



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:32 PM EDT

PDB ID : 2O7E / pdb_00002o7e
Title : Tyrosine ammonia-lyase from Rhodobacter sphaeroides (His89Phe variant), bound to 2-aminoindan-2-phosphonic acid
Authors : Louie, G.V.; Bowman, M.E.; Moffitt, M.C.; Baiga, T.J.; Moore, B.S.; Noel, J.P.
Deposited on : 2006-12-11
Resolution : 1.75 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	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.48.1

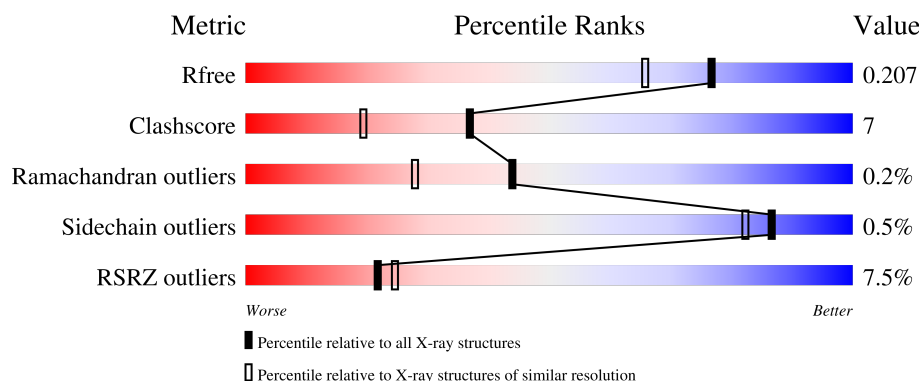
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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	521	<div> <div>10%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	B	521	<div> <div>7%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	C	521	<div> <div>7%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	D	521	<div> <div>8%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	E	521	<div> <div>7%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	521	<div><div></div><div>4%</div><div>85%</div><div>12%</div><div>..</div></div>
1	G	521	<div><div></div><div>4%</div><div>85%</div><div>12%</div><div>..</div></div>
1	H	521	<div><div></div><div>12%</div><div>84%</div><div>12%</div><div>..</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33671 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 Putative histidine ammonia-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			3814	2366	729	705	14			
1	B	515	Total	C	N	O	S	0	0	0
			3814	2366	729	705	14			
1	C	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			
1	D	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			
1	E	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			
1	F	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			
1	G	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			
1	H	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			

There are 32 discrepancies between the modelled and reference sequences:

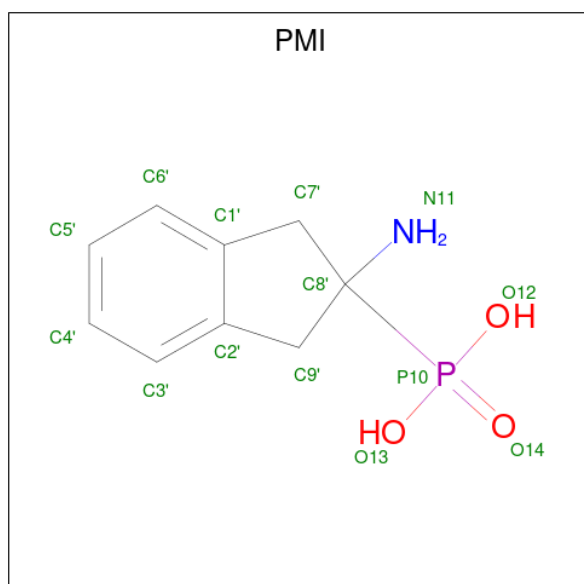
Chain	Residue	Modelled	Actual	Comment	Reference
A	89	PHE	HIS	engineered mutation	UNP Q3IWB0
A	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
A	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
A	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
B	89	PHE	HIS	engineered mutation	UNP Q3IWB0
B	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
B	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
B	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
C	89	PHE	HIS	engineered mutation	UNP Q3IWB0
C	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
C	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
C	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
D	89	PHE	HIS	engineered mutation	UNP Q3IWB0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
D	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
D	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
E	89	PHE	HIS	engineered mutation	UNP Q3IWB0
E	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
E	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
E	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
F	89	PHE	HIS	engineered mutation	UNP Q3IWB0
F	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
F	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
F	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
G	89	PHE	HIS	engineered mutation	UNP Q3IWB0
G	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
G	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
G	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
H	89	PHE	HIS	engineered mutation	UNP Q3IWB0
H	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
H	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
H	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0

- Molecule 2 is (2-AMINO-2,3-DIHYDRO-1H-INDEN-2-YL)PHOSPHONIC ACID (CCD ID: PMI) (formula: C₉H₁₂NO₃P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			14	9	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			14	9	1	3	1		
2	C	1	Total	C	N	O	P	0	0
			14	9	1	3	1		
2	D	1	Total	C	N	O	P	0	0
			14	9	1	3	1		
2	E	1	Total	C	N	O	P	0	0
			14	9	1	3	1		
2	F	1	Total	C	N	O	P	0	0
			14	9	1	3	1		
2	G	1	Total	C	N	O	P	0	0
			14	9	1	3	1		
2	H	1	Total	C	N	O	P	0	0
			14	9	1	3	1		

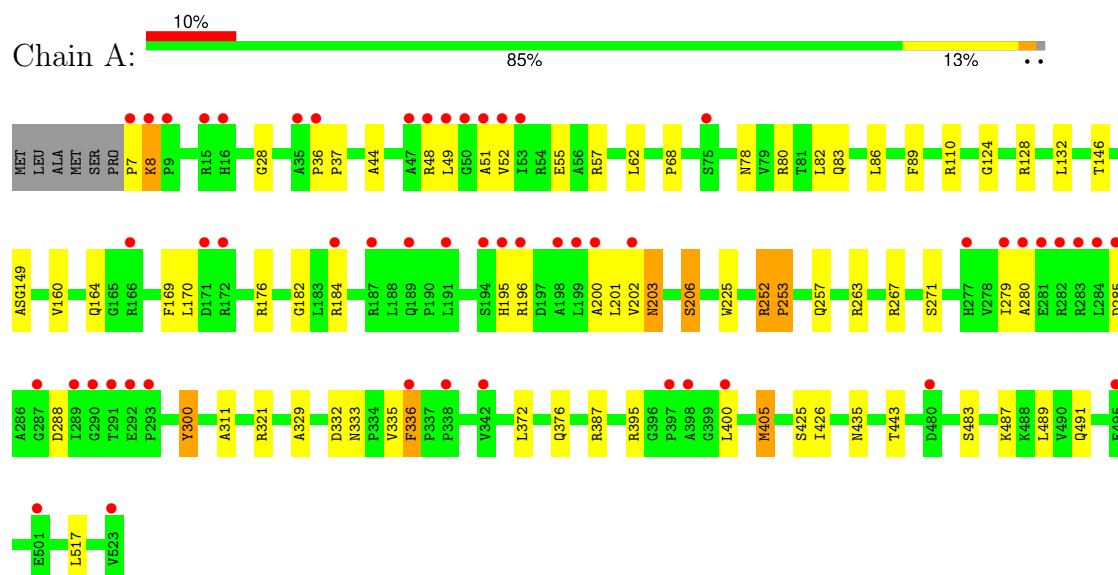
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	325	Total	O	0	0
			325	325		
3	B	373	Total	O	0	0
			373	373		
3	C	414	Total	O	0	0
			414	414		
3	D	355	Total	O	0	0
			355	355		
3	E	380	Total	O	0	0
			380	380		
3	F	479	Total	O	0	0
			479	479		
3	G	413	Total	O	0	0
			413	413		
3	H	350	Total	O	0	0
			350	350		

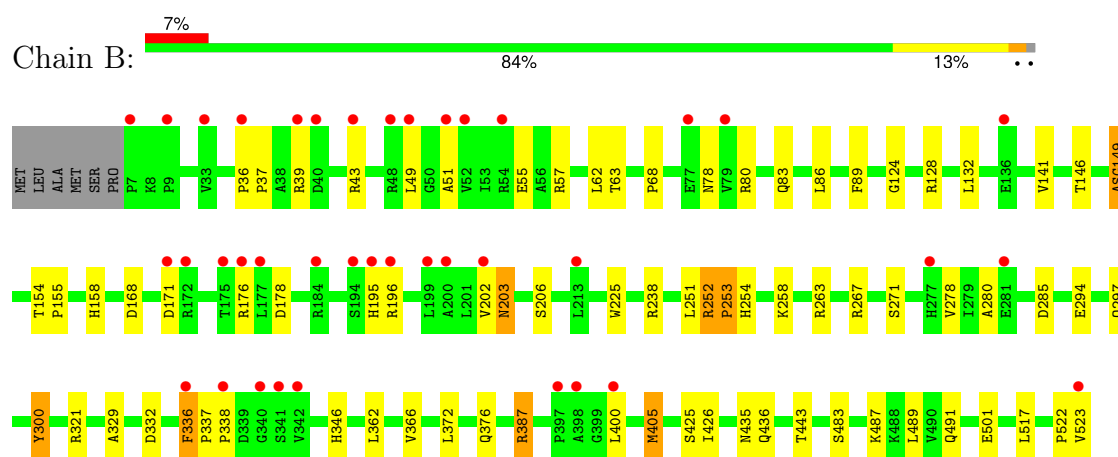
3 Residue-property plots [i](#)

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.

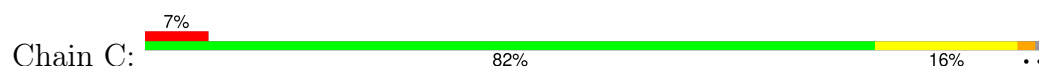
• Molecule 1: Putative histidine ammonia-lyase

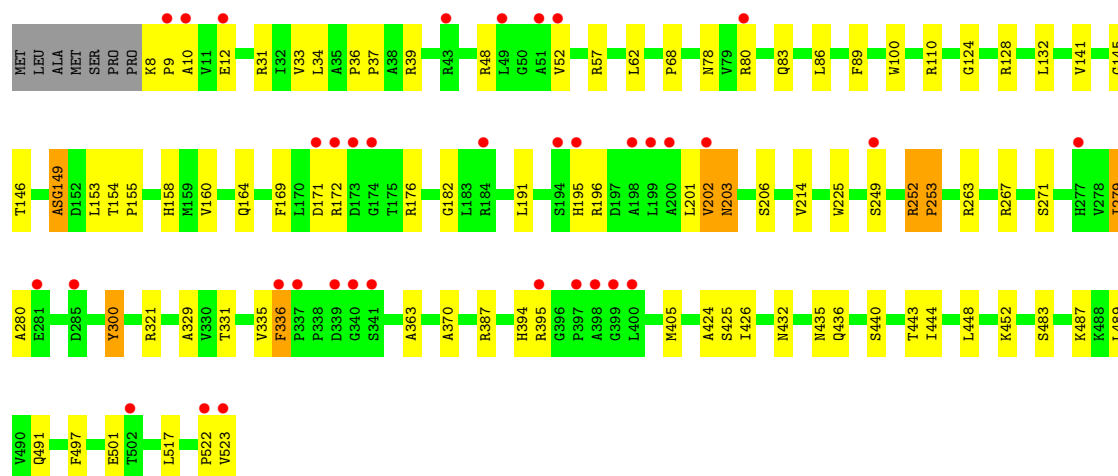


• Molecule 1: Putative histidine ammonia-lyase

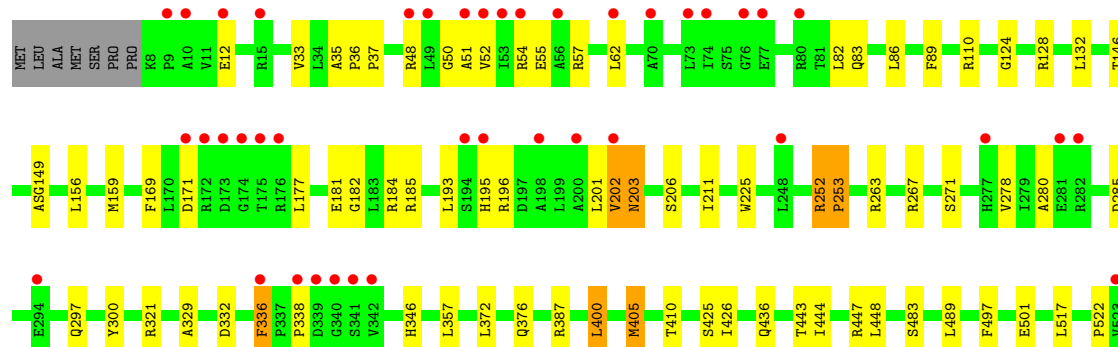
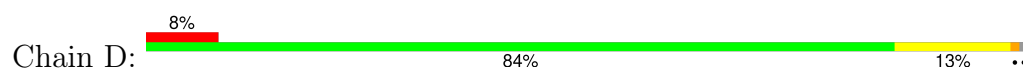


