



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:39 PM UTC

PDB ID : 4YR8 / pdb_00004yr8
Title : Crystal structure of JNK in complex with a regulator protein
Authors : Liu, X.; Wang, J.; Wu, J.W.; Wang, Z.X.
Deposited on : 2015-03-14
Resolution : 2.40 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

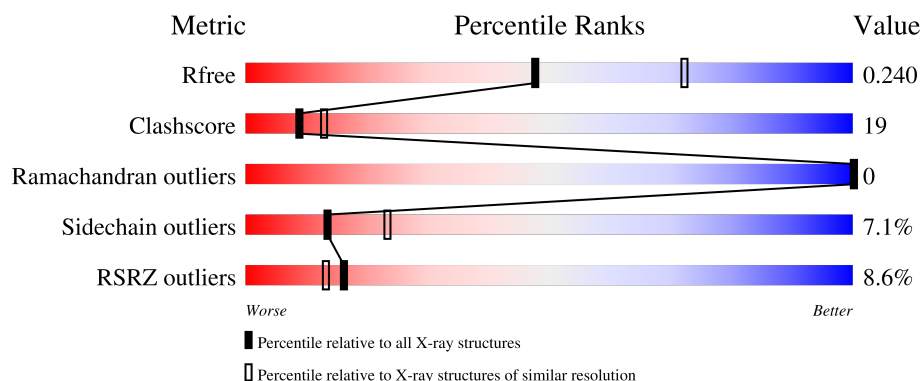
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	371	 6% 64% 20% 14%
1	C	371	 11% 53% 26% 6% 14%
1	E	371	 6% 51% 28% 5% 15%
1	F	371	 12% 52% 24% 19%
2	B	167	 2% 63% 17% 16%

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Mol	Chain	Length	Quality of chain
2	D	167	3% 58% 24% 15%
2	G	167	5% 51% 28% 16%
2	H	167	5% 62% 22% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14988 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 Mitogen-activated protein kinase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	317	Total	C	N	O	S	0	0	0
			2551	1639	430	463	19			
1	A	320	Total	C	N	O	S	0	0	0
			2582	1661	433	469	19			
1	C	318	Total	C	N	O	S	0	0	0
			2565	1652	431	463	19			
1	F	300	Total	C	N	O	S	0	1	0
			2412	1558	404	431	19			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	364	LEU	-	expression tag	UNP P45983
E	365	GLU	-	expression tag	UNP P45983
E	366	HIS	-	expression tag	UNP P45983
E	367	HIS	-	expression tag	UNP P45983
E	368	HIS	-	expression tag	UNP P45983
E	369	HIS	-	expression tag	UNP P45983
E	370	HIS	-	expression tag	UNP P45983
E	371	HIS	-	expression tag	UNP P45983
A	364	LEU	-	expression tag	UNP P45983
A	365	GLU	-	expression tag	UNP P45983
A	366	HIS	-	expression tag	UNP P45983
A	367	HIS	-	expression tag	UNP P45983
A	368	HIS	-	expression tag	UNP P45983
A	369	HIS	-	expression tag	UNP P45983
A	370	HIS	-	expression tag	UNP P45983
A	371	HIS	-	expression tag	UNP P45983
C	364	LEU	-	expression tag	UNP P45983
C	365	GLU	-	expression tag	UNP P45983
C	366	HIS	-	expression tag	UNP P45983
C	367	HIS	-	expression tag	UNP P45983
C	368	HIS	-	expression tag	UNP P45983

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Chain	Residue	Modelled	Actual	Comment	Reference
C	369	HIS	-	expression tag	UNP P45983
C	370	HIS	-	expression tag	UNP P45983
C	371	HIS	-	expression tag	UNP P45983
F	364	LEU	-	expression tag	UNP P45983
F	365	GLU	-	expression tag	UNP P45983
F	366	HIS	-	expression tag	UNP P45983
F	367	HIS	-	expression tag	UNP P45983
F	368	HIS	-	expression tag	UNP P45983
F	369	HIS	-	expression tag	UNP P45983
F	370	HIS	-	expression tag	UNP P45983
F	371	HIS	-	expression tag	UNP P45983

- Molecule 2 is a protein called Dual specificity protein phosphatase 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	141	Total	C	N	O	S	0	0	0
			1121	719	191	202	9			
2	B	141	Total	C	N	O	S	0	1	0
			1129	724	194	202	9			
2	D	142	Total	C	N	O	S	0	0	0
			1130	725	193	203	9			
2	H	143	Total	C	N	O	S	0	0	0
			1138	729	195	205	9			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	135	MET	-	expression tag	UNP Q9BY84
G	136	GLY	-	expression tag	UNP Q9BY84
G	137	SER	-	expression tag	UNP Q9BY84
G	138	SER	-	expression tag	UNP Q9BY84
G	139	HIS	-	expression tag	UNP Q9BY84
G	140	HIS	-	expression tag	UNP Q9BY84
G	141	HIS	-	expression tag	UNP Q9BY84
G	142	HIS	-	expression tag	UNP Q9BY84
G	143	HIS	-	expression tag	UNP Q9BY84
G	144	HIS	-	expression tag	UNP Q9BY84
G	145	SER	-	expression tag	UNP Q9BY84
G	146	SER	-	expression tag	UNP Q9BY84
G	147	GLY	-	expression tag	UNP Q9BY84
G	148	LEU	-	expression tag	UNP Q9BY84
G	149	VAL	-	expression tag	UNP Q9BY84

