4:H:6:ILE:HD12	4:H:41:CYS:CB	2.50	0.41
1:A:13:TYR:CD1	1:A:74:TRP:CZ2	3.06	0.41
1:A:134:VAL:HG23	1:A:197:LEU:HD22	2.02	0.41
1:B:89:ALA:O	1:B:272:GLY:O	2.38	0.41
2:C:134:LEU:O	2:C:134:LEU:CG	2.68	0.41
1:D:113:ILE:HD13	1:D:266:GLY:HA3	2.03	0.41
3:F:89:VAL:CG1	3:F:90:LEU:O	2.68	0.41
3:F:102:GLU:O	3:F:102:GLU:HG3	2.19	0.41
3:G:170:ARG:HE	3:G:170:ARG:HB3	1.66	0.41
4:H:104:ARG:HG3	4:H:143:ASP:OD2	2.20	0.41
1:A:159:LEU:HD11	1:A:181:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:SER:HA	1:A:189:PRO:HD3	1.96	0.41
2:C:72:LYS:HE2	2:C:97:LYS:HE3	2.03	0.41
2:C:100:ARG:CG	2:C:264:VAL:HG22	2.42	0.41
3:E:24:VAL:CG2	3:E:39:ILE:HG21	2.50	0.41
3:G:6:ILE:HA	3:G:7:PRO:HD3	1.95	0.41
4:H:136:ALA:HB3	4:H:137:PRO:CD	2.51	0.41
1:D:131:HIS:HA	1:D:236:GLY:O	2.21	0.40
1:D:189:PRO:HA	1:D:223:ILE:CD1	2.48	0.40
3:E:53:LEU:HD13	3:E:174:VAL:CG2	2.51	0.40
3:E:178:VAL:HG22	3:E:178:VAL:H	1.48	0.40
1:A:132:THR:HG21	1:A:235:CYS:HA	2.03	0.40
2:C:71:ILE:HD12	2:C:98:VAL:CG1	2.51	0.40
2:C:132:THR:CG2	2:C:236:GLY:H	2.35	0.40
2:C:187:ARG:HD3	3:G:184:ARG:HE	1.86	0.40
1:D:26:VAL:HG11	1:D:61:HIS:CE1	2.57	0.40
1:D:128:GLU:O	1:D:239:PHE:HA	2.22	0.40
3:E:151:THR:H	3:E:151:THR:HG1	1.58	0.40
3:F:34:ARG:HB2	3:F:41:CYS:HB2	2.03	0.40
3:G:68:LEU:O	3:G:71:LYS:O	2.39	0.40
3:G:180:TYR:O	3:G:184:ARG:HB2	2.20	0.40
1:A:132:THR:HB	1:A:236:GLY:H	1.86	0.40
1:B:139:LEU:HD12	1:B:139:LEU:HA	1.84	0.40
3:E:179:SER:HA	3:E:182:THR:HG22	2.01	0.40
1:B:3:PHE:CD2	1:B:3:PHE:C	2.95	0.40
1:B:241:ILE:HD13	1:B:241:ILE:HG21	1.81	0.40
2:C:153:LEU:HD23	2:C:162:ILE:HG13	2.03	0.40
3:F:37:LYS:HE2	3:F:38:ASP:OD2	2.21	0.40
3:G:16:MET:HE1	3:G:26:PHE:CZ	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:GLU:OE1	3:G:1:MET:N[4_554]	2.13	0.07

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	273/275 (99%)	238 (87%)	25 (9%)	10 (4%)	3	4
1	B	273/275 (99%)	242 (89%)	24 (9%)	7 (3%)	5	7
1	D	272/275 (99%)	237 (87%)	25 (9%)	10 (4%)	3	4
2	C	273/275 (99%)	238 (87%)	17 (6%)	18 (7%)	1	1
3	E	200/208 (96%)	183 (92%)	11 (6%)	6 (3%)	4	5
3	F	201/208 (97%)	183 (91%)	11 (6%)	7 (4%)	3	4
3	G	202/208 (97%)	180 (89%)	15 (7%)	7 (4%)	3	4
4	H	200/208 (96%)	190 (95%)	6 (3%)	4 (2%)	7	11
All	All	1894/1932 (98%)	1691 (89%)	134 (7%)	69 (4%)	3	4