• Molecule 1: Putative histidine ammonia-lyase

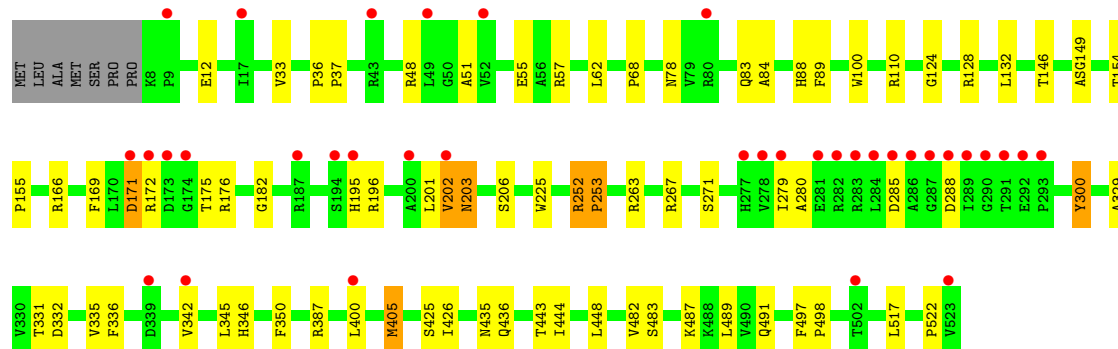
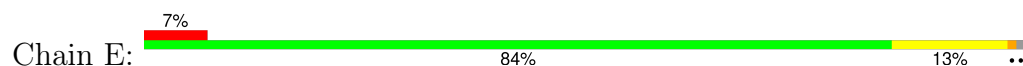




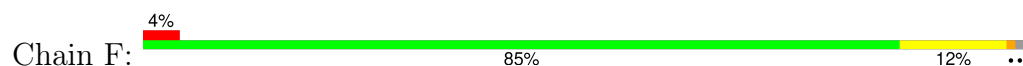
- Molecule 1: Putative histidine ammonia-lyase

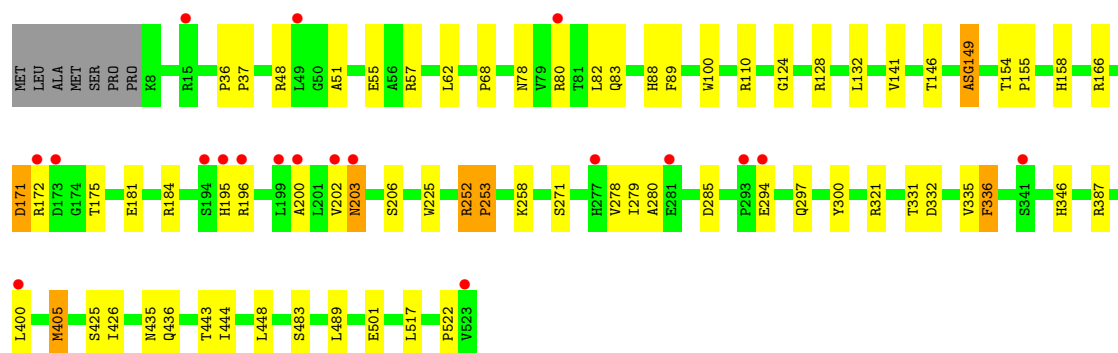


- Molecule 1: Putative histidine ammonia-lyase

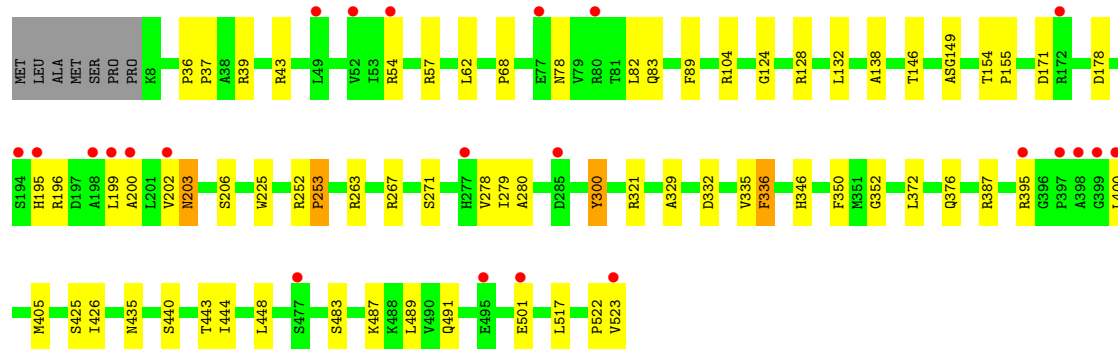
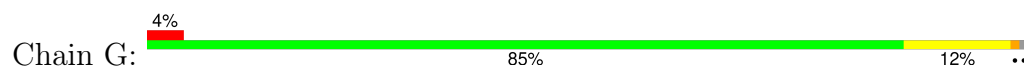


- Molecule 1: Putative histidine ammonia-lyase

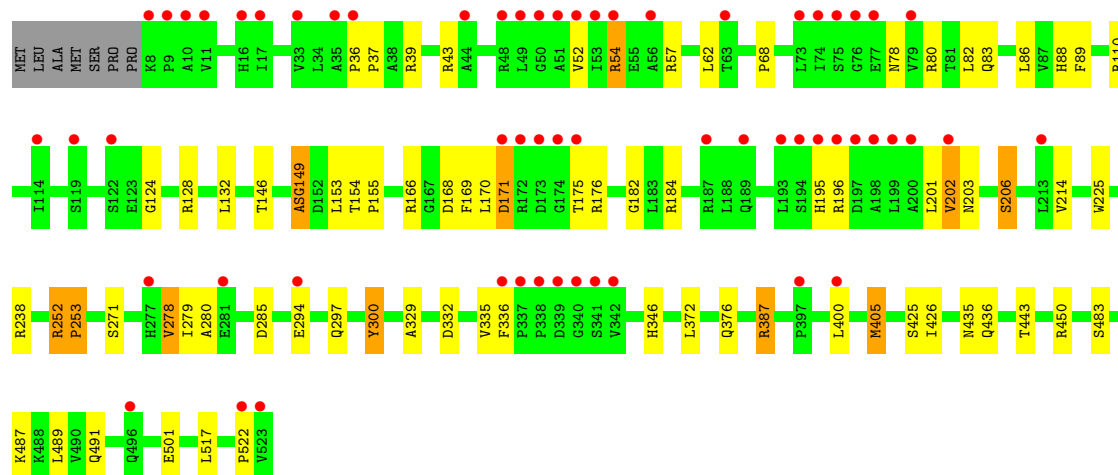
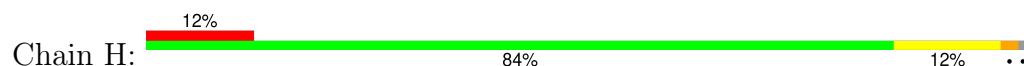




• Molecule 1: Putative histidine ammonia-lyase



• Molecule 1: Putative histidine ammonia-lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.57Å 154.84Å 164.53Å 90.00° 94.16° 90.00°	Depositor
Resolution (Å)	500.00 – 1.75 164.09 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.4 (500.00-1.75) 96.3 (164.09-1.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.75Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.189 , 0.210 0.187 , 0.207	Depositor DCC
R_{free} test set	21241 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33671	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.42	1/3863 (0.0%)	0.90	12/5254 (0.2%)
1	B	0.41	1/3863 (0.0%)	0.89	14/5254 (0.3%)
1	C	0.43	0/3855	0.90	18/5243 (0.3%)
1	D	0.41	1/3855 (0.0%)	0.90	17/5243 (0.3%)
1	E	0.42	1/3855 (0.0%)	0.89	11/5243 (0.2%)
1	F	0.45	1/3855 (0.0%)	0.91	13/5243 (0.2%)
1	G	0.43	0/3855	0.90	14/5243 (0.3%)
1	H	0.41	1/3855 (0.0%)	0.87	10/5243 (0.2%)
All	All	0.42	6/30856 (0.0%)	0.89	109/41966 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	405	MET	SD-CE	-8.24	1.58	1.79
1	H	405	MET	SD-CE	-6.81	1.62	1.79
1	B	405	MET	SD-CE	-6.15	1.64	1.79
1	D	405	MET	SD-CE	-5.51	1.65	1.79
1	A	405	MET	SD-CE	-5.22	1.66	1.79
1	E	405	MET	SD-CE	-5.07	1.66	1.79