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Chain	Residue	Modelled	Actual	Comment	Reference
G	150	PRO	-	expression tag	UNP Q9BY84
G	151	ARG	-	expression tag	UNP Q9BY84
G	152	GLY	-	expression tag	UNP Q9BY84
G	153	SER	-	expression tag	UNP Q9BY84
G	154	HIS	-	expression tag	UNP Q9BY84
G	155	MET	-	expression tag	UNP Q9BY84
B	135	MET	-	expression tag	UNP Q9BY84
B	136	GLY	-	expression tag	UNP Q9BY84
B	137	SER	-	expression tag	UNP Q9BY84
B	138	SER	-	expression tag	UNP Q9BY84
B	139	HIS	-	expression tag	UNP Q9BY84
B	140	HIS	-	expression tag	UNP Q9BY84
B	141	HIS	-	expression tag	UNP Q9BY84
B	142	HIS	-	expression tag	UNP Q9BY84
B	143	HIS	-	expression tag	UNP Q9BY84
B	144	HIS	-	expression tag	UNP Q9BY84
B	145	SER	-	expression tag	UNP Q9BY84
B	146	SER	-	expression tag	UNP Q9BY84
B	147	GLY	-	expression tag	UNP Q9BY84
B	148	LEU	-	expression tag	UNP Q9BY84
B	149	VAL	-	expression tag	UNP Q9BY84
B	150	PRO	-	expression tag	UNP Q9BY84
B	151	ARG	-	expression tag	UNP Q9BY84
B	152	GLY	-	expression tag	UNP Q9BY84
B	153	SER	-	expression tag	UNP Q9BY84
B	154	HIS	-	expression tag	UNP Q9BY84
B	155	MET	-	expression tag	UNP Q9BY84
D	135	MET	-	expression tag	UNP Q9BY84
D	136	GLY	-	expression tag	UNP Q9BY84
D	137	SER	-	expression tag	UNP Q9BY84
D	138	SER	-	expression tag	UNP Q9BY84
D	139	HIS	-	expression tag	UNP Q9BY84
D	140	HIS	-	expression tag	UNP Q9BY84
D	141	HIS	-	expression tag	UNP Q9BY84
D	142	HIS	-	expression tag	UNP Q9BY84
D	143	HIS	-	expression tag	UNP Q9BY84
D	144	HIS	-	expression tag	UNP Q9BY84
D	145	SER	-	expression tag	UNP Q9BY84
D	146	SER	-	expression tag	UNP Q9BY84
D	147	GLY	-	expression tag	UNP Q9BY84
D	148	LEU	-	expression tag	UNP Q9BY84
D	149	VAL	-	expression tag	UNP Q9BY84

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Chain	Residue	Modelled	Actual	Comment	Reference
D	150	PRO	-	expression tag	UNP Q9BY84
D	151	ARG	-	expression tag	UNP Q9BY84
D	152	GLY	-	expression tag	UNP Q9BY84
D	153	SER	-	expression tag	UNP Q9BY84
D	154	HIS	-	expression tag	UNP Q9BY84
D	155	MET	-	expression tag	UNP Q9BY84
H	135	MET	-	expression tag	UNP Q9BY84
H	136	GLY	-	expression tag	UNP Q9BY84
H	137	SER	-	expression tag	UNP Q9BY84
H	138	SER	-	expression tag	UNP Q9BY84
H	139	HIS	-	expression tag	UNP Q9BY84
H	140	HIS	-	expression tag	UNP Q9BY84
H	141	HIS	-	expression tag	UNP Q9BY84
H	142	HIS	-	expression tag	UNP Q9BY84
H	143	HIS	-	expression tag	UNP Q9BY84
H	144	HIS	-	expression tag	UNP Q9BY84
H	145	SER	-	expression tag	UNP Q9BY84
H	146	SER	-	expression tag	UNP Q9BY84
H	147	GLY	-	expression tag	UNP Q9BY84
H	148	LEU	-	expression tag	UNP Q9BY84
H	149	VAL	-	expression tag	UNP Q9BY84
H	150	PRO	-	expression tag	UNP Q9BY84
H	151	ARG	-	expression tag	UNP Q9BY84
H	152	GLY	-	expression tag	UNP Q9BY84
H	153	SER	-	expression tag	UNP Q9BY84
H	154	HIS	-	expression tag	UNP Q9BY84
H	155	MET	-	expression tag	UNP Q9BY84