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	ALA
1	A	174	SER
1	A	227	LEU
1	A	271	GLU
1	B	141	GLU
1	B	273	LYS
2	C	61	HIS
2	C	64	ARG
2	C	65	TYR
2	C	66	SER
2	C	68	GLU
2	C	69	SER
2	C	134	LEU
2	C	227	LEU
2	C	261	GLU
2	C	262	LYS
1	D	134	VAL

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Mol	Chain	Res	Type
1	D	271	GLU
1	D	272	GLY
3	E	72	GLU
3	F	29	GLU
3	F	103	LYS
3	F	202	SER
3	G	136	ALA
4	H	38	ASP
4	H	136	ALA
1	A	5	ASP
1	A	68	ASP
1	B	43	ARG
1	B	149	LYS
1	B	158	ASN
2	C	63	LYS
2	C	133	GLY
2	C	259	ASN
1	D	4	LEU
1	D	146	LEU
3	G	37	LYS
3	G	38	ASP
4	H	139	ALA
1	B	18	LYS
2	C	139	LEU
3	E	119	SER
3	F	102	GLU
3	G	36	GLY
3	G	102	GLU
4	H	132	SER
1	A	64	ARG
1	A	170	LYS
1	A	246	SER
1	D	68	ASP
1	D	69	SER
1	D	261	GLU
3	E	201	ASP
3	F	101	GLY
3	G	72	GLU
1	A	43	ARG
2	C	140	LYS
2	C	233	GLU
1	D	135	TYR

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Mol	Chain	Res	Type
1	D	259	ASN
3	E	85	ILE
3	E	96	ARG
2	C	5	ASP
3	G	202	SER
3	E	32	ILE
1	B	66	SER
2	C	37	GLY
3	F	97	GLY
3	F	39	ILE

5.3.2 Protein sidechains (i)

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	247/247 (100%)	193 (78%)	54 (22%)	1 1
1	B	247/247 (100%)	190 (77%)	57 (23%)	1 1
1	D	246/247 (100%)	188 (76%)	58 (24%)	1 1
2	C	246/247 (100%)	191 (78%)	55 (22%)	1 1
3	E	181/187 (97%)	136 (75%)	45 (25%)	0 1
3	F	182/187 (97%)	141 (78%)	41 (22%)	1 1
3	G	183/187 (98%)	141 (77%)	42 (23%)	1 1
4	H	181/187 (97%)	145 (80%)	36 (20%)	1 2
All	All	1713/1736 (99%)	1325 (77%)	388 (23%)	1 1

All (388) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	4	LEU
1	A	17	THR
1	A	33	GLU
1	A	43	ARG

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Mol	Chain	Res	Type
1	A	54	PHE
1	A	55	THR
1	A	56	LYS
1	A	61	HIS
1	A	62	ARG
1	A	66	SER
1	A	68	ASP
1	A	70	GLN
1	A	71	ILE
1	A	73	VAL
1	A	83	SER
1	A	85	SER
1	A	87	LEU
1	A	96	GLU
1	A	103	LEU
1	A	122	GLU
1	A	125	VAL
1	A	132	THR
1	A	134	VAL
1	A	144	LYS
1	A	145	ASP
1	A	146	LEU
1	A	147	HIS
1	A	152	ASN
1	A	154	ILE
1	A	156	THR
1	A	159	LEU
1	A	161	GLU
1	A	162	ILE
1	A	166	SER
1	A	167	HIS
1	A	171	ILE
1	A	172	ASP
1	A	178	LYS
1	A	187	ARG
1	A	196	ASP
1	A	200	SER
1	A	223	ILE
1	A	225	LEU
1	A	229	ARG
1	A	232	GLU
1	A	233	GLU