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	202	VAL	N-CA-C	8.64	121.60	112.96
1	F	278	VAL	N-CA-C	-8.24	98.02	108.89
1	C	202	VAL	N-CA-C	7.96	120.92	112.96
1	B	202	VAL	N-CA-C	7.85	120.81	112.96
1	F	252	ARG	CA-C-N	7.85	129.65	119.84
1	F	252	ARG	C-N-CA	7.85	129.65	119.84
1	D	202	VAL	N-CA-C	7.57	120.53	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	VAL	N-CA-C	7.34	120.30	112.96
1	E	252	ARG	CA-C-N	7.23	128.88	119.84
1	E	252	ARG	C-N-CA	7.23	128.88	119.84
1	D	206	SER	N-CA-C	7.21	119.14	111.28
1	B	206	SER	N-CA-C	7.14	119.06	111.28
1	C	497	PHE	CA-C-N	7.13	124.87	119.66
1	C	497	PHE	C-N-CA	7.13	124.87	119.66
1	C	206	SER	N-CA-C	7.02	119.79	111.71
1	A	336	PHE	CA-C-N	6.68	127.27	120.38
1	A	336	PHE	C-N-CA	6.68	127.27	120.38
1	E	425	SER	N-CA-C	6.67	119.39	111.71
1	D	278	VAL	N-CA-C	-6.65	100.11	108.89
1	E	206	SER	N-CA-C	6.55	119.24	111.71
1	G	252	ARG	CA-C-N	6.50	127.97	119.84
1	G	252	ARG	C-N-CA	6.50	127.97	119.84
1	C	336	PHE	CA-C-N	6.47	127.04	120.38
1	C	336	PHE	C-N-CA	6.47	127.04	120.38
1	H	278	VAL	N-CA-C	-6.44	101.25	109.30
1	G	203	ASN	N-CA-C	6.40	119.58	110.68
1	H	252	ARG	CA-C-N	6.33	127.76	119.84
1	H	252	ARG	C-N-CA	6.33	127.76	119.84
1	A	252	ARG	CA-C-N	6.16	127.53	119.84
1	A	252	ARG	C-N-CA	6.16	127.53	119.84
1	F	206	SER	N-CA-C	6.15	118.78	111.71
1	G	336	PHE	CA-C-N	6.14	126.70	120.38
1	G	336	PHE	C-N-CA	6.14	126.70	120.38
1	G	278	VAL	N-CA-C	-6.08	99.82	108.58
1	A	425	SER	N-CA-C	6.05	118.67	111.71
1	G	202	VAL	N-CA-C	6.02	120.46	113.42
1	H	387	ARG	N-CA-C	6.01	119.54	111.24
1	C	171	ASP	N-CA-C	-5.99	101.91	110.59
1	D	252	ARG	CA-C-N	5.94	127.26	119.84
1	D	252	ARG	C-N-CA	5.94	127.26	119.84
1	F	171	ASP	N-CA-C	-5.93	102.00	110.59
1	A	206	SER	N-CA-C	5.90	118.50	111.71
1	C	252	ARG	CA-C-N	5.89	127.20	119.84
1	C	252	ARG	C-N-CA	5.89	127.20	119.84
1	H	253	PRO	N-CA-C	5.89	124.60	112.47
1	B	253	PRO	N-CA-C	5.86	124.54	112.47
1	G	425	SER	N-CA-C	5.86	119.25	111.75
1	D	203	ASN	N-CA-C	5.85	118.82	110.68
1	D	425	SER	N-CA-C	5.84	118.43	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	300	TYR	N-CA-C	5.83	118.41	111.71
1	D	253	PRO	N-CA-C	5.80	124.42	112.47
1	G	171	ASP	N-CA-C	-5.80	101.87	110.46
1	B	336	PHE	CA-C-N	5.79	126.34	120.38
1	B	336	PHE	C-N-CA	5.79	126.34	120.38
1	H	206	SER	N-CA-C	5.77	118.31	111.33
1	E	253	PRO	N-CA-C	5.76	124.33	112.47
1	F	387	ARG	N-CA-C	5.76	119.33	111.39
1	C	425	SER	N-CA-C	5.75	119.11	111.75
1	F	203	ASN	N-CA-C	5.74	120.07	111.81
1	H	425	SER	N-CA-C	5.73	119.09	111.75
1	D	497	PHE	CA-C-N	5.73	123.84	119.66
1	D	497	PHE	C-N-CA	5.73	123.84	119.66
1	B	425	SER	N-CA-C	5.72	119.07	111.75
1	A	387	ARG	N-CA-C	5.67	119.06	111.24
1	E	203	ASN	N-CA-C	5.63	119.92	111.81
1	D	336	PHE	CA-C-N	5.62	126.17	120.38
1	D	336	PHE	C-N-CA	5.62	126.17	120.38
1	G	206	SER	N-CA-C	5.62	118.17	111.71
1	C	253	PRO	N-CA-C	5.61	124.03	112.47
1	A	253	PRO	N-CA-C	5.60	124.01	112.47
1	H	300	TYR	N-CA-C	5.58	118.13	111.71
1	E	387	ARG	N-CA-C	5.53	119.03	111.39
1	G	300	TYR	N-CA-C	5.53	118.07	111.71
1	E	171	ASP	N-CA-C	-5.43	102.71	110.59
1	A	203	ASN	N-CA-C	5.42	118.21	110.68
1	G	253	PRO	N-CA-C	5.40	123.59	112.47
1	G	387	ARG	N-CA-C	5.38	118.67	111.24
1	F	253	PRO	N-CA-C	5.36	123.52	112.47
1	H	171	ASP	N-CA-C	-5.36	102.81	110.59
1	H	202	VAL	N-CA-C	5.32	118.74	113.53
1	C	279	ILE	N-CA-C	5.30	116.03	110.62
1	E	202	VAL	N-CA-C	5.30	119.62	113.42
1	F	425	SER	N-CA-C	5.30	118.53	111.75
1	B	254	HIS	N-CA-C	-5.28	102.99	109.65
1	C	300	TYR	N-CA-C	5.27	117.77	111.71
1	D	400	LEU	N-CA-C	-5.27	105.54	111.28
1	C	164	GLN	N-CA-C	-5.26	106.54	113.17
1	G	440	SER	N-CA-C	5.24	118.84	112.23
1	A	300	TYR	N-CA-C	5.24	116.99	111.28
1	B	171	ASP	N-CA-C	-5.22	102.27	110.36
1	D	193	LEU	N-CA-C	5.21	117.99	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	300	TYR	N-CA-C	5.20	117.69	111.71
1	F	336	PHE	CA-C-N	5.20	125.73	120.38
1	F	336	PHE	C-N-CA	5.20	125.73	120.38
1	C	387	ARG	N-CA-C	5.19	118.40	111.24
1	A	395	ARG	N-CA-C	-5.16	101.70	109.85
1	E	300	TYR	N-CA-C	5.16	117.64	111.71
1	F	300	TYR	N-CA-C	5.15	117.64	111.71
1	B	387	ARG	N-CA-C	5.12	118.30	111.24
1	C	203	ASN	N-CA-C	5.10	119.15	111.81
1	D	387	ARG	N-CA-C	5.08	118.25	111.24
1	C	440	SER	N-CA-C	5.06	118.61	112.23
1	B	252	ARG	CA-C-N	5.04	126.14	119.84
1	B	252	ARG	C-N-CA	5.04	126.14	119.84
1	B	278	VAL	N-CA-C	-5.02	101.11	108.54
1	E	84	ALA	N-CA-C	-5.02	105.89	111.36
1	D	171	ASP	N-CA-C	-5.01	102.60	110.17
1	C	370	ALA	N-CA-C	-5.01	106.01	111.82
1	B	203	ASN	N-CA-C	5.00	119.01	111.81

There are no chirality outliers.

There are no planarity outliers.

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	3814	0	3857	62	0
1	B	3814	0	3858	59	0
1	C	3807	0	3850	66	0
1	D	3807	0	3849	56	0
1	E	3807	0	3850	55	0
1	F	3807	0	3850	61	0
1	G	3807	0	3849	54	0
1	H	3807	0	3850	72	0
2	A	14	0	9	1	0
2	B	14	0	9	3	0
2	C	14	0	9	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	14	0	9	1	0
2	E	14	0	9	3	0
2	F	14	0	9	2	0
2	G	14	0	9	2	0
2	H	14	0	9	3	0
3	A	325	0	0	9	0
3	B	373	0	0	7	0
3	C	414	0	0	12	0
3	D	355	0	0	4	0
3	E	380	0	0	5	0
3	F	479	0	0	11	0
3	G	413	0	0	8	0
3	H	350	0	0	9	0
All	All	33671	0	30885	430	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 7.