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	H	1	Total Cl 1 1	0	0

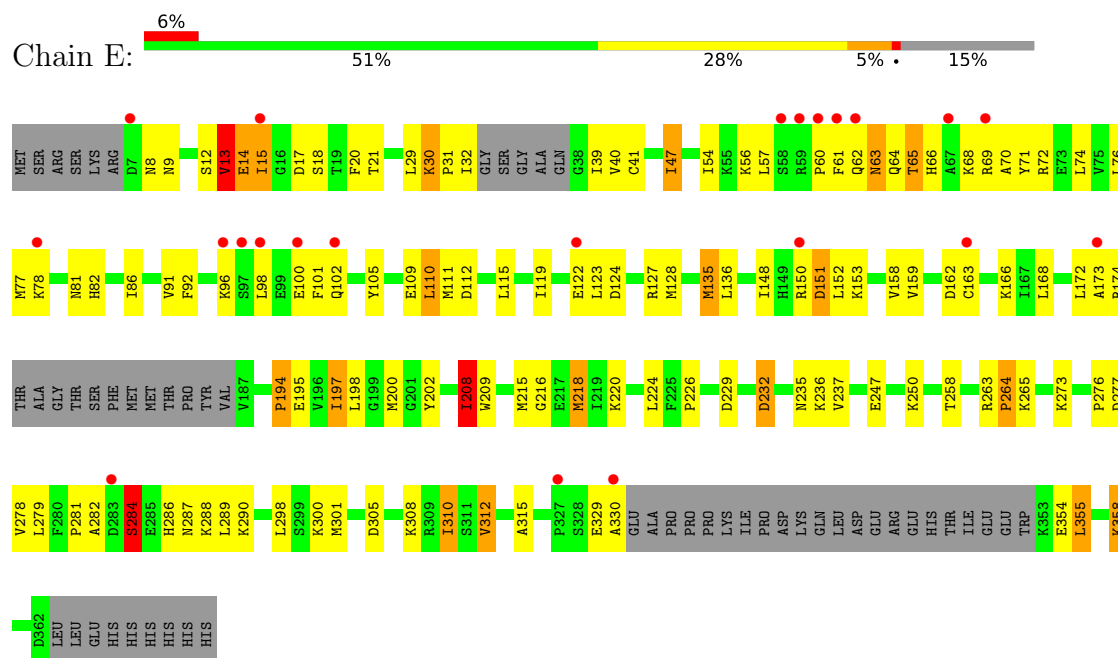
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	81	Total 81	O 81	0	0
4	G	23	Total 23	O 23	0	0
4	A	71	Total 71	O 71	0	0
4	B	43	Total 43	O 43	0	0
4	C	55	Total 55	O 55	0	0
4	D	20	Total 20	O 20	0	0
4	F	50	Total 50	O 50	0	0
4	H	13	Total 13	O 13	0	0

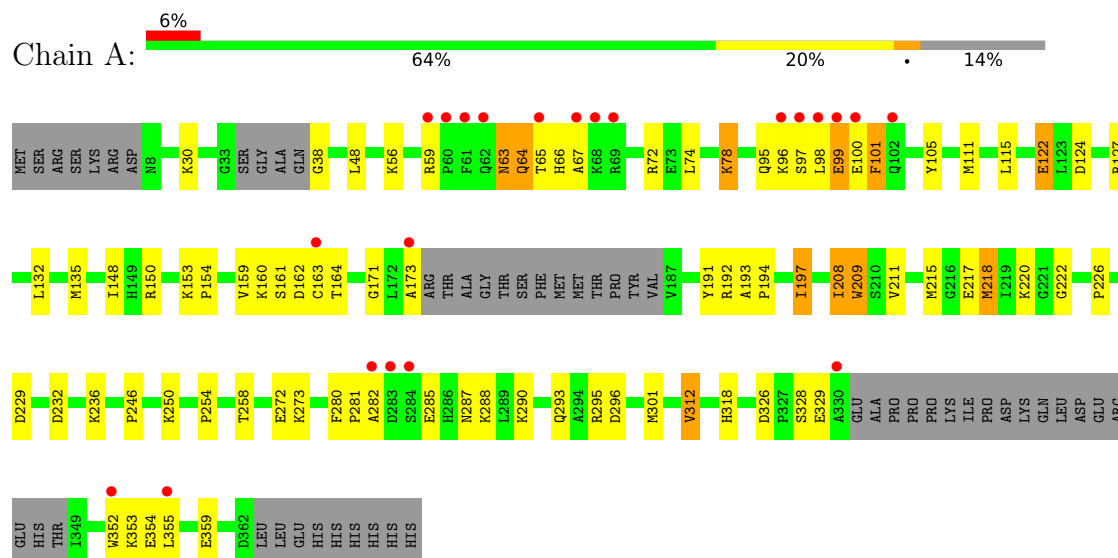
3 Residue-property plots [i](#)

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.

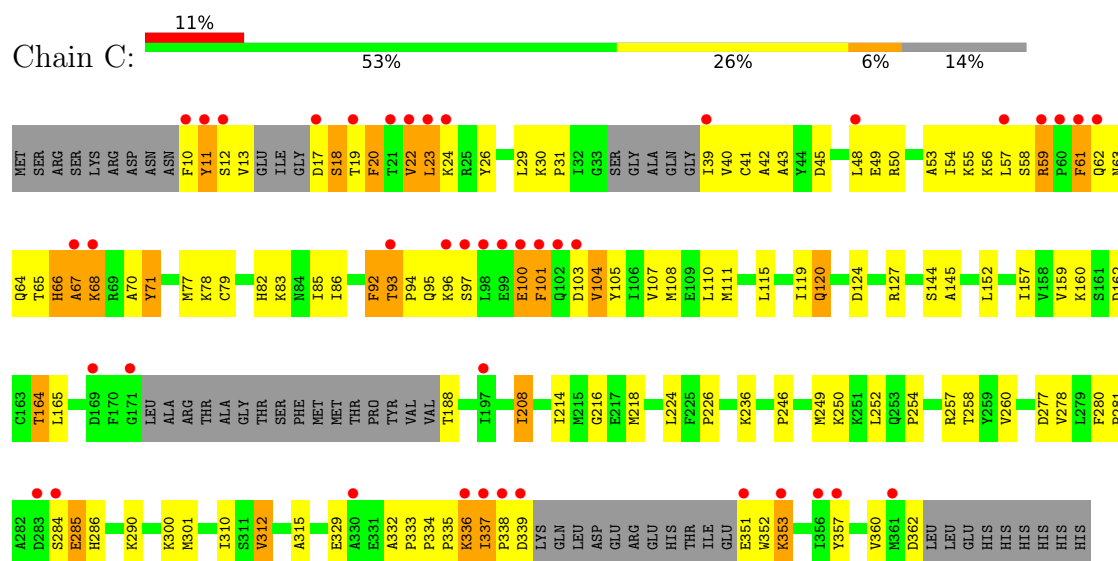
• Molecule 1: Mitogen-activated protein kinase 8