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Mol	Chain	Res	Type
1	A	248	ARG
1	A	250	VAL
1	A	262	LYS
1	A	264	VAL
1	A	270	LEU
1	A	273	LYS
1	A	274	THR
1	B	7	GLU
1	B	18	LYS
1	B	22	SER
1	B	33	GLU
1	B	41	LEU
1	B	42	ASP
1	B	43	ARG
1	B	49	SER
1	B	54	PHE
1	B	56	LYS
1	B	59	LEU
1	B	62	ARG
1	B	66	SER
1	B	71	ILE
1	B	83	SER
1	B	85	SER
1	B	87	LEU
1	B	103	LEU
1	B	111	GLU
1	B	113	ILE
1	B	122	GLU
1	B	132	THR
1	B	136	GLU
1	B	139	LEU
1	B	140	LYS
1	B	145	ASP
1	B	146	LEU
1	B	150	VAL
1	B	156	THR
1	B	158	ASN
1	B	161	GLU
1	B	163	GLU
1	B	165	LEU
1	B	168	MET
1	B	169	LYS

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Mol	Chain	Res	Type
1	B	173	LEU
1	B	175	ARG
1	B	179	ILE
1	B	186	ARG
1	B	188	SER
1	B	215	LYS
1	B	219	VAL
1	B	222	GLU
1	B	225	LEU
1	B	227	LEU
1	B	229	ARG
1	B	231	ILE
1	B	232	GLU
1	B	237	LEU
1	B	238	ILE
1	B	248	ARG
1	B	250	VAL
1	B	262	LYS
1	B	264	VAL
1	B	267	SER
1	B	273	LYS
1	B	275	CYS
2	C	1	MET
2	C	4	LEU
2	C	22	SER
2	C	34	GLU
2	C	41	LEU
2	C	43	ARG
2	C	46	ASN
2	C	47	LEU
2	C	49	SER
2	C	54	PHE
2	C	55	THR
2	C	61	HIS
2	C	62	ARG
2	C	63	LYS
2	C	65	TYR
2	C	71	ILE
2	C	72	LYS
2	C	80	TYR
2	C	85	SER
2	C	87	LEU

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Mol	Chain	Res	Type
2	C	100	ARG
2	C	102	SER
2	C	103	LEU
2	C	122	GLU
2	C	132	THR
2	C	134	LEU
2	C	141	GLU
2	C	144	LYS
2	C	148	GLU
2	C	153	LEU
2	C	154	ILE
2	C	158	ASN
2	C	159	LEU
2	C	161	GLU
2	C	165	LEU
2	C	169	LYS
2	C	179	ILE
2	C	194	THR
2	C	199	LEU
2	C	205	LEU
2	C	215	LYS
2	C	222	GLU
2	C	225	LEU
2	C	231	ILE
2	C	232	GLU
2	C	238	ILE
2	C	247	SER
2	C	248	ARG
2	C	250	VAL
2	C	264	VAL
2	C	267	SER
2	C	270	LEU
2	C	271	GLU
2	C	273	LYS
2	C	274	THR
1	D	4	LEU
1	D	5	ASP
1	D	15	LYS
1	D	19	LYS
1	D	40	PHE
1	D	41	LEU
1	D	43	ARG

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Mol	Chain	Res	Type
1	D	54	PHE
1	D	55	THR
1	D	68	ASP
1	D	81	ARG
1	D	85	SER
1	D	87	LEU
1	D	90	GLU
1	D	98	VAL
1	D	103	LEU
1	D	106	SER
1	D	118	SER
1	D	125	VAL
1	D	132	THR
1	D	134	VAL
1	D	137	ASP
1	D	138	LEU
1	D	139	LEU
1	D	140	LYS
1	D	141	GLU
1	D	142	ILE
1	D	148	GLU
1	D	151	LEU
1	D	152	ASN
1	D	154	ILE
1	D	156	THR
1	D	159	LEU
1	D	167	HIS
1	D	168	MET
1	D	169	LYS
1	D	170	LYS
1	D	171	ILE
1	D	173	LEU
1	D	174	SER
1	D	175	ARG
1	D	178	LYS
1	D	186	ARG
1	D	187	ARG
1	D	188	SER
1	D	193	LYS
1	D	197	LEU
1	D	200	SER
1	D	205	LEU