All (430) 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:83:GLN:HE22	1:H:196:ARG:HA	1.17	1.08
1:A:83:GLN:HE22	1:A:196:ARG:HA	1.21	1.02
1:B:83:GLN:HE22	1:B:196:ARG:HA	1.25	0.97
1:F:200:ALA:HB2	3:F:3012:HOH:O	1.64	0.97
1:G:83:GLN:HE22	1:G:196:ARG:HA	1.28	0.96
2:C:701:PMI:H5'	1:D:405:MET:HE3	1.49	0.95
1:D:83:GLN:HE22	1:D:196:ARG:HA	1.30	0.94
2:E:701:PMI:H5'	1:F:405:MET:HE3	1.47	0.93
2:G:701:PMI:H5'	1:H:405:MET:HE3	1.52	0.91
1:C:83:GLN:HE22	1:C:196:ARG:HA	1.38	0.89
1:A:405:MET:HE3	2:B:701:PMI:H5'	1.53	0.87
2:A:701:PMI:H5'	1:B:405:MET:HE3	1.57	0.85
1:F:83:GLN:HE22	1:F:196:ARG:HA	1.41	0.84
1:E:405:MET:HE3	2:F:701:PMI:H5'	1.59	0.84
1:H:83:GLN:NE2	1:H:196:ARG:HA	1.93	0.82
1:G:405:MET:HE3	2:H:701:PMI:H5'	1.61	0.81
1:F:62:LEU:HD21	1:F:196:ARG:HB3	1.62	0.81
1:A:62:LEU:HD21	1:A:196:ARG:HB3	1.64	0.79
1:B:51:ALA:O	1:B:55:GLU:HG3	1.83	0.79
1:G:83:GLN:NE2	1:G:196:ARG:HA	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ALA:HB2	3:A:2945:HOH:O	1.82	0.78
1:B:68:PRO:HG3	1:B:435:ASN:HB2	1.68	0.76
1:A:83:GLN:NE2	1:A:196:ARG:HA	1.99	0.76
1:B:62:LEU:HD21	1:B:196:ARG:HB3	1.68	0.75
1:D:83:GLN:NE2	1:D:196:ARG:HA	2.02	0.74
1:E:196:ARG:HD3	1:E:336:PHE:HE2	1.52	0.74
1:B:196:ARG:HD3	1:B:336:PHE:HE2	1.53	0.74
1:C:405:MET:HE3	2:D:701:PMI:H5'	1.69	0.73
1:E:83:GLN:HE22	1:E:196:ARG:HA	1.52	0.72
1:G:487:LYS:O	1:G:491:GLN:HG3	1.88	0.72
1:G:62:LEU:HD21	1:G:196:ARG:HB3	1.70	0.72
1:E:487:LYS:O	1:E:491:GLN:HG3	1.90	0.72
1:D:62:LEU:HD21	1:D:196:ARG:HB3	1.70	0.71
1:D:196:ARG:HD3	1:D:336:PHE:HE2	1.54	0.71
1:H:62:LEU:HD21	1:H:196:ARG:HB3	1.71	0.71
1:A:68:PRO:HG3	1:A:435:ASN:HB2	1.72	0.71
1:C:487:LYS:O	1:C:491:GLN:HG3	1.90	0.71
1:D:50:GLY:O	1:D:54:ARG:HG3	1.91	0.70
1:B:83:GLN:NE2	1:B:196:ARG:HA	2.05	0.70
1:B:487:LYS:O	1:B:491:GLN:HG3	1.92	0.69
1:F:68:PRO:HG3	1:F:435:ASN:HB2	1.73	0.69
1:B:251:LEU:HD13	1:C:335:VAL:HG21	1.75	0.69
1:B:258:LYS:HD2	3:B:3514:HOH:O	1.94	0.68
1:C:83:GLN:OE1	1:C:195:HIS:O	2.11	0.68
1:A:196:ARG:HD3	1:A:336:PHE:CE2	2.29	0.68
1:H:196:ARG:HD3	1:H:336:PHE:CE2	2.29	0.68
1:A:51:ALA:O	1:A:55:GLU:HG3	1.94	0.67
1:E:62:LEU:HD21	1:E:196:ARG:HB3	1.76	0.67
1:G:200:ALA:HB2	3:G:2988:HOH:O	1.95	0.66
1:D:51:ALA:O	1:D:55:GLU:HG3	1.95	0.66
1:F:196:ARG:HD3	1:F:336:PHE:CE2	2.30	0.66
1:C:196:ARG:HD3	1:C:336:PHE:HE2	1.60	0.66
1:F:83:GLN:NE2	1:F:196:ARG:HA	2.09	0.66
1:E:51:ALA:O	1:E:55:GLU:HG3	1.97	0.65
1:G:68:PRO:HG3	1:G:435:ASN:HB2	1.77	0.65
1:D:196:ARG:HD3	1:D:336:PHE:CE2	2.30	0.65
1:C:62:LEU:HD21	1:C:196:ARG:HB3	1.79	0.65
1:D:297:GLN:HG3	3:D:3086:HOH:O	1.96	0.65
1:H:196:ARG:HD3	1:H:336:PHE:HE2	1.59	0.65
1:E:83:GLN:OE1	1:E:195:HIS:O	2.15	0.64
1:B:196:ARG:HD3	1:B:336:PHE:CE2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:ARG:HD3	1:E:336:PHE:CE2	2.31	0.64
1:C:48:ARG:HH11	1:C:48:ARG:HG2	1.63	0.63
1:H:238:ARG:HH11	1:H:387:ARG:NH2	1.96	0.63
1:H:214:VAL:HB	1:H:450:ARG:NH2	2.14	0.62
1:E:89:PHE:CE1	1:F:405:MET:HE2	2.35	0.62
1:F:83:GLN:OE1	1:F:195:HIS:O	2.18	0.62
1:F:171:ASP:OD2	1:F:175:THR:HB	1.99	0.62
1:A:280:ALA:O	1:D:57:ARG:HD2	1.99	0.62
1:A:372:LEU:O	1:A:376:GLN:HG3	2.00	0.62
1:F:124:GLY:O	1:F:128:ARG:HG2	1.99	0.61
1:H:487:LYS:O	1:H:491:GLN:HG3	2.01	0.61
1:F:36:PRO:HB2	1:F:37:PRO:HD3	1.84	0.60
1:H:206:SER:OG	3:H:1354:HOH:O	2.12	0.60
1:B:280:ALA:O	1:C:57:ARG:HD2	2.01	0.60
1:C:83:GLN:NE2	1:C:196:ARG:HA	2.12	0.60
1:C:145:GLY:HA2	1:D:410:THR:HG23	1.84	0.60
1:A:271:SER:HB2	1:A:483:SER:HB3	1.84	0.60
1:A:279:ILE:HD11	1:D:346:HIS:CE1	2.37	0.60
1:C:196:ARG:HD3	1:C:336:PHE:CE2	2.37	0.59
1:E:48:ARG:HH11	1:E:48:ARG:HG2	1.67	0.59
1:F:321:ARG:HH21	1:G:321:ARG:HH21	1.50	0.59
1:G:271:SER:HB2	1:G:483:SER:HB3	1.83	0.59
1:D:36:PRO:HB2	1:D:37:PRO:HD3	1.83	0.59
1:G:132:LEU:HD13	1:G:132:LEU:C	2.27	0.59
1:G:196:ARG:HD3	1:G:336:PHE:CE2	2.37	0.59
1:C:68:PRO:HG3	1:C:435:ASN:HB2	1.85	0.59
1:B:141:VAL:HG13	1:B:158:HIS:HB2	1.85	0.58
1:F:196:ARG:HD3	1:F:336:PHE:HE2	1.66	0.58
1:H:68:PRO:HG3	1:H:435:ASN:HB2	1.86	0.58
1:D:83:GLN:OE1	1:D:195:HIS:O	2.22	0.58
2:G:701:PMI:C5'	1:H:405:MET:HE3	2.30	0.58
1:C:124:GLY:O	1:C:128:ARG:HG2	2.03	0.58
1:G:83:GLN:HE22	1:G:196:ARG:CA	2.10	0.57
1:G:83:GLN:NE2	1:G:195:HIS:O	2.38	0.56
1:H:271:SER:HB2	1:H:483:SER:HB3	1.86	0.56
2:E:701:PMI:H5'	1:F:405:MET:CE	2.28	0.56
1:E:271:SER:HB2	1:E:483:SER:HB3	1.87	0.56
1:C:48:ARG:HG2	1:C:48:ARG:NH1	2.21	0.56
1:E:57:ARG:HD2	1:H:280:ALA:O	2.06	0.56
1:E:280:ALA:O	1:H:57:ARG:HD2	2.06	0.56
1:A:78:ASN:HB3	1:B:400:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:THR:HG22	3:F:2088:HOH:O	2.05	0.55
1:A:132:LEU:C	1:A:132:LEU:HD13	2.31	0.55
1:A:225:TRP:CE2	1:A:517:LEU:HD22	2.41	0.55
1:B:57:ARG:HD2	1:C:280:ALA:O	2.07	0.55
1:F:82:LEU:HD12	3:F:2155:HOH:O	2.05	0.55
1:H:39:ARG:HG3	1:H:39:ARG:HH11	1.72	0.55
1:H:297:GLN:HG3	3:H:2410:HOH:O	2.06	0.55
1:H:238:ARG:NH1	1:H:387:ARG:NH2	2.56	0.54
1:F:51:ALA:O	1:F:55:GLU:HG3	2.06	0.54
1:F:280:ALA:O	1:G:57:ARG:HD2	2.06	0.54
1:G:82:LEU:HD12	3:G:1625:HOH:O	2.08	0.54
1:E:400:LEU:HD21	1:F:78:ASN:HB3	1.88	0.54
1:E:89:PHE:CZ	1:F:405:MET:HE2	2.43	0.54
1:D:146:THR:HG22	3:D:2324:HOH:O	2.07	0.54
1:E:405:MET:HE2	1:F:89:PHE:CZ	2.43	0.54
1:H:335:VAL:HG11	3:H:1982:HOH:O	2.08	0.54
1:E:132:LEU:C	1:E:132:LEU:HD13	2.32	0.54
1:F:335:VAL:HG11	3:F:1411:HOH:O	2.08	0.54
1:H:83:GLN:OE1	1:H:195:HIS:O	2.25	0.54
1:A:57:ARG:HD2	1:D:280:ALA:O	2.08	0.54
1:B:271:SER:HB2	1:B:483:SER:HB3	1.90	0.53
1:D:184:ARG:HG2	1:D:184:ARG:HH11	1.72	0.53
1:B:329:ALA:HB1	1:C:252:ARG:HA	1.89	0.53
1:H:489:LEU:C	1:H:489:LEU:HD23	2.32	0.53
1:E:335:VAL:HG11	3:E:1376:HOH:O	2.08	0.53
1:B:124:GLY:O	1:B:128:ARG:HG2	2.08	0.53
3:C:2230:HOH:O	1:D:82:LEU:HD12	2.08	0.53
1:H:132:LEU:C	1:H:132:LEU:HD13	2.34	0.53
1:A:83:GLN:OE1	1:A:195:HIS:O	2.26	0.53
1:C:271:SER:HB2	1:C:483:SER:HB3	1.90	0.53
1:H:83:GLN:HE22	1:H:196:ARG:CA	2.04	0.53
1:H:54:ARG:HG2	1:H:54:ARG:HH11	1.73	0.53
1:C:89:PHE:CE1	1:D:405:MET:HE2	2.44	0.53
1:D:169:PHE:CD2	1:D:182:GLY:HA3	2.43	0.53
1:D:271:SER:HB2	1:D:483:SER:HB3	1.91	0.53
1:A:196:ARG:HD3	1:A:336:PHE:HE2	1.70	0.53
1:B:436:GLN:HG2	1:C:300:TYR:CZ	2.44	0.53
1:B:68:PRO:HG3	1:B:435:ASN:CB	2.39	0.52
1:F:426:ILE:HD13	3:G:3571:HOH:O	2.09	0.52
1:F:48:ARG:HG2	1:F:48:ARG:HH11	1.73	0.52
1:F:225:TRP:CE2	1:F:517:LEU:HD22	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:VAL:HG13	1:F:158:HIS:HB2	1.91	0.52
1:G:78:ASN:HB3	1:H:400:LEU:HD21	1.91	0.52
1:G:225:TRP:CE2	1:G:517:LEU:HD22	2.45	0.52
1:G:489:LEU:HD23	1:G:489:LEU:C	2.34	0.52
1:E:48:ARG:HG2	1:E:48:ARG:NH1	2.25	0.52
1:E:88:HIS:NE2	1:E:166:ARG:NH2	2.50	0.52
1:B:83:GLN:OE1	1:B:195:HIS:O	2.27	0.51
1:C:176:ARG:HD2	3:C:3285:HOH:O	2.09	0.51
1:G:523:VAL:OXT	1:G:523:VAL:HG12	2.08	0.51
1:D:203:ASN:O	1:D:332:ASP:HA	2.10	0.51
1:E:225:TRP:CE2	1:E:517:LEU:HD22	2.46	0.51
1:G:83:GLN:CD	1:G:195:HIS:O	2.53	0.51
1:H:83:GLN:CD	1:H:195:HIS:O	2.54	0.51
1:A:196:ARG:HD3	1:A:336:PHE:CZ	2.46	0.51
1:A:176:ARG:HD2	3:A:3332:HOH:O	2.10	0.51
1:H:225:TRP:CE2	1:H:517:LEU:HD22	2.46	0.51
1:A:487:LYS:O	1:A:491:GLN:HG3	2.11	0.51
1:H:184:ARG:HG2	1:H:184:ARG:HH11	1.76	0.51
1:E:252:ARG:HA	1:H:329:ALA:HB1	1.92	0.51
1:B:523:VAL:OXT	1:B:523:VAL:HG12	2.11	0.51
1:C:78:ASN:HB3	1:D:400:LEU:HD21	1.93	0.51
1:G:146:THR:HG22	3:G:1967:HOH:O	2.10	0.51
3:A:3436:HOH:O	1:D:426:ILE:HD13	2.11	0.51
1:F:279:ILE:HD11	1:G:346:HIS:CE1	2.46	0.51
1:B:132:LEU:HD13	1:B:132:LEU:C	2.35	0.50
1:G:89:PHE:CZ	1:H:405:MET:HE2	2.45	0.50
1:A:52:VAL:HG13	1:A:57:ARG:HB2	1.93	0.50
1:D:52:VAL:HG13	1:D:57:ARG:HB2	1.93	0.50
1:A:426:ILE:HD13	3:D:3398:HOH:O	2.11	0.50
1:E:78:ASN:HB3	1:F:400:LEU:HD21	1.94	0.50
1:F:80:ARG:HG2	3:F:2717:HOH:O	2.10	0.50
1:B:36:PRO:HB2	1:B:37:PRO:HD3	1.92	0.50
1:E:68:PRO:HG3	1:E:435:ASN:HB2	1.92	0.50
1:E:83:GLN:NE2	1:E:196:ARG:HA	2.23	0.50
1:F:271:SER:HB2	1:F:483:SER:HB3	1.93	0.50
1:E:110:ARG:HD3	1:E:201:LEU:HA	1.94	0.50
2:C:701:PMI:C5'	1:D:405:MET:HE3	2.30	0.50
1:E:489:LEU:HD23	1:E:489:LEU:C	2.36	0.50
1:F:57:ARG:HD2	1:G:280:ALA:O	2.12	0.50
1:A:405:MET:HE2	1:B:89:PHE:CE1	2.47	0.50
1:E:279:ILE:HD11	1:H:346:HIS:CE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:VAL:HG11	3:A:1711:HOH:O	2.12	0.49
1:H:124:GLY:O	1:H:128:ARG:HG2	2.13	0.49
1:D:83:GLN:CD	1:D:195:HIS:O	2.56	0.49
1:E:154:THR:HB	1:E:155:PRO:CD	2.43	0.49
1:H:146:THR:HG22	3:H:2163:HOH:O	2.12	0.49
1:A:329:ALA:HB1	1:D:252:ARG:HA	1.94	0.49
1:E:346:HIS:CE1	1:H:279:ILE:HD11	2.48	0.49
1:C:36:PRO:HB2	1:C:37:PRO:HD3	1.93	0.49
1:E:146:THR:HG22	3:E:1932:HOH:O	2.11	0.49
1:F:489:LEU:C	1:F:489:LEU:HD23	2.37	0.49
1:C:225:TRP:CE2	1:C:517:LEU:HD22	2.47	0.49
1:D:184:ARG:HG2	1:D:184:ARG:NH1	2.27	0.49
1:H:83:GLN:NE2	1:H:195:HIS:O	2.46	0.49
1:A:7:PRO:O	1:A:8:LYS:C	2.55	0.49
1:B:168:ASP:HB2	1:B:176:ARG:HH21	1.78	0.48
1:A:86:LEU:HA	1:A:89:PHE:CE2	2.49	0.48
1:B:489:LEU:HD23	1:B:489:LEU:C	2.38	0.48
1:B:225:TRP:CE2	1:B:517:LEU:HD22	2.49	0.48
1:A:311:ALA:HB1	1:D:357:LEU:HD12	1.95	0.48
1:B:252:ARG:HA	1:C:329:ALA:HB1	1.96	0.48
1:B:346:HIS:CE1	1:C:279:ILE:HD11	2.48	0.48
1:E:203:ASN:O	1:E:332:ASP:HA	2.14	0.48
1:A:83:GLN:CD	1:A:195:HIS:O	2.57	0.48
1:D:83:GLN:HE22	1:D:196:ARG:CA	2.15	0.48
1:H:52:VAL:HG13	1:H:57:ARG:HB2	1.96	0.48
1:A:321:ARG:HH21	1:D:321:ARG:HH21	1.61	0.48
1:F:68:PRO:HG3	1:F:435:ASN:CB	2.44	0.48
1:G:124:GLY:O	1:G:128:ARG:HG2	2.13	0.48
1:C:132:LEU:C	1:C:132:LEU:HD13	2.38	0.47
1:H:86:LEU:HA	1:H:89:PHE:CE2	2.49	0.47