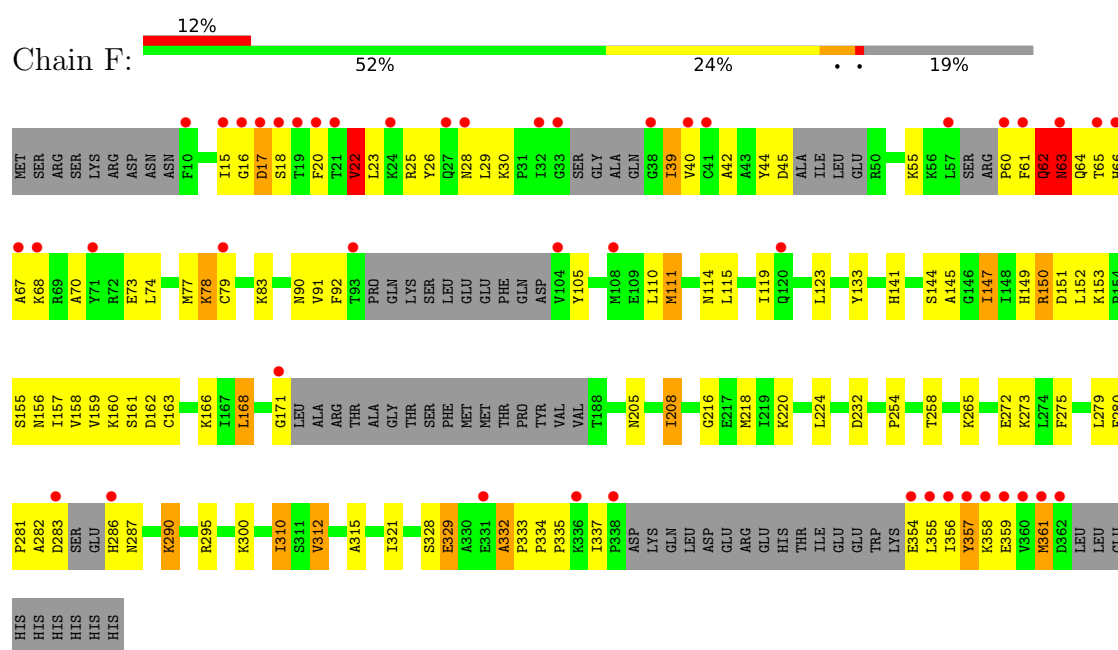
• Molecule 1: Mitogen-activated protein kinase 8



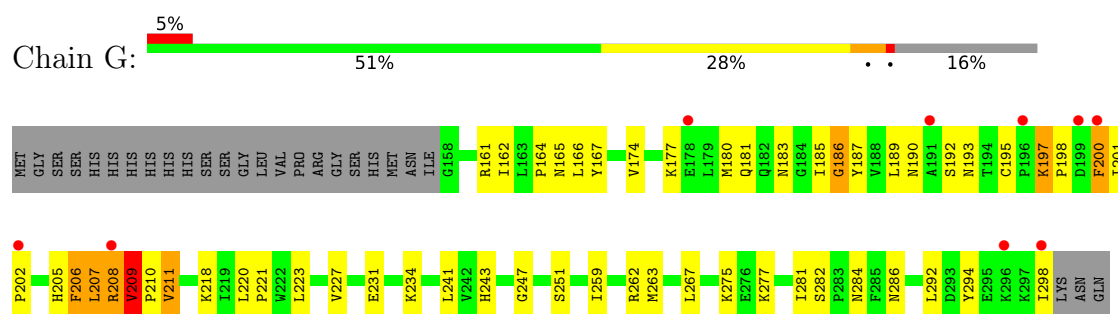
- Molecule 1: Mitogen-activated protein kinase 8



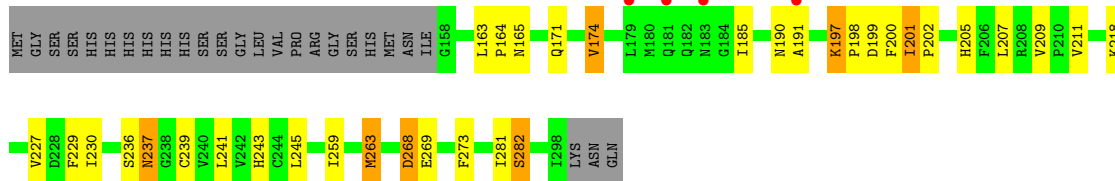
- Molecule 1: Mitogen-activated protein kinase 8



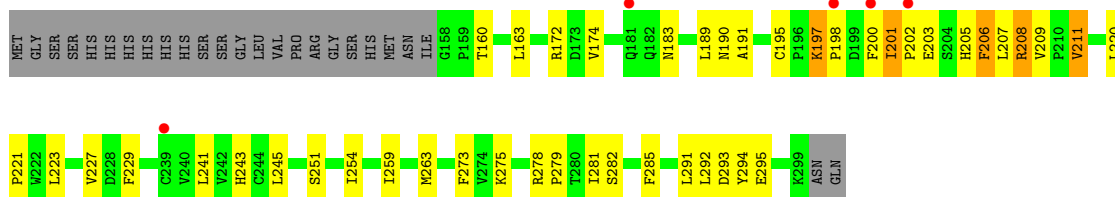
- Molecule 2: Dual specificity protein phosphatase 16