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Mol	Chain	Res	Type
1	D	210	SER
1	D	219	VAL
1	D	225	LEU
1	D	227	LEU
1	D	229	ARG
1	D	233	GLU
1	D	238	ILE
1	D	250	VAL
1	D	264	VAL
3	E	1	MET
3	E	2	LEU
3	E	10	ARG
3	E	11	LEU
3	E	14	LYS
3	E	20	LYS
3	E	22	THR
3	E	25	ILE
3	E	28	ARG
3	E	31	SER
3	E	38	ASP
3	E	44	VAL
3	E	45	ARG
3	E	51	THR
3	E	63	CYS
3	E	67	VAL
3	E	72	GLU
3	E	74	SER
3	E	75	LEU
3	E	76	ILE
3	E	80	PHE
3	E	87	ARG
3	E	96	ARG
3	E	102	GLU
3	E	103	LYS
3	E	104	ARG
3	E	114	GLN
3	E	118	GLU
3	E	130	LYS
3	E	134	GLU
3	E	142	SER
3	E	150	GLU
3	E	151	THR

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Mol	Chain	Res	Type
3	E	153	ARG
3	E	157	GLU
3	E	160	LEU
3	E	173	VAL
3	E	180	TYR
3	E	181	ARG
3	E	182	THR
3	E	184	ARG
3	E	185	GLU
3	E	186	GLU
3	E	193	LYS
3	E	194	LEU
3	F	1	MET
3	F	10	ARG
3	F	11	LEU
3	F	20	LYS
3	F	22	THR
3	F	27	GLU
3	F	32	ILE
3	F	33	LEU
3	F	38	ASP
3	F	40	VAL
3	F	67	VAL
3	F	72	GLU
3	F	73	THR
3	F	74	SER
3	F	75	LEU
3	F	77	GLN
3	F	80	PHE
3	F	83	THR
3	F	85	ILE
3	F	88	MET
3	F	103	LYS
3	F	104	ARG
3	F	107	THR
3	F	111	ASN
3	F	113	THR
3	F	114	GLN
3	F	125	ARG
3	F	133	VAL
3	F	148	ILE
3	F	151	THR

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Mol	Chain	Res	Type
3	F	153	ARG
3	F	155	LEU
3	F	160	LEU
3	F	168	VAL
3	F	170	ARG
3	F	173	VAL
3	F	176	ASN
3	F	178	VAL
3	F	185	GLU
3	F	197	VAL
3	F	201	ASP
3	G	1	MET
3	G	10	ARG
3	G	11	LEU
3	G	14	LYS
3	G	28	ARG
3	G	31	SER
3	G	32	ILE
3	G	33	LEU
3	G	37	LYS
3	G	47	PHE
3	G	51	THR
3	G	53	LEU
3	G	67	VAL
3	G	73	THR
3	G	74	SER
3	G	75	LEU
3	G	77	GLN
3	G	80	PHE
3	G	87	ARG
3	G	100	GLU
3	G	103	LYS
3	G	113	THR
3	G	114	GLN
3	G	120	LYS
3	G	124	CYS
3	G	138	ILE
3	G	141	LEU
3	G	153	ARG
3	G	160	LEU
3	G	165	GLU
3	G	169	ILE

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Mol	Chain	Res	Type
3	G	170	ARG
3	G	173	VAL
3	G	178	VAL
3	G	180	TYR
3	G	183	LYS
3	G	184	ARG
3	G	189	SER
3	G	194	LEU
3	G	196	GLU
3	G	200	HIS
3	G	203	ASN
4	H	1	MET
4	H	2	LEU
4	H	11	LEU
4	H	28	ARG
4	H	30	SER
4	H	31	SER
4	H	34	ARG
4	H	39	ILE
4	H	41	CYS
4	H	51	THR
4	H	75	LEU
4	H	76	ILE
4	H	77	GLN
4	H	80	PHE
4	H	87	ARG
4	H	94	LYS
4	H	96	ARG
4	H	113	THR
4	H	123	HIS
4	H	125	ARG
4	H	130	LYS
4	H	132	SER
4	H	138	ILE
4	H	142	SER
4	H	145	ILE
4	H	153	ARG
4	H	155	LEU
4	H	165	GLU
4	H	174	VAL
4	H	178	VAL
4	H	181	ARG