1:A:203:ASN:O	1:A:332:ASP:HA	2.14	0.47
1:G:395:ARG:CZ	1:G:501:GLU:HG2	2.44	0.47
1:H:372:LEU:O	1:H:376:GLN:HG3	2.14	0.47
1:H:80:ARG:HH11	1:H:80:ARG:HG3	1.78	0.47
1:H:171:ASP:OD2	1:H:175:THR:HB	2.14	0.47
1:C:523:VAL:OXT	1:C:523:VAL:HG12	2.13	0.47
1:A:400:LEU:HD21	1:B:78:ASN:HB3	1.95	0.47
1:G:196:ARG:HH21	1:G:199:LEU:HD23	1.80	0.47
1:G:400:LEU:HD21	1:H:78:ASN:HB3	1.97	0.47
1:A:206:SER:OG	3:A:1478:HOH:O	2.21	0.47
1:C:12:GLU:HA	1:C:33:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:TRP:CE2	1:C:522:PRO:HG3	2.50	0.47
1:C:363:ALA:HB1	1:C:452:LYS:HD2	1.97	0.47
1:C:100:TRP:CZ2	1:C:172:ARG:HG2	2.50	0.47
1:A:169:PHE:CD2	1:A:182:GLY:HA3	2.50	0.47
1:D:48:ARG:NH2	1:D:338:PRO:O	2.48	0.47
1:F:171:ASP:C	1:F:171:ASP:OD1	2.58	0.47
1:H:36:PRO:N	1:H:37:PRO:HD2	2.29	0.47
1:H:294:GLU:OE1	1:H:387:ARG:NH2	2.48	0.47
1:D:444:ILE:O	1:D:448:LEU:HG	2.15	0.47
1:D:489:LEU:C	1:D:489:LEU:HD23	2.40	0.47
1:B:436:GLN:HG2	1:C:300:TYR:CE2	2.50	0.46
1:C:83:GLN:CD	1:C:195:HIS:O	2.57	0.46
1:C:86:LEU:HA	1:C:89:PHE:CE2	2.50	0.46
1:C:89:PHE:CZ	1:D:405:MET:HE2	2.50	0.46
1:C:444:ILE:O	1:C:448:LEU:HG	2.14	0.46
1:A:405:MET:HE2	1:B:89:PHE:CZ	2.50	0.46
1:D:124:GLY:O	1:D:128:ARG:HG2	2.14	0.46
1:F:436:GLN:HG2	1:G:300:TYR:CZ	2.50	0.46
1:C:154:THR:HB	1:C:155:PRO:CD	2.45	0.46
1:F:501:GLU:HB2	3:F:2400:HOH:O	2.15	0.46
1:G:39:ARG:HD2	1:G:43:ARG:NH2	2.30	0.46
1:G:335:VAL:HG11	3:G:1135:HOH:O	2.13	0.46
1:G:196:ARG:HD3	1:G:336:PHE:CZ	2.50	0.46
1:H:184:ARG:HG2	1:H:184:ARG:NH1	2.30	0.46
1:G:36:PRO:N	1:G:37:PRO:HD2	2.31	0.46
1:G:83:GLN:OE1	1:G:195:HIS:O	2.33	0.46
1:B:86:LEU:HA	1:B:89:PHE:CE2	2.50	0.46
1:A:252:ARG:HA	1:D:329:ALA:HB1	1.98	0.46
1:B:225:TRP:CE2	1:B:522:PRO:HD3	2.51	0.46
1:C:489:LEU:C	1:C:489:LEU:HD23	2.40	0.46
1:G:203:ASN:O	1:G:332:ASP:HA	2.15	0.46
1:B:149:MDO:HB21	2:B:701:PMI:H7'1	1.87	0.46
1:C:34:LEU:HD23	1:C:39:ARG:HG2	1.97	0.46
1:E:342:VAL:HG21	1:E:345:LEU:CD2	2.46	0.46
1:F:88:HIS:NE2	1:F:166:ARG:NH2	2.53	0.46
1:H:170:LEU:HD23	1:H:176:ARG:HG2	1.98	0.46
1:H:39:ARG:O	1:H:43:ARG:HG3	2.15	0.46
1:H:203:ASN:O	1:H:332:ASP:HA	2.16	0.46
1:C:146:THR:HG22	3:C:1832:HOH:O	2.15	0.46
1:D:181:GLU:OE1	1:D:181:GLU:HA	2.16	0.46
1:F:83:GLN:CD	1:F:195:HIS:O	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:171:ASP:C	1:H:171:ASP:OD1	2.59	0.46
1:A:49:LEU:HD21	1:A:196:ARG:H	1.82	0.45
1:C:110:ARG:NH2	1:C:331:THR:O	2.49	0.45
1:E:12:GLU:HA	1:E:33:VAL:HG13	1.98	0.45
1:H:153:LEU:HB2	3:H:2465:HOH:O	2.15	0.45
1:A:36:PRO:N	1:A:37:PRO:HD2	2.30	0.45
1:A:110:ARG:HD3	1:A:201:LEU:HA	1.98	0.45
1:F:132:LEU:C	1:F:132:LEU:HD13	2.40	0.45
1:F:258:LYS:HD2	3:F:5378:HOH:O	2.17	0.45
1:A:83:GLN:HE22	1:A:196:ARG:CA	2.09	0.45
1:B:80:ARG:HB2	3:B:4971:HOH:O	2.17	0.45
1:D:177:LEU:HD21	1:D:185:ARG:NH1	2.31	0.45
1:D:263:ARG:O	1:D:267:ARG:HG2	2.16	0.45
1:H:176:ARG:HD2	3:H:3379:HOH:O	2.16	0.45
1:C:432:ASN:HA	3:C:1165:HOH:O	2.16	0.45
1:E:263:ARG:O	1:E:267:ARG:HG2	2.17	0.45
1:E:405:MET:CE	1:F:89:PHE:CZ	2.99	0.45
1:F:80:ARG:HB2	3:F:2468:HOH:O	2.15	0.45
1:G:54:ARG:HD2	3:G:2686:HOH:O	2.17	0.45
1:E:110:ARG:NH2	1:E:331:THR:O	2.50	0.45
1:F:294:GLU:HG2	3:F:5120:HOH:O	2.16	0.45
1:H:450:ARG:HG2	1:H:450:ARG:HH11	1.82	0.45
1:A:263:ARG:O	1:A:267:ARG:HG2	2.17	0.45
1:H:110:ARG:HD3	1:H:201:LEU:HA	1.99	0.45
1:A:124:GLY:O	1:A:128:ARG:HG2	2.17	0.45
1:D:225:TRP:CE2	1:D:517:LEU:HD22	2.52	0.45
3:E:1223:HOH:O	1:H:278:VAL:HG12	2.16	0.45
2:E:701:PMI:C5'	1:F:405:MET:HE3	2.33	0.45
1:F:225:TRP:CE2	1:F:522:PRO:HD3	2.51	0.45
1:B:63:THR:HG22	3:B:4988:HOH:O	2.16	0.45
1:C:203:ASN:CG	3:C:3002:HOH:O	2.60	0.45
1:H:82:LEU:HD12	3:H:2439:HOH:O	2.15	0.45
1:A:160:VAL:O	1:A:164:GLN:HG3	2.17	0.44
3:B:3548:HOH:O	1:C:426:ILE:HD13	2.17	0.44
1:G:225:TRP:CE2	1:G:522:PRO:HD3	2.52	0.44
1:C:110:ARG:HD3	1:C:201:LEU:HA	1.99	0.44
1:D:132:LEU:HD13	1:D:132:LEU:C	2.42	0.44
1:G:444:ILE:O	1:G:448:LEU:HG	2.17	0.44
1:A:80:ARG:HB2	3:A:2221:HOH:O	2.16	0.44
1:C:424:ALA:HB2	1:C:448:LEU:HD12	1.98	0.44
1:H:238:ARG:NH1	1:H:387:ARG:HH22	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ARG:HD3	1:A:257:GLN:OE1	2.16	0.44
1:C:225:TRP:CD2	1:C:522:PRO:HG3	2.53	0.44
1:G:196:ARG:HD3	1:G:336:PHE:HE2	1.80	0.44
1:D:372:LEU:O	1:D:376:GLN:HG3	2.17	0.44
1:G:405:MET:HE2	1:H:89:PHE:CZ	2.53	0.44
1:B:154:THR:HB	1:B:155:PRO:CD	2.47	0.44
1:F:154:THR:HB	1:F:155:PRO:CD	2.47	0.44
1:F:181:GLU:OE1	1:F:184:ARG:NH1	2.51	0.44
1:G:263:ARG:O	1:G:267:ARG:HG2	2.18	0.44
1:A:196:ARG:HH11	1:A:336:PHE:HE2	1.66	0.44
1:B:285:ASP:C	1:B:285:ASP:OD2	2.61	0.44
1:D:285:ASP:C	1:D:285:ASP:OD2	2.60	0.44
1:B:501:GLU:HB2	3:B:2922:HOH:O	2.18	0.44
1:C:149:MDO:HB21	2:C:701:PMI:H7'1	1.82	0.44
1:C:263:ARG:O	1:C:267:ARG:HG2	2.17	0.44
1:F:297:GLN:HG3	3:F:2987:HOH:O	2.17	0.44
1:H:225:TRP:CE2	1:H:522:PRO:HD3	2.53	0.44
1:C:153:LEU:HD21	3:C:3002:HOH:O	2.17	0.43
1:E:436:GLN:HG2	1:H:300:TYR:CZ	2.53	0.43
1:H:80:ARG:HG3	1:H:80:ARG:NH1	2.33	0.43
1:A:203:ASN:ND2	1:A:333:ASN:HB3	2.33	0.43
1:A:405:MET:HE3	2:B:701:PMI:C5'	2.36	0.43
1:C:128:ARG:HG3	1:C:191:LEU:HD12	2.00	0.43
1:C:160:VAL:HG13	1:C:191:LEU:HD23	2.00	0.43
1:F:285:ASP:OD2	1:F:285:ASP:C	2.61	0.43
1:H:168:ASP:HB2	1:H:176:ARG:HH21	1.83	0.43
1:B:238:ARG:HH21	1:B:387:ARG:HH21	1.64	0.43
1:D:12:GLU:HG2	1:D:35:ALA:HB2	2.01	0.43
1:E:405:MET:HE2	1:F:89:PHE:CE1	2.54	0.43
1:H:39:ARG:HD3	1:H:43:ARG:HH21	1.83	0.43
1:A:285:ASP:OD1	1:A:288:ASP:OD2	2.37	0.43
1:C:249:SER:HB2	3:C:5194:HOH:O	2.18	0.43
1:C:394:HIS:HE1	3:C:2881:HOH:O	2.01	0.43
1:D:86:LEU:HA	1:D:89:PHE:CE2	2.53	0.43
1:E:83:GLN:CD	1:E:195:HIS:O	2.61	0.43
1:H:149:MDO:HB21	2:H:701:PMI:H7'1	1.85	0.43
1:H:214:VAL:HB	1:H:450:ARG:HH21	1.83	0.43
1:A:489:LEU:C	1:A:489:LEU:HD23	2.43	0.43
1:D:12:GLU:HA	1:D:33:VAL:HG13	2.00	0.43
1:F:80:ARG:HG3	1:F:80:ARG:HH11	1.84	0.43
1:H:285:ASP:OD2	1:H:285:ASP:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:TYR:CZ	1:D:436:GLN:HG2	2.53	0.43
1:D:156:LEU:O	1:D:159:MET:HB3	2.19	0.43
1:A:44:ALA:O	1:A:48:ARG:HG3	2.19	0.43
1:B:294:GLU:HG3	1:B:387:ARG:NH2	2.34	0.42
1:E:36:PRO:HB2	1:E:37:PRO:HD3	2.00	0.42
1:G:405:MET:HE3	2:H:701:PMI:C5'	2.39	0.42
1:B:178:ASP:OD2	1:B:178:ASP:C	2.62	0.42
1:B:426:ILE:HD13	3:C:3493:HOH:O	2.17	0.42
1:F:149:MDO:HB21	2:F:701:PMI:H7'1	1.85	0.42
1:F:196:ARG:HD3	1:F:336:PHE:CZ	2.55	0.42
1:G:89:PHE:CE1	1:H:405:MET:HE2	2.55	0.42
1:C:52:VAL:HG23	3:C:1574:HOH:O	2.18	0.42
1:F:346:HIS:CE1	1:G:279:ILE:HD11	2.54	0.42
1:A:184:ARG:HG2	1:A:184:ARG:HH11	1.84	0.42
1:F:252:ARG:HA	1:G:329:ALA:HB1	2.01	0.42
1:G:154:THR:HB	1:G:155:PRO:CD	2.50	0.42
1:B:372:LEU:O	1:B:376:GLN:HG3	2.19	0.42
1:E:100:TRP:CZ2	1:E:172:ARG:HG2	2.54	0.42
1:B:146:THR:HG22	3:B:2492:HOH:O	2.20	0.42
1:E:171:ASP:OD2	1:E:175:THR:HB	2.19	0.42
1:E:225:TRP:CE2	1:E:522:PRO:HD3	2.55	0.42
3:E:3348:HOH:O	1:H:426:ILE:HD13	2.20	0.42
1:C:12:GLU:HA	1:C:33:VAL:CG1	2.50	0.42
1:E:426:ILE:HD13	3:H:3422:HOH:O	2.19	0.42
1:E:444:ILE:O	1:E:448:LEU:HG	2.20	0.42
3:F:3660:HOH:O	1:G:426:ILE:HD13	2.20	0.42
1:C:214:VAL:HG13	3:C:4020:HOH:O	2.20	0.41
1:D:225:TRP:CE2	1:D:522:PRO:HD3	2.55	0.41
1:F:444:ILE:O	1:F:448:LEU:HG	2.19	0.41
1:B:39:ARG:HD2	1:B:43:ARG:NH2	2.35	0.41
1:B:321:ARG:HH21	1:C:321:ARG:HH21	1.67	0.41
1:E:169:PHE:CD2	1:E:182:GLY:HA3	2.55	0.41
1:A:200:ALA:CB	3:A:2945:HOH:O	2.53	0.41
1:B:49:LEU:HD21	1:B:196:ARG:H	1.85	0.41
1:B:263:ARG:O	1:B:267:ARG:HG2	2.19	0.41
1:A:89:PHE:CZ	1:B:405:MET:CE	3.03	0.41
1:B:297:GLN:HG3	3:B:3097:HOH:O	2.21	0.41
1:B:300:TYR:CZ	1:C:436:GLN:HG2	2.55	0.41
1:C:169:PHE:CD2	1:C:182:GLY:HA3	2.55	0.41
1:D:83:GLN:NE2	1:D:195:HIS:O	2.53	0.41
1:E:497:PHE:HA	1:E:498:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:GLN:HE22	1:F:196:ARG:CA	2.23	0.41
1:D:211:ILE:HD13	1:D:447:ARG:HG3	2.03	0.41
1:E:482:VAL:O	1:E:487:LYS:HE2	2.21	0.41
1:F:110:ARG:NH2	1:F:331:THR:O	2.53	0.41
1:G:352:GLY:HA2	3:G:1417:HOH:O	2.19	0.41
1:A:170:LEU:CD2	1:A:176:ARG:HG2	2.51	0.41
1:G:200:ALA:CB	3:G:2988:HOH:O	2.60	0.41
1:B:141:VAL:HG13	1:B:158:HIS:CB	2.51	0.41
1:G:372:LEU:O	1:G:376:GLN:HG3	2.20	0.41
1:H:88:HIS:NE2	1:H:166:ARG:NH2	2.59	0.41
1:A:82:LEU:HD12	3:A:1805:HOH:O	2.21	0.41
1:B:337:PRO:HA	1:B:338:PRO:HD3	1.96	0.41
1:B:362:LEU:O	1:B:366:VAL:HG23	2.21	0.41
1:D:501:GLU:HB2	3:D:2374:HOH:O	2.20	0.41
1:E:300:TYR:CZ	1:H:436:GLN:HG2	2.56	0.41
1:F:203:ASN:O	1:F:332:ASP:HA	2.21	0.41
1:G:104:ARG:HG3	1:G:138:ALA:HB2	2.03	0.41
1:G:350:PHE:CD1	1:G:350:PHE:C	2.99	0.41
1:H:501:GLU:HB2	3:H:3619:HOH:O	2.21	0.41
1:A:89:PHE:CZ	1:B:405:MET:HE2	2.55	0.41
1:C:141:VAL:HG13	1:C:158:HIS:HB2	2.02	0.41
1:E:124:GLY:O	1:E:128:ARG:HG2	2.21	0.41
1:E:329:ALA:HB1	1:H:252:ARG:HA	2.01	0.41
1:A:68:PRO:HG3	1:A:435:ASN:CB	2.46	0.40
1:C:8:LYS:HA	1:C:9:PRO:HD3	1.95	0.40
1:C:195:HIS:CE1	3:C:2333:HOH:O	2.74	0.40
1:E:350:PHE:CD1	1:E:350:PHE:C	2.99	0.40
1:G:178:ASP:OD1	1:G:178:ASP:C	2.64	0.40
1:H:154:THR:HB	1:H:155:PRO:CD	2.51	0.40
1:A:8:LYS:HE3	1:A:28:GLY:O	2.21	0.40
1:C:395:ARG:NH1	1:C:501:GLU:HG2	2.35	0.40
1:D:110:ARG:HD3	1:D:201:LEU:HA	2.02	0.40
1:F:100:TRP:CH2	1:F:172:ARG:HD3	2.57	0.40
1:G:68:PRO:HG3	1:G:435:ASN:CB	2.46	0.40
1:B:203:ASN:O	1:B:332:ASP:HA	2.21	0.40
1:D:51:ALA:HA	1:D:54:ARG:NH1	2.37	0.40
1:E:285:ASP:OD1	1:E:288:ASP:OD2	2.39	0.40
1:A:146:THR:HG22	3:A:2274:HOH:O	2.21	0.40
1:C:10:ALA:HB2	1:C:31:ARG:NH2	2.37	0.40
1:E:176:ARG:HD2	3:E:3308:HOH:O	2.21	0.40
1:H:169:PHE:CD2	1:H:182:GLY:HA3	2.57	0.40