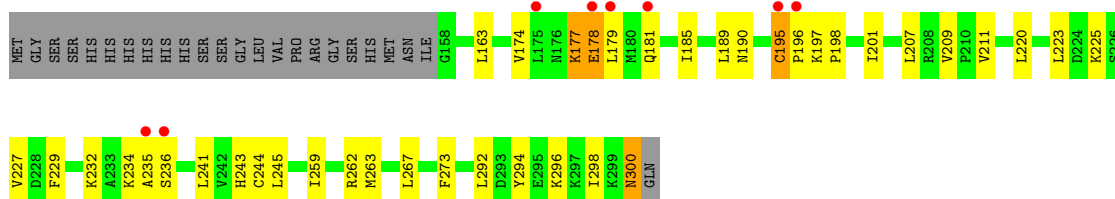
- Molecule 2: Dual specificity protein phosphatase 16



- Molecule 2: Dual specificity protein phosphatase 16



- Molecule 2: Dual specificity protein phosphatase 16



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.15Å 74.85Å 134.81Å 76.94° 84.32° 67.44°	Depositor
Resolution (Å)	38.02 – 2.40 38.02 – 2.40	Depositor EDS
% Data completeness (in resolution range)	83.8 (38.02-2.40) 83.6 (38.02-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.35 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.217 , 0.239 0.220 , 0.240	Depositor DCC
R_{free} test set	3406 reflections (4.25%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14988	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: CL

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	0.80	3/2636 (0.1%)	1.09	14/3559 (0.4%)
1	C	0.87	5/2622 (0.2%)	1.04	9/3542 (0.3%)
1	E	1.52	27/2603 (1.0%)	1.09	6/3514 (0.2%)
1	F	0.91	1/2465 (0.0%)	1.07	15/3325 (0.5%)
2	B	0.94	2/1156 (0.2%)	1.04	4/1561 (0.3%)
2	D	0.85	4/1154 (0.3%)	1.10	9/1558 (0.6%)
2	G	1.22	3/1145 (0.3%)	1.21	6/1547 (0.4%)
2	H	0.72	0/1162	1.04	4/1569 (0.3%)
All	All	1.03	45/14943 (0.3%)	1.08	67/20175 (0.3%)

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	91	VAL	C-O	-7.17	1.16	1.24
2	D	282	SER	N-CA	-6.91	1.39	1.46
1	C	71	TYR	C-N	-6.31	1.25	1.33
1	E	232	ASP	N-CA	-6.29	1.38	1.46
1	E	218	MET	C-O	-6.17	1.16	1.24
1	A	153	LYS	C-O	-6.15	1.17	1.24
1	E	54	ILE	C-O	-6.06	1.17	1.24
2	D	201	ILE	CA-CB	5.94	1.59	1.54
1	C	68	LYS	C-N	-5.93	1.25	1.34
1	E	208	ILE	C-O	-5.91	1.17	1.24
2	G	166	LEU	C-O	-5.87	1.17	1.23
1	E	153	LYS	C-O	-5.68	1.18	1.24
1	E	110	LEU	C-O	-5.66	1.17	1.24
1	C	20	PHE	N-CA	-5.62	1.39	1.46
1	E	12	SER	C-O	-5.58	1.17	1.23
2	G	189	LEU	C-O	-5.51	1.17	1.24
1	E	13	VAL	C-O	-5.50	1.18	1.23
2	G	211	VAL	C-O	-5.48	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	151	ASP	C-O	-5.47	1.18	1.23
1	E	209	TRP	C-O	-5.42	1.17	1.24
2	B	268	ASP	C-O	-5.37	1.17	1.24
2	B	269	GLU	C-O	-5.36	1.17	1.24
1	E	112	ASP	C-O	-5.35	1.17	1.24
1	E	82	HIS	C-O	-5.33	1.17	1.23
1	F	147	ILE	C-O	-5.32	1.18	1.24
1	E	152	LEU	C-O	-5.32	1.17	1.24
1	C	43	ALA	CA-C	-5.29	1.46	1.52
1	E	197	ILE	C-O	-5.27	1.17	1.24
2	D	291	LEU	C-O	-5.25	1.17	1.24
1	A	287	ASN	C-O	-5.23	1.18	1.24
1	E	136	LEU	C-O	-5.22	1.18	1.24
1	E	310	ILE	C-O	-5.18	1.17	1.24
1	E	47	ILE	C-O	-5.17	1.18	1.24
1	E	232	ASP	C-O	-5.15	1.18	1.24
1	E	237	VAL	C-O	-5.14	1.18	1.24
1	E	14	GLU	C-O	-5.14	1.17	1.24
1	E	135	MET	C-O	-5.14	1.18	1.24
1	E	198	LEU	C-O	-5.13	1.17	1.24
1	E	194	PRO	C-O	-5.13	1.17	1.24
1	A	209	TRP	C-O	-5.11	1.18	1.24
2	D	294	TYR	C-O	-5.05	1.18	1.24
1	E	264	PRO	N-CD	5.03	1.54	1.47
1	E	9	ASN	C-O	-5.03	1.17	1.23
1	C	50	ARG	CA-C	-5.02	1.46	1.52
1	E	109	GLU	C-O	-5.01	1.17	1.23