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Mol	Chain	Res	Type
4	H	182	THR
4	H	184	ARG
4	H	185	GLU
4	H	189	SER
4	H	194	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	70	GLN
1	A	101	ASN
1	A	131	HIS
1	A	147	HIS
1	A	191	HIS
1	B	131	HIS
1	B	158	ASN
1	B	259	ASN
2	C	70	GLN
2	C	158	ASN
2	C	213	GLN
1	D	46	ASN
1	D	152	ASN
3	E	55	HIS
3	E	123	HIS
3	F	77	GLN
3	F	84	ASN
3	F	172	HIS
3	F	200	HIS
3	G	55	HIS
3	G	176	ASN
4	H	77	GLN
4	H	176	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
5	HIS	D	1276	-	6,11,11	1.08	1 (16%)	5,14,14	2.99	3 (60%)
5	HIS	H	1203	-	6,11,11	0.85	0	5,14,14	1.52	1 (20%)
5	HIS	C	1275	-	6,11,11	1.04	1 (16%)	5,14,14	1.64	2 (40%)
5	HIS	H	1204	-	6,11,11	0.96	1 (16%)	5,14,14	1.64	1 (20%)
6	PO4	H	1202	-	4,4,4	1.02	0	6,6,6	0.21	0
6	PO4	F	1203	-	4,4,4	1.15	0	6,6,6	0.72	0
5	HIS	E	1204	-	6,11,11	1.26	1 (16%)	5,14,14	1.71	2 (40%)
5	HIS	E	1205	-	6,11,11	1.24	1 (16%)	5,14,14	2.10	2 (40%)
5	HIS	G	1206	-	6,11,11	1.02	1 (16%)	5,14,14	2.27	2 (40%)
6	PO4	E	1203	-	4,4,4	1.19	0	6,6,6	0.50	0
6	PO4	G	1205	-	4,4,4	0.93	0	6,6,6	0.58	0
6	PO4	E	1202	-	4,4,4	1.30	0	6,6,6	0.98	0
6	PO4	G	1204	-	4,4,4	1.09	0	6,6,6	0.67	0
5	HIS	F	1204	-	6,11,11	1.02	1 (16%)	5,14,14	2.14	2 (40%)

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
5	HIS	D	1276	-	-	6/8/8/8	0/1/1/1
5	HIS	H	1203	-	-	4/8/8/8	0/1/1/1
5	HIS	C	1275	-	-	4/8/8/8	0/1/1/1
5	HIS	H	1204	-	-	4/8/8/8	0/1/1/1
5	HIS	E	1204	-	-	5/8/8/8	0/1/1/1
5	HIS	E	1205	-	-	4/8/8/8	0/1/1/1
5	HIS	G	1206	-	-	5/8/8/8	0/1/1/1
5	HIS	F	1204	-	-	6/8/8/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1205	HIS	OXT-C	-2.53	1.22	1.30
5	D	1276	HIS	OXT-C	-2.38	1.23	1.30
5	C	1275	HIS	OXT-C	-2.29	1.23	1.30
5	E	1204	HIS	CA-N	2.24	1.60	1.48
5	G	1206	HIS	OXT-C	-2.21	1.23	1.30
5	F	1204	HIS	OXT-C	-2.18	1.23	1.30
5	H	1204	HIS	OXT-C	-2.03	1.24	1.30