There are no symmetry-related clashes.

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	510/521 (98%)	498 (98%)	10 (2%)	2 (0%)	30	16
1	B	510/521 (98%)	502 (98%)	7 (1%)	1 (0%)	44	28
1	C	509/521 (98%)	502 (99%)	6 (1%)	1 (0%)	44	28
1	D	509/521 (98%)	501 (98%)	7 (1%)	1 (0%)	44	28
1	E	509/521 (98%)	500 (98%)	8 (2%)	1 (0%)	44	28
1	F	509/521 (98%)	501 (98%)	7 (1%)	1 (0%)	44	28
1	G	509/521 (98%)	503 (99%)	5 (1%)	1 (0%)	44	28
1	H	509/521 (98%)	497 (98%)	11 (2%)	1 (0%)	44	28
All	All	4074/4168 (98%)	4004 (98%)	61 (2%)	9 (0%)	44	28

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	253	PRO
1	E	253	PRO
1	A	8	LYS
1	A	253	PRO
1	H	253	PRO
1	B	253	PRO
1	C	253	PRO
1	D	253	PRO
1	G	253	PRO

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	384/389 (99%)	383 (100%)	1 (0%)	91	88
1	B	384/389 (99%)	383 (100%)	1 (0%)	91	88
1	C	383/389 (98%)	380 (99%)	3 (1%)	79	71
1	D	383/389 (98%)	381 (100%)	2 (0%)	86	82
1	E	383/389 (98%)	381 (100%)	2 (0%)	86	82
1	F	383/389 (98%)	382 (100%)	1 (0%)	91	88
1	G	383/389 (98%)	382 (100%)	1 (0%)	91	88
1	H	383/389 (98%)	380 (99%)	3 (1%)	79	71
All	All	3066/3112 (98%)	3052 (100%)	14 (0%)	86	82

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	THR
1	B	443	THR
1	C	80	ARG
1	C	202	VAL
1	C	443	THR
1	D	202	VAL
1	D	443	THR
1	E	202	VAL
1	E	443	THR
1	F	443	THR
1	G	443	THR
1	H	54	ARG
1	H	202	VAL
1	H	443	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	376	GLN
1	A	491	GLN
1	B	83	GLN

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Mol	Chain	Res	Type
1	B	164	GLN
1	B	353	GLN
1	B	394	HIS
1	B	520	GLN
1	C	83	GLN
1	C	164	GLN
1	C	277	HIS
1	C	394	HIS
1	D	83	GLN
1	D	164	GLN
1	D	394	HIS
1	D	491	GLN
1	E	83	GLN
1	E	164	GLN
1	E	189	GLN
1	E	394	HIS
1	E	491	GLN
1	E	516	HIS
1	F	83	GLN
1	F	164	GLN
1	F	394	HIS
1	F	401	ASN
1	F	491	GLN
1	G	83	GLN
1	G	164	GLN
1	G	203	ASN
1	G	353	GLN
1	G	394	HIS
1	H	78	ASN
1	H	83	GLN
1	H	394	HIS
1	H	508	GLN

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	MDO	G	149	1,2	11,13,14	2.44	4 (36%)	15,18,20	2.51	7 (46%)
1	MDO	D	149	1,2	11,13,14	2.25	4 (36%)	15,18,20	2.39	6 (40%)
1	MDO	C	149	1,2	11,13,14	2.48	4 (36%)	15,18,20	2.39	7 (46%)
1	MDO	F	149	1,2	11,13,14	2.42	4 (36%)	15,18,20	2.38	6 (40%)
1	MDO	A	149	1,2	11,13,14	2.33	4 (36%)	15,18,20	2.58	7 (46%)
1	MDO	B	149	1,2	11,13,14	2.44	4 (36%)	15,18,20	2.48	7 (46%)
1	MDO	H	149	1,2	11,13,14	2.39	4 (36%)	15,18,20	2.43	5 (33%)
1	MDO	E	149	1,2	11,13,14	2.42	4 (36%)	15,18,20	2.47	7 (46%)