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	LYS	O-C-N	-12.44	112.13	121.84
1	C	61	PHE	N-CA-C	10.22	124.37	112.72
1	C	11	TYR	N-CA-C	10.16	122.91	110.41
2	G	209	VAL	N-CA-C	-9.74	98.51	108.15
1	F	332	ALA	N-CA-C	-8.86	99.95	110.13
2	G	200	PHE	N-CA-C	8.75	123.53	111.55
1	F	17	ASP	N-CA-C	-8.59	102.97	113.19
1	F	62	GLN	N-CA-C	8.31	121.08	111.11
1	F	68	LYS	N-CA-C	-8.07	102.88	112.89
1	C	67	ALA	N-CA-C	-7.50	103.04	111.14
1	A	282	ALA	N-CA-C	7.40	120.40	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	208	ARG	N-CA-C	-7.14	98.59	109.95
2	B	191	ALA	N-CA-C	7.00	120.70	112.72
2	B	245	LEU	N-CA-C	6.96	119.46	111.11
1	C	96	LYS	N-CA-C	6.92	118.90	111.36
2	H	244	CYS	N-CA-C	-6.69	100.02	108.45
1	A	148	ILE	CB-CA-C	6.68	121.40	111.31
2	G	186	GLY	CA-C-N	-6.57	111.27	123.03
2	G	186	GLY	C-N-CA	-6.57	111.27	123.03
2	H	177	LYS	N-CA-C	6.50	118.95	111.02
2	B	282	SER	N-CA-CB	-6.45	103.05	111.23
1	A	148	ILE	N-CA-C	-6.43	99.01	108.97
1	E	235	ASN	N-CA-C	6.27	118.63	111.11
2	D	282	SER	N-CA-CB	-6.24	103.36	111.09
1	A	48	LEU	N-CA-C	-6.14	105.82	113.38
1	C	285	GLU	CB-CA-C	6.14	120.39	109.65
2	D	200	PHE	CA-C-N	-6.11	118.02	123.33
2	D	200	PHE	C-N-CA	-6.11	118.02	123.33
2	D	295	GLU	N-CA-C	-6.09	104.64	111.28
1	E	282	ALA	N-CA-C	6.07	119.16	111.69
1	F	282	ALA	N-CA-C	6.06	118.39	109.24
1	A	99	GLU	N-CA-C	-6.06	104.76	111.36
1	C	285	GLU	N-CA-C	-6.05	97.98	108.69
2	G	162	ILE	N-CA-C	-6.00	107.04	111.90
1	F	62	GLN	CB-CA-C	-5.99	101.22	110.81
1	E	101	PHE	N-CA-C	5.96	119.45	110.64
1	E	92	PHE	N-CA-C	5.87	117.71	108.96
1	E	284	SER	N-CA-C	-5.84	100.37	109.72
1	A	64	GLN	N-CA-C	5.79	120.35	113.28
1	C	20	PHE	N-CA-C	-5.55	100.67	109.76
1	C	61	PHE	N-CA-CB	-5.51	102.50	110.70
1	F	63	ASN	N-CA-C	-5.48	101.34	110.17
1	F	22	VAL	CB-CA-C	5.47	118.68	111.19
1	A	281	PRO	N-CA-C	5.46	120.16	111.26
1	A	101	PHE	N-CA-C	5.43	118.06	109.96
2	B	230	ILE	N-CA-C	-5.43	105.42	110.53
1	F	310	ILE	CB-CA-C	-5.40	105.40	111.45
1	A	63	ASN	N-CA-C	-5.40	101.29	108.74
2	D	160	THR	N-CA-C	5.39	117.52	108.73
2	D	197	LYS	N-CA-C	-5.38	102.46	110.20
1	F	90	ASN	N-CA-C	5.36	116.68	108.42
1	A	197	ILE	CB-CA-C	-5.35	103.59	112.26
1	C	92	PHE	N-CA-C	5.35	116.98	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	287	ASN	N-CA-C	5.30	117.32	107.99
2	D	211	VAL	N-CA-C	5.30	117.69	108.95
2	H	235	ALA	N-CA-C	-5.24	107.44	113.88
2	D	183	ASN	N-CA-C	-5.23	103.62	110.53
1	A	164	THR	N-CA-C	-5.23	101.94	110.20
1	A	280	PHE	CA-C-N	5.21	125.51	119.93
1	A	280	PHE	C-N-CA	5.21	125.51	119.93
1	F	39	ILE	N-CA-C	5.11	116.17	109.21
2	H	195	CYS	N-CA-C	5.09	121.06	109.81
1	F	361	MET	N-CA-C	5.08	119.11	113.02
1	F	357	TYR	N-CA-C	5.07	116.62	111.14
2	D	245	LEU	N-CA-C	5.07	119.68	111.37
1	E	65	THR	N-CA-C	5.05	117.56	111.40
1	F	168	LEU	N-CA-C	5.01	119.41	112.45

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	2582	0	2597	53	0
1	C	2565	0	2572	149	0
1	E	2551	0	2569	103	0
1	F	2412	0	2431	85	0
2	B	1129	0	1154	33	0
2	D	1130	0	1154	40	0
2	G	1121	0	1141	73	0
2	H	1138	0	1160	23	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	71	0	0	4	0
4	B	43	0	0	1	0
4	C	55	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	20	0	0	2	0
4	E	81	0	0	5	0
4	F	50	0	0	2	0
4	G	23	0	0	2	0
4	H	13	0	0	0	0
All	All	14988	0	14778	548	0