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1276	HIS	OXT-C-O	-5.44	111.74	124.08
5	G	1206	HIS	OXT-C-O	-4.02	114.96	124.08
5	F	1204	HIS	OXT-C-O	-3.59	115.94	124.08
5	E	1205	HIS	OXT-C-O	-3.38	116.41	124.08
5	E	1205	HIS	CD2-NE2-CE1	2.53	109.71	105.72
5	E	1204	HIS	OXT-C-O	-2.52	118.37	124.08
5	F	1204	HIS	CD2-NE2-CE1	2.49	109.66	105.72
5	D	1276	HIS	CD2-NE2-CE1	2.48	109.64	105.72
5	D	1276	HIS	CB-CG-CD2	2.47	132.17	127.75
5	H	1203	HIS	CB-CG-CD2	2.46	132.13	127.75
5	C	1275	HIS	OXT-C-O	-2.28	118.90	124.08
5	H	1204	HIS	CB-CG-CD2	2.27	131.80	127.75
5	G	1206	HIS	CB-CG-CD2	2.17	131.62	127.75
5	E	1204	HIS	CD2-NE2-CE1	2.08	109.01	105.72
5	C	1275	HIS	CD2-NE2-CE1	2.05	108.97	105.72

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1275	HIS	CA-CB-CG-ND1
5	C	1275	HIS	CA-CB-CG-CD2
5	D	1276	HIS	O-C-CA-N
5	D	1276	HIS	C-CA-CB-CG
5	E	1204	HIS	O-C-CA-N
5	E	1204	HIS	CA-CB-CG-ND1
5	E	1204	HIS	CA-CB-CG-CD2
5	G	1206	HIS	N-CA-CB-CG
5	G	1206	HIS	C-CA-CB-CG
5	G	1206	HIS	CA-CB-CG-ND1
5	H	1203	HIS	CA-CB-CG-ND1
5	H	1204	HIS	OXT-C-CA-N
5	C	1275	HIS	OXT-C-CA-N
5	D	1276	HIS	OXT-C-CA-N
5	H	1203	HIS	OXT-C-CA-N
5	E	1204	HIS	OXT-C-CA-N
5	E	1205	HIS	OXT-C-CA-N
5	D	1276	HIS	N-CA-CB-CG
5	C	1275	HIS	O-C-CA-N
5	H	1203	HIS	O-C-CA-N
5	H	1204	HIS	O-C-CA-N
5	F	1204	HIS	OXT-C-CA-N
5	G	1206	HIS	OXT-C-CA-N
5	E	1204	HIS	O-C-CA-CB
5	E	1205	HIS	CA-CB-CG-ND1
5	F	1204	HIS	CA-CB-CG-ND1
5	F	1204	HIS	CA-CB-CG-CD2
5	H	1203	HIS	CA-CB-CG-CD2
5	F	1204	HIS	O-C-CA-N
5	G	1206	HIS	O-C-CA-N
5	H	1204	HIS	O-C-CA-CB
5	D	1276	HIS	OXT-C-CA-CB
5	E	1205	HIS	O-C-CA-CB
5	E	1205	HIS	OXT-C-CA-CB
5	D	1276	HIS	O-C-CA-CB
5	F	1204	HIS	O-C-CA-CB
5	H	1204	HIS	OXT-C-CA-CB
5	F	1204	HIS	OXT-C-CA-CB

There are no ring outliers.

9 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1203	HIS	12	0
5	C	1275	HIS	7	0
5	H	1204	HIS	11	0
6	H	1202	PO4	2	0
5	E	1204	HIS	9	0
5	E	1205	HIS	6	0
5	G	1206	HIS	6	0
6	E	1202	PO4	2	0
5	F	1204	HIS	8	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	33:GLU	C	34:GLU	N	0.94