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	MDO	G	149	1,2	-	1/4/23/24	0/1/1/1
1	MDO	D	149	1,2	-	1/4/23/24	0/1/1/1
1	MDO	C	149	1,2	-	1/4/23/24	0/1/1/1
1	MDO	F	149	1,2	-	2/4/23/24	0/1/1/1
1	MDO	A	149	1,2	-	1/4/23/24	0/1/1/1
1	MDO	B	149	1,2	-	1/4/23/24	0/1/1/1
1	MDO	H	149	1,2	-	1/4/23/24	0/1/1/1
1	MDO	E	149	1,2	-	1/4/23/24	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	149	MDO	O2-C2	5.57	1.34	1.23
1	C	149	MDO	O2-C2	5.52	1.34	1.23
1	B	149	MDO	O2-C2	5.39	1.34	1.23
1	F	149	MDO	O2-C2	5.33	1.33	1.23
1	H	149	MDO	O2-C2	5.28	1.33	1.23
1	G	149	MDO	O2-C2	5.26	1.33	1.23
1	D	149	MDO	O2-C2	5.09	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	MDO	O2-C2	5.09	1.33	1.23
1	C	149	MDO	C2-N3	-4.36	1.30	1.40
1	H	149	MDO	C2-N3	-4.18	1.30	1.40
1	B	149	MDO	C2-N3	-4.04	1.30	1.40
1	G	149	MDO	C2-N3	-4.03	1.30	1.40
1	E	149	MDO	C2-N3	-4.00	1.30	1.40
1	F	149	MDO	C2-N3	-3.93	1.31	1.40
1	A	149	MDO	C2-N3	-3.82	1.31	1.40
1	D	149	MDO	C2-N3	-3.78	1.31	1.40
1	F	149	MDO	CA2-N2	-2.98	1.34	1.39
1	A	149	MDO	CA2-N2	-2.92	1.34	1.39
1	G	149	MDO	CA2-N2	-2.84	1.34	1.39
1	B	149	MDO	CA2-N2	-2.83	1.34	1.39
1	C	149	MDO	CA2-N2	-2.79	1.34	1.39
1	F	149	MDO	CA2-C2	-2.78	1.37	1.43
1	H	149	MDO	CA2-N2	-2.77	1.34	1.39
1	E	149	MDO	CA2-N2	-2.71	1.34	1.39
1	G	149	MDO	CA2-C2	-2.65	1.37	1.43
1	B	149	MDO	CA2-C2	-2.59	1.38	1.43
1	D	149	MDO	CA2-N2	-2.58	1.34	1.39
1	D	149	MDO	CA2-C2	-2.56	1.38	1.43
1	A	149	MDO	CA2-C2	-2.46	1.38	1.43
1	C	149	MDO	CA2-C2	-2.43	1.38	1.43
1	E	149	MDO	CA2-C2	-2.36	1.38	1.43
1	H	149	MDO	CA2-C2	-2.22	1.38	1.43

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	149	MDO	CA2-C2-N3	6.63	109.07	103.50
1	A	149	MDO	CA2-C2-N3	6.60	109.04	103.50
1	G	149	MDO	CA2-C2-N3	6.41	108.88	103.50
1	E	149	MDO	CA2-C2-N3	6.32	108.81	103.50
1	C	149	MDO	CA2-C2-N3	6.32	108.81	103.50
1	B	149	MDO	CA2-C2-N3	6.23	108.73	103.50
1	D	149	MDO	CA2-C2-N3	6.19	108.69	103.50
1	F	149	MDO	CA2-C2-N3	6.14	108.66	103.50
1	A	149	MDO	O2-C2-CA2	-4.35	128.24	131.02
1	F	149	MDO	O2-C2-CA2	-4.34	128.25	131.02
1	B	149	MDO	O2-C2-CA2	-3.87	128.55	131.02
1	G	149	MDO	O2-C2-CA2	-3.82	128.58	131.02
1	H	149	MDO	O2-C2-CA2	-3.65	128.69	131.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	MDO	O2-C2-CA2	-3.48	128.80	131.02
1	C	149	MDO	O2-C2-CA2	-3.47	128.81	131.02
1	E	149	MDO	O2-C2-CA2	-3.27	128.93	131.02
1	H	149	MDO	C2-CA2-N2	-3.13	106.71	108.95
1	B	149	MDO	C3-CA3-N3	-3.02	105.55	112.43
1	G	149	MDO	C3-CA3-N3	-2.96	105.70	112.43
1	A	149	MDO	C2-CA2-N2	-2.93	106.85	108.95
1	E	149	MDO	C2-CA2-N2	-2.91	106.86	108.95
1	D	149	MDO	N3-C1-N2	-2.89	109.21	111.48
1	E	149	MDO	C3-CA3-N3	-2.84	105.96	112.43
1	A	149	MDO	C2-N3-C1	-2.83	106.76	108.07
1	D	149	MDO	C2-CA2-N2	-2.80	106.95	108.95
1	B	149	MDO	N3-C1-N2	-2.79	109.28	111.48
1	D	149	MDO	C2-N3-C1	-2.76	106.79	108.07
1	G	149	MDO	C2-CA2-N2	-2.66	107.04	108.95
1	C	149	MDO	C2-CA2-N2	-2.65	107.06	108.95
1	B	149	MDO	C2-CA2-N2	-2.62	107.07	108.95
1	G	149	MDO	N3-C1-N2	-2.61	109.42	111.48
1	F	149	MDO	C2-N3-C1	-2.60	106.86	108.07
1	E	149	MDO	N3-C1-N2	-2.60	109.44	111.48
1	C	149	MDO	C3-CA3-N3	-2.56	106.61	112.43
1	E	149	MDO	C2-N3-C1	-2.52	106.90	108.07
1	A	149	MDO	CA2-N2-C1	2.49	107.62	105.39
1	C	149	MDO	N3-C1-N2	-2.48	109.53	111.48
1	D	149	MDO	CA2-N2-C1	2.39	107.54	105.39
1	A	149	MDO	N3-C1-N2	-2.37	109.61	111.48
1	F	149	MDO	N3-C1-N2	-2.37	109.61	111.48
1	E	149	MDO	CA2-N2-C1	2.37	107.52	105.39
1	G	149	MDO	C2-N3-C1	-2.29	107.01	108.07
1	H	149	MDO	N3-C1-N2	-2.28	109.69	111.48
1	G	149	MDO	CA2-N2-C1	2.23	107.39	105.39
1	F	149	MDO	CA2-N2-C1	2.23	107.39	105.39
1	F	149	MDO	C2-CA2-N2	-2.22	107.36	108.95
1	B	149	MDO	CA2-N2-C1	2.21	107.37	105.39
1	H	149	MDO	CA2-N2-C1	2.19	107.36	105.39
1	C	149	MDO	CA2-N2-C1	2.11	107.29	105.39
1	A	149	MDO	C3-CA3-N3	-2.09	107.66	112.43
1	B	149	MDO	C2-N3-C1	-2.09	107.10	108.07
1	C	149	MDO	C2-N3-C1	-2.03	107.13	108.07

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	149	MDO	N2-C1-CA1-CB
1	B	149	MDO	N2-C1-CA1-CB
1	C	149	MDO	N2-C1-CA1-CB
1	E	149	MDO	N2-C1-CA1-CB
1	F	149	MDO	N2-C1-CA1-CB
1	G	149	MDO	N2-C1-CA1-CB
1	H	149	MDO	N2-C1-CA1-CB
1	D	149	MDO	N3-C1-CA1-CB
1	F	149	MDO	N3-C1-CA1-CB

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	149	MDO	1	0
1	F	149	MDO	1	0
1	B	149	MDO	1	0
1	H	149	MDO	1	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	PMI	F	701	1	12,15,15	2.16	4 (33%)	18,24,24	1.37	2 (11%)
2	PMI	H	701	1	12,15,15	2.10	4 (33%)	18,24,24	1.29	2 (11%)
2	PMI	C	701	1	12,15,15	2.10	3 (25%)	18,24,24	1.37	2 (11%)
2	PMI	E	701	1	12,15,15	2.06	3 (25%)	18,24,24	1.40	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PMI	A	701	1	12,15,15	2.14	4 (33%)	18,24,24	1.39	2 (11%)
2	PMI	B	701	1	12,15,15	2.13	4 (33%)	18,24,24	1.38	2 (11%)
2	PMI	D	701	1	12,15,15	2.13	4 (33%)	18,24,24	1.31	2 (11%)
2	PMI	G	701	1	12,15,15	2.07	4 (33%)	18,24,24	1.36	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PMI	F	701	1	-	0/6/19/19	0/2/2/2
2	PMI	H	701	1	-	0/6/19/19	0/2/2/2
2	PMI	C	701	1	-	0/6/19/19	0/2/2/2
2	PMI	E	701	1	-	0/6/19/19	0/2/2/2
2	PMI	A	701	1	-	0/6/19/19	0/2/2/2
2	PMI	B	701	1	-	0/6/19/19	0/2/2/2
2	PMI	D	701	1	-	0/6/19/19	0/2/2/2
2	PMI	G	701	1	-	0/6/19/19	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	PMI	C1'-C2'	5.67	1.49	1.39
2	B	701	PMI	C1'-C2'	5.63	1.49	1.39
2	F	701	PMI	C1'-C2'	5.58	1.49	1.39
2	C	701	PMI	C1'-C2'	5.48	1.49	1.39
2	E	701	PMI	C1'-C2'	5.47	1.49	1.39
2	D	701	PMI	C1'-C2'	5.47	1.49	1.39
2	H	701	PMI	C1'-C2'	5.44	1.49	1.39
2	G	701	PMI	C1'-C2'	5.36	1.49	1.39
2	F	701	PMI	C4'-C5'	2.59	1.43	1.38
2	D	701	PMI	C5'-C6'	2.58	1.43	1.38
2	A	701	PMI	C4'-C5'	2.53	1.43	1.38
2	B	701	PMI	C4'-C5'	2.51	1.43	1.38
2	E	701	PMI	C4'-C5'	2.46	1.43	1.38
2	H	701	PMI	C4'-C5'	2.44	1.43	1.38
2	C	701	PMI	C5'-C6'	2.44	1.43	1.38
2	H	701	PMI	C5'-C6'	2.43	1.43	1.38
2	C	701	PMI	C4'-C5'	2.42	1.43	1.38
2	F	701	PMI	C5'-C6'	2.39	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	PMI	C5'-C6'	2.39	1.43	1.38
2	G	701	PMI	C5'-C6'	2.39	1.43	1.38
2	B	701	PMI	C5'-C6'	2.39	1.43	1.38
2	D	701	PMI	C4'-C5'	2.36	1.43	1.38
2	G	701	PMI	C4'-C5'	2.32	1.43	1.38
2	H	701	PMI	C4'-C3'	2.31	1.42	1.38
2	E	701	PMI	C5'-C6'	2.30	1.42	1.38
2	D	701	PMI	C4'-C3'	2.21	1.42	1.38
2	A	701	PMI	C4'-C3'	2.12	1.42	1.38
2	G	701	PMI	C4'-C3'	2.09	1.42	1.38
2	B	701	PMI	C4'-C3'	2.08	1.42	1.38
2	F	701	PMI	C4'-C3'	2.02	1.42	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	PMI	C9'-C8'-C7'	4.71	110.52	104.06
2	B	701	PMI	C9'-C8'-C7'	4.66	110.47	104.06
2	E	701	PMI	C9'-C8'-C7'	4.66	110.45	104.06
2	F	701	PMI	C9'-C8'-C7'	4.58	110.35	104.06
2	G	701	PMI	C9'-C8'-C7'	4.56	110.33	104.06
2	C	701	PMI	C9'-C8'-C7'	4.56	110.32	104.06
2	D	701	PMI	C9'-C8'-C7'	4.45	110.18	104.06
2	H	701	PMI	C9'-C8'-C7'	4.34	110.02	104.06
2	E	701	PMI	C5'-C6'-C1'	-2.27	117.56	120.88
2	C	701	PMI	C5'-C6'-C1'	-2.17	117.70	120.88
2	F	701	PMI	C5'-C6'-C1'	-2.16	117.72	120.88
2	A	701	PMI	C5'-C6'-C1'	-2.14	117.74	120.88
2	B	701	PMI	C5'-C6'-C1'	-2.12	117.77	120.88
2	G	701	PMI	C5'-C6'-C1'	-2.11	117.80	120.88
2	D	701	PMI	C5'-C6'-C1'	-2.03	117.90	120.88
2	H	701	PMI	C5'-C6'-C1'	-2.02	117.92	120.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	701	PMI	2	0
2	H	701	PMI	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	PMI	3	0
2	E	701	PMI	3	0
2	A	701	PMI	1	0
2	B	701	PMI	3	0
2	D	701	PMI	1	0
2	G	701	PMI	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	514/521 (98%)	0.57	53 (10%) 13 15	12, 21, 41, 56	0
1	B	514/521 (98%)	0.25	39 (7%) 21 24	9, 18, 37, 52	0
1	C	513/521 (98%)	0.11	36 (7%) 24 27	9, 17, 33, 46	0
1	D	513/521 (98%)	0.37	41 (7%) 20 22	8, 19, 39, 52	0
1	E	513/521 (98%)	0.21	36 (7%) 24 27	9, 17, 36, 62	0
1	F	513/521 (98%)	-0.07	19 (3%) 45 52	7, 14, 29, 41	0
1	G	513/521 (98%)	0.02	23 (4%) 39 43	7, 16, 31, 46	0
1	H	513/521 (98%)	0.42	60 (11%) 10 12	8, 19, 40, 55	0
All	All	4106/4168 (98%)	0.24	307 (7%) 22 24	7, 18, 37, 62	0