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

All (548) 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)
2:G:207:LEU:HD12	2:G:208:ARG:N	1.31	1.40
1:C:63:ASN:CB	1:C:65:THR:HG22	1.71	1.19
1:C:101:PHE:CE2	1:C:357:TYR:HB2	1.82	1.14
2:B:198:PRO:HG2	2:B:201:ILE:HB	1.27	1.12
2:G:180:MET:HE1	2:G:185:ILE:HG21	1.26	1.11
1:C:63:ASN:HB2	1:C:65:THR:HG22	1.27	1.10
1:C:101:PHE:HE2	1:C:357:TYR:HB2	0.98	1.10
2:G:207:LEU:HD12	2:G:207:LEU:C	1.69	1.09
1:F:67:ALA:HB1	1:F:356:ILE:HD11	1.24	1.09
1:C:92:PHE:CE1	1:C:105:TYR:CD2	2.42	1.07
1:A:64:GLN:HG3	1:A:352:TRP:HE1	0.92	1.06
1:C:145:ALA:CB	1:C:335:PRO:HG2	1.88	1.04
2:G:180:MET:CE	2:G:185:ILE:HG21	1.90	1.01
1:C:145:ALA:HB2	1:C:335:PRO:HG2	1.02	1.01
1:C:145:ALA:HB2	1:C:335:PRO:CG	1.89	1.01
2:G:206:PHE:CD1	2:G:207:LEU:N	2.28	1.00
2:G:180:MET:HE1	2:G:185:ILE:CG2	1.90	1.00
1:C:65:THR:HG23	1:C:66:HIS:ND1	1.76	0.99
1:C:101:PHE:HE2	1:C:357:TYR:CB	1.74	0.99
2:G:207:LEU:CD1	2:G:208:ARG:N	2.24	0.98
1:A:64:GLN:HG3	1:A:352:TRP:NE1	1.78	0.98
1:C:101:PHE:CE2	1:C:357:TYR:CD1	2.53	0.97
2:G:180:MET:CE	2:G:185:ILE:CG2	2.43	0.95
1:A:326:ASP:HB3	1:A:329:GLU:HG3	1.45	0.95
1:E:63:ASN:OD1	1:E:65:THR:HG22	1.68	0.94
1:C:95:GLN:HG2	1:C:101:PHE:HA	1.51	0.93
2:D:191:ALA:HA	2:D:209:VAL:HB	1.48	0.93
1:C:63:ASN:HB3	1:C:65:THR:HG22	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:THR:HG23	1:C:66:HIS:CE1	2.05	0.91
2:G:206:PHE:CD1	2:G:206:PHE:C	2.48	0.90
1:C:101:PHE:CD2	1:C:357:TYR:CD1	2.58	0.90
2:G:207:LEU:HD12	2:G:208:ARG:H	1.33	0.90
1:C:332:ALA:HB1	1:C:333:PRO:HD2	1.52	0.89
1:E:63:ASN:HD21	1:E:66:HIS:H	1.17	0.89
2:G:174:VAL:HG12	2:G:198:PRO:HB3	1.55	0.89
2:B:198:PRO:CG	2:B:201:ILE:HB	2.04	0.88
1:E:226:PRO:O	1:E:236:LYS:HE2	1.73	0.87
1:C:66:HIS:O	1:C:70:ALA:CB	2.24	0.86
2:G:207:LEU:C	2:G:207:LEU:CD1	2.49	0.85
2:D:190:ASN:HD21	2:D:195:CYS:HB2	1.41	0.85
2:G:207:LEU:HD11	2:G:208:ARG:O	1.76	0.85
1:C:12:SER:O	1:C:13:VAL:CG2	2.24	0.84
1:C:39:ILE:HG23	1:C:40:VAL:HG23	1.59	0.84
1:F:145:ALA:HB3	1:F:147:ILE:HD12	1.56	0.84
2:B:198:PRO:HG2	2:B:201:ILE:CB	2.07	0.84
1:C:65:THR:CG2	1:C:66:HIS:CE1	2.61	0.83
1:C:101:PHE:CE2	1:C:357:TYR:HD1	1.95	0.83
1:A:63:ASN:ND2	1:A:65:THR:H	1.76	0.83
1:A:97:SER:HB3	1:A:100:GLU:HB2	1.61	0.82
1:C:56:LYS:HE2	1:C:58:SER:OG	1.79	0.82
1:E:215:MET:HE2	1:E:298:LEU:HG	1.61	0.82
2:D:197:LYS:CG	2:D:198:PRO:HD2	2.08	0.82
1:C:92:PHE:CE1	1:C:105:TYR:HD2	1.99	0.81
2:D:197:LYS:HG3	2:D:206:PHE:CD2	2.16	0.81
2:B:202:PRO:HG2	2:B:205:HIS:HB2	1.62	0.80
1:C:63:ASN:HB2	1:C:65:THR:CG2	2.11	0.80
1:A:162:ASP:O	1:A:163:CYS:HB2	1.79	0.80
2:G:207:LEU:CD1	2:G:208:ARG:O	2.30	0.79
1:E:194:PRO:HA	1:E:197:ILE:HD12	1.63	0.79
1:C:93:THR:HB	1:C:103:ASP:O	1.82	0.79
1:C:29:LEU:O	1:C:30:LYS:HD3	1.82	0.79
1:C:57:LEU:HB2	1:C:104:VAL:O	1.82	0.79
1:C:101:PHE:CD1	1:C:101:PHE:C	2.61	0.78
1:C:65:THR:CG2	1:C:66:HIS:ND1	2.47	0.78
1:E:128:MET:HG2	1:E:218:MET:HE2	1.64	0.78
1:C:101:PHE:CE2	1:C:357:TYR:CB	2.58	0.78