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	275/275 (100%)	-0.10	6 (2%)	62	65	9, 27, 50, 61	3 (1%)
1	B	275/275 (100%)	-0.09	11 (4%)	38	42	10, 27, 53, 65	6 (2%)
1	D	274/275 (99%)	-0.04	15 (5%)	25	27	8, 28, 49, 61	4 (1%)
2	C	275/275 (100%)	-0.13	13 (4%)	31	34	11, 26, 54, 78	7 (2%)
3	E	202/208 (97%)	-0.01	10 (4%)	28	31	28, 50, 86, 98	2 (0%)
3	F	203/208 (97%)	-0.08	4 (1%)	65	68	10, 27, 50, 62	1 (0%)
3	G	204/208 (98%)	-0.07	10 (4%)	29	32	11, 27, 48, 60	0
4	H	202/208 (97%)	-0.22	2 (0%)	82	84	9, 27, 46, 58	3 (1%)
All	All	1910/1932 (98%)	-0.09	71 (3%)	41	45	8, 28, 58, 98	26 (1%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	202	SER	8.0
2	C	65	TYR	7.6
1	D	68	ASP	6.0
2	C	64	ARG	5.4
3	F	203	ASN	5.3
2	C	66	SER	5.2
1	D	2	ASP	4.8
3	G	203	ASN	4.5
3	G	204	GLU	4.5
2	C	167	HIS	4.4
2	C	63	LYS	4.2
3	F	202	SER	3.8
2	C	275	CYS	3.6
3	E	101	GLY	3.6
1	B	65	TYR	3.6
3	E	102	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	167	HIS	3.4
3	E	123	HIS	3.4
2	C	61	HIS	3.1
1	D	166	SER	3.0
1	B	68	ASP	2.9
1	D	167	HIS	2.9
2	C	67	PRO	2.9
1	B	170	LYS	2.8
3	E	99	PRO	2.8
1	D	259	ASN	2.8
1	B	148	GLU	2.8
1	B	259	ASN	2.7
1	B	260	GLY	2.7
1	D	67	PRO	2.7
3	G	153	ARG	2.7
3	G	10	ARG	2.6
1	A	145	ASP	2.6
1	D	232	GLU	2.6
1	A	148	GLU	2.6
3	G	200	HIS	2.6
3	G	201	ASP	2.6
2	C	31	LYS	2.5
1	A	33	GLU	2.5
4	H	37	LYS	2.5
1	B	67	PRO	2.5
1	D	275	CYS	2.5
1	D	122	GLU	2.4
3	E	153	ARG	2.4
3	F	121	GLY	2.4
1	B	66	SER	2.4
1	D	65	TYR	2.4
3	E	202	SER	2.4
3	F	199	GLU	2.4
3	E	156	LYS	2.3
1	D	148	GLU	2.2
1	A	141	GLU	2.2
1	D	66	SER	2.2
1	B	167	HIS	2.2
1	D	186	ARG	2.2
1	D	172	ASP	2.2
1	B	101	ASN	2.2
2	C	36	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	118	GLU	2.2
3	G	198	ILE	2.1
3	E	72	GLU	2.1
1	D	36	ALA	2.1
2	C	166	SER	2.1
3	G	202	SER	2.1
2	C	259	ASN	2.1
2	C	122	GLU	2.1
3	G	95	GLY	2.1
3	G	151	THR	2.0
1	A	152	ASN	2.0
3	E	96	ARG	2.0
1	B	152	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
5	HIS	F	1204	11/11	0.71	0.42	40,65,69,72	11
5	HIS	H	1203	11/11	0.73	0.24	63,68,76,78	11
5	HIS	E	1204	11/11	0.80	0.30	40,52,55,59	11
5	HIS	E	1205	11/11	0.80	0.28	40,64,71,72	11
5	HIS	G	1206	11/11	0.82	0.19	70,74,82,87	10
5	HIS	C	1275	11/11	0.88	0.20	57,62,64,66	10
5	HIS	H	1204	11/11	0.88	0.22	67,71,77,77	10
6	PO4	F	1203	5/5	0.89	0.15	61,63,68,69	5
6	PO4	H	1202	5/5	0.89	0.17	71,71,74,74	5
5	HIS	D	1276	11/11	0.90	0.16	40,58,76,78	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PO4	E	1203	5/5	0.92	0.21	63,63,67,69	5
6	PO4	G	1205	5/5	0.93	0.17	41,47,49,53	5
6	PO4	G	1204	5/5	0.96	0.12	63,66,67,68	0
6	PO4	E	1202	5/5	0.97	0.10	43,43,48,54	5

6.5 Other polymers (i)

There are no such residues in this entry.