All (307) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	523	VAL	7.9
1	E	523	VAL	7.8
1	D	523	VAL	6.9
1	B	277	HIS	6.6
1	F	523	VAL	6.4
1	H	277	HIS	6.0
1	H	523	VAL	5.9
1	D	277	HIS	5.9
1	F	277	HIS	5.8
1	E	290	GLY	5.7
1	G	523	VAL	5.4
1	C	397	PRO	5.3
1	A	289	ILE	5.2
1	C	523	VAL	5.1
1	H	77	GLU	5.1
1	A	523	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	E	277	HIS	4.9
1	H	9	PRO	4.9
1	H	281	GLU	4.9
1	A	172	ARG	4.9
1	A	49	LEU	4.8
1	D	9	PRO	4.8
1	B	7	PRO	4.8
1	H	52	VAL	4.5
1	A	291	THR	4.4
1	A	290	GLY	4.4
1	A	51	ALA	4.4
1	A	277	HIS	4.4
1	D	340	GLY	4.4
1	A	400	LEU	4.3
1	H	194	SER	4.3
1	D	52	VAL	4.3
1	D	281	GLU	4.2
1	E	284	LEU	4.2
1	A	292	GLU	4.2
1	A	281	GLU	4.2
1	E	281	GLU	4.2
1	A	7	PRO	4.1
1	E	291	THR	4.1
1	G	277	HIS	4.1
1	E	289	ILE	4.1
1	B	341	SER	4.0
1	A	285	ASP	4.0
1	C	400	LEU	4.0
1	E	292	GLU	3.9
1	F	200	ALA	3.9
1	B	172	ARG	3.9
1	G	49	LEU	3.8
1	G	202	VAL	3.8
1	B	195	HIS	3.8
1	D	341	SER	3.7
1	A	293	PRO	3.6
1	A	52	VAL	3.6
1	E	202	VAL	3.6
1	C	172	ARG	3.6
1	C	398	ALA	3.6
1	F	281	GLU	3.6
1	D	342	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	194	SER	3.6
1	H	202	VAL	3.6
1	H	199	LEU	3.6
1	B	200	ALA	3.5
1	G	398	ALA	3.5
1	D	49	LEU	3.5
1	A	287	GLY	3.5
1	E	283	ARG	3.5
1	G	400	LEU	3.5
1	A	8	LYS	3.5
1	E	80	ARG	3.5
1	A	342	VAL	3.4
1	D	194	SER	3.4
1	E	286	ALA	3.4
1	H	56	ALA	3.4
1	E	287	GLY	3.4
1	E	194	SER	3.4
1	A	202	VAL	3.3
1	E	172	ARG	3.3
1	H	49	LEU	3.3
1	D	175	THR	3.3
1	C	194	SER	3.3
1	D	54	ARG	3.2
1	H	76	GLY	3.2
1	G	397	PRO	3.2
1	A	336	PHE	3.2
1	B	9	PRO	3.2
1	C	195	HIS	3.2
1	B	184	ARG	3.1
1	E	400	LEU	3.1
1	E	502	THR	3.1
1	C	199	LEU	3.1
1	D	336	PHE	3.1
1	B	54	ARG	3.1
1	A	195	HIS	3.1
1	G	200	ALA	3.1
1	F	195	HIS	3.1
1	E	200	ALA	3.0
1	H	51	ALA	3.0
1	B	202	VAL	3.0
1	E	342	VAL	3.0
1	H	342	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	336	PHE	3.0
1	H	336	PHE	3.0
1	D	200	ALA	3.0
1	H	198	ALA	3.0
1	A	194	SER	3.0
1	D	76	GLY	3.0
1	H	74	ILE	3.0
1	C	281	GLU	3.0
1	H	48	ARG	3.0
1	H	172	ARG	3.0
1	A	50	GLY	3.0
1	D	51	ALA	3.0
1	B	48	ARG	2.9
1	C	43	ARG	2.9
1	F	202	VAL	2.9
1	H	11	VAL	2.9
1	E	285	ASP	2.9
1	D	15	ARG	2.9
1	B	397	PRO	2.9
1	E	279	ILE	2.9
1	H	195	HIS	2.9
1	H	200	ALA	2.9
1	A	9	PRO	2.9
1	D	77	GLU	2.9
1	F	49	LEU	2.9
1	F	199	LEU	2.9
1	H	193	LEU	2.9
1	A	282	ARG	2.9
1	F	294	GLU	2.9
1	H	294	GLU	2.9
1	D	171	ASP	2.9
1	C	277	HIS	2.8
1	B	52	VAL	2.8
1	A	200	ALA	2.8
1	A	280	ALA	2.8
1	D	173	ASP	2.8
1	C	184	ARG	2.8
1	C	202	VAL	2.8
1	B	175	THR	2.8
1	H	75	SER	2.8
1	G	199	LEU	2.8
1	A	279	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	48	ARG	2.8
1	E	339	ASP	2.7
1	B	49	LEU	2.7
1	C	49	LEU	2.7
1	H	400	LEU	2.7
1	H	79	VAL	2.7
1	C	336	PHE	2.7
1	C	173	ASP	2.7
1	H	341	SER	2.7
1	H	189	GLN	2.7
1	D	339	ASP	2.7
1	E	9	PRO	2.7
1	B	281	GLU	2.7
1	H	171	ASP	2.7
1	H	33	VAL	2.7
1	D	195	HIS	2.6
1	E	195	HIS	2.6
1	E	278	VAL	2.6
1	E	282	ARG	2.6
1	A	284	LEU	2.6
1	H	196	ARG	2.6
1	B	194	SER	2.6
1	C	285	ASP	2.6
1	H	496	GLN	2.6
1	D	176	ARG	2.6
1	F	196	ARG	2.6
1	A	189	GLN	2.6
1	A	283	ARG	2.6
1	D	172	ARG	2.5
1	C	52	VAL	2.5
1	E	52	VAL	2.5
1	B	400	LEU	2.5
1	B	39	ARG	2.5
1	B	43	ARG	2.5
1	C	171	ASP	2.5
1	E	171	ASP	2.5
1	B	77	GLU	2.5
1	D	294	GLU	2.5
1	A	48	ARG	2.5
1	H	8	LYS	2.5
1	G	194	SER	2.5
1	A	36	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	33	VAL	2.5
1	C	337	PRO	2.5
1	F	15	ARG	2.5
1	D	10	ALA	2.5
1	H	10	ALA	2.5
1	B	136	GLU	2.5
1	A	199	LEU	2.4
1	H	73	LEU	2.4
1	G	195	HIS	2.4
1	H	54	ARG	2.4
1	E	173	ASP	2.4
1	D	202	VAL	2.4
1	E	17	ILE	2.4
1	C	339	ASP	2.4
1	D	56	ALA	2.4
1	H	35	ALA	2.4
1	C	340	GLY	2.4
1	A	495	GLU	2.4
1	B	196	ARG	2.4
1	F	172	ARG	2.4
1	G	80	ARG	2.4
1	A	47	ALA	2.4
1	D	198	ALA	2.4
1	G	52	VAL	2.4
1	G	501	GLU	2.4
1	B	177	LEU	2.4
1	H	114	ILE	2.3
1	A	166	ARG	2.3
1	F	80	ARG	2.3
1	A	480	ASP	2.3
1	E	49	LEU	2.3
1	H	63	THR	2.3
1	A	15	ARG	2.3
1	B	176	ARG	2.3
1	H	337	PRO	2.3
1	H	397	PRO	2.3
1	H	53	ILE	2.3
1	G	285	ASP	2.3
1	H	339	ASP	2.3
1	C	395	ARG	2.3
1	E	43	ARG	2.3
1	H	119	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	397	PRO	2.3
1	H	17	ILE	2.3
1	B	40	ASP	2.3
1	C	200	ALA	2.3
1	D	70	ALA	2.3
1	A	184	ARG	2.3
1	D	174	GLY	2.3
1	E	187	ARG	2.3
1	H	50	GLY	2.3
1	H	213	LEU	2.3
1	A	53	ILE	2.2
1	D	282	ARG	2.2
1	G	395	ARG	2.2
1	C	399	GLY	2.2
1	A	501	GLU	2.2
1	D	12	GLU	2.2
1	H	175	THR	2.2
1	A	75	SER	2.2
1	C	249	SER	2.2
1	D	62	LEU	2.2
1	D	73	LEU	2.2
1	A	187	ARG	2.2
1	A	196	ARG	2.2
1	C	80	ARG	2.2
1	G	54	ARG	2.2
1	C	12	GLU	2.2
1	D	53	ILE	2.2
1	H	16	HIS	2.2
1	B	398	ALA	2.2
1	H	44	ALA	2.2
1	C	341	SER	2.2
1	H	187	ARG	2.2
1	B	342	VAL	2.2
1	G	495	GLU	2.2
1	A	338	PRO	2.2
1	B	338	PRO	2.2
1	F	293	PRO	2.2
1	B	51	ALA	2.2
1	F	341	SER	2.2
1	B	171	ASP	2.2
1	C	502	THR	2.2
1	F	173	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	199	LEU	2.2
1	E	174	GLY	2.2
1	A	35	ALA	2.1
1	D	80	ARG	2.1
1	G	477	SER	2.1
1	E	288	ASP	2.1
1	H	36	PRO	2.1
1	B	340	GLY	2.1
1	G	399	GLY	2.1
1	A	191	LEU	2.1
1	D	248	LEU	2.1
1	G	77	GLU	2.1
1	A	171	ASP	2.1
1	H	197	ASP	2.1
1	C	10	ALA	2.1
1	C	51	ALA	2.1
1	B	36	PRO	2.1
1	C	522	PRO	2.1
1	H	338	PRO	2.1
1	B	79	VAL	2.1
1	B	213	LEU	2.1
1	A	398	ALA	2.1
1	G	198	ALA	2.1
1	A	16	HIS	2.1
1	D	74	ILE	2.1
1	C	174	GLY	2.1
1	E	293	PRO	2.1
1	H	173	ASP	2.1
1	F	203	ASN	2.1
1	A	198	ALA	2.0
1	H	174	GLY	2.0
1	H	340	GLY	2.0
1	H	522	PRO	2.0
1	F	400	LEU	2.0
1	G	172	ARG	2.0
1	C	198	ALA	2.0
1	H	122	SER	2.0
1	C	9	PRO	2.0
1	D	338	PRO	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	MDO	H	149	13/14	0.91	0.10	16,19,26,26	0
1	MDO	B	149	13/14	0.93	0.08	16,19,23,26	0
1	MDO	F	149	13/14	0.95	0.08	12,15,20,21	0
1	MDO	G	149	13/14	0.95	0.07	13,14,17,19	0
1	MDO	A	149	13/14	0.95	0.06	15,18,21,21	0
1	MDO	C	149	13/14	0.96	0.05	13,14,18,19	0
1	MDO	D	149	13/14	0.96	0.07	18,20,22,24	0
1	MDO	E	149	13/14	0.96	0.06	12,14,18,18	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(Å ²)	Q<0.9
2	PMI	B	701	14/14	0.90	0.12	26,29,31,31	0
2	PMI	H	701	14/14	0.91	0.12	25,31,32,33	0
2	PMI	E	701	14/14	0.92	0.11	20,24,26,27	0
2	PMI	D	701	14/14	0.93	0.10	26,27,29,32	0
2	PMI	A	701	14/14	0.93	0.10	23,26,28,29	0
2	PMI	F	701	14/14	0.93	0.11	21,25,27,28	0
2	PMI	C	701	14/14	0.93	0.10	19,22,23,23	0
2	PMI	G	701	14/14	0.95	0.09	21,22,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.