1:A:95:GLN:HG2	1:A:100:GLU:O	1.84	0.78
1:F:74:LEU:CD2	1:F:359:GLU:HB3	2.14	0.78
1:E:65:THR:HG23	1:E:66:HIS:HD2	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:LEU:C	1:F:111:MET:HE3	2.11	0.76
1:E:13:VAL:HG23	1:E:15:ILE:HD11	1.66	0.76
2:G:186:GLY:C	2:G:187:TYR:HD1	1.92	0.76
1:F:74:LEU:HD21	1:F:359:GLU:HB3	1.68	0.76
1:C:66:HIS:O	1:C:70:ALA:HB3	1.87	0.75
1:E:63:ASN:ND2	1:E:66:HIS:H	1.83	0.74
1:A:101:PHE:O	1:A:353:LYS:NZ	2.21	0.74
1:A:150:ARG:HH22	1:A:173:ALA:C	1.95	0.74
2:G:206:PHE:C	2:G:206:PHE:HD1	1.96	0.74
2:D:197:LYS:HG2	2:D:198:PRO:HD2	1.69	0.74
2:G:202:PRO:HG2	2:G:205:HIS:HB2	1.68	0.73
1:C:93:THR:HG22	1:C:360:VAL:HG11	1.71	0.73
2:G:180:MET:CE	2:G:185:ILE:HG22	2.17	0.73
2:G:180:MET:HE3	2:G:185:ILE:HG22	1.71	0.73
1:F:115:LEU:O	1:F:119:ILE:HG13	1.89	0.73
1:E:287:ASN:HB2	4:E:403:HOH:O	1.89	0.72
1:C:92:PHE:HE1	1:C:105:TYR:CD2	2.05	0.72
1:F:67:ALA:HA	1:F:70:ALA:HB3	1.72	0.72
2:G:197:LYS:HG3	2:G:198:PRO:HD2	1.69	0.72
1:C:12:SER:C	1:C:13:VAL:HG23	2.14	0.72
1:C:12:SER:O	1:C:13:VAL:HG23	1.88	0.71
2:H:207:LEU:HD22	2:H:229:PHE:HB2	1.72	0.71
1:F:60:PRO:HD2	1:F:61:PHE:CD1	2.26	0.71
1:C:144:SER:HB3	1:C:334:PRO:HB3	1.72	0.71
1:C:12:SER:O	1:C:13:VAL:HG22	1.91	0.71
1:F:22:VAL:HG13	1:F:26:TYR:HD2	1.55	0.70
1:E:278:VAL:HG22	2:H:262:ARG:NH1	2.06	0.70
1:C:56:LYS:HG2	1:C:58:SER:OG	1.92	0.70
1:C:93:THR:CB	1:C:103:ASP:O	2.40	0.70
1:C:188:THR:N	4:C:401:HOH:O	2.24	0.70
2:D:174:VAL:HG12	2:D:241:LEU:HD23	1.72	0.70
1:E:208:ILE:HD11	1:E:312:VAL:HG12	1.73	0.69
1:C:31:PRO:HA	1:C:41:CYS:HA	1.74	0.69
1:F:67:ALA:CB	1:F:356:ILE:HD11	2.13	0.69
1:C:95:GLN:CG	1:C:101:PHE:HA	2.21	0.69
1:C:101:PHE:CD2	1:C:357:TYR:HD1	2.06	0.69
2:G:186:GLY:C	2:G:187:TYR:CD1	2.71	0.69
2:G:220:LEU:N	2:G:221:PRO:HD2	2.08	0.69
2:H:178:GLU:O	2:H:181:GLN:N	2.25	0.69
1:C:310:ILE:HD13	1:C:315:ALA:HB2	1.75	0.68
1:F:111:MET:HE3	1:F:111:MET:CA	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:281:ILE:HG13	2:D:281:ILE:O	1.94	0.68
1:C:29:LEU:HD23	1:C:41:CYS:SG	2.34	0.68
1:E:286:HIS:O	1:E:290:LYS:HG2	1.94	0.67
2:B:197:LYS:CG	2:B:198:PRO:HD2	2.24	0.67
1:E:65:THR:HG23	1:E:66:HIS:CD2	2.29	0.67
1:E:208:ILE:CD1	1:E:312:VAL:HG12	2.25	0.67
2:B:197:LYS:HG3	2:B:198:PRO:HD2	1.77	0.67
1:C:22:VAL:HG13	1:C:26:TYR:HD2	1.58	0.67
1:C:120:GLN:HA	1:C:120:GLN:NE2	2.10	0.66
1:C:101:PHE:CE2	1:C:357:TYR:CG	2.84	0.66
2:G:180:MET:HE3	2:G:185:ILE:CG2	2.25	0.66
1:F:216:GLY:HA3	1:F:224:LEU:HD11	1.77	0.66
1:F:111:MET:CE	1:F:111:MET:HA	2.26	0.66
1:E:124:ASP:OD2	1:E:127:ARG:NH2	2.25	0.66
1:C:115:LEU:O	1:C:119:ILE:HG13	1.96	0.66
1:C:22:VAL:CG1	1:C:26:TYR:HB2	2.26	0.65
1:F:16:GLY:C	1:F:18:SER:H	2.04	0.65
1:E:31:PRO:HA	1:E:41:CYS:HB3	1.77	0.65
1:C:11:TYR:HD2	1:C:12:SER:O	1.80	0.65
1:E:15:ILE:HD12	1:E:15:ILE:N	2.12	0.65
1:A:122:GLU:H	1:A:122:GLU:CD	2.04	0.65
2:H:185:ILE:HD13	2:H:241:LEU:HB2	1.79	0.65
2:D:259:ILE:HG23	2:D:263:MET:HE3	1.78	0.65
1:F:44:TYR:O	1:F:45:ASP:HB2	1.95	0.65
1:C:12:SER:OG	1:C:13:VAL:N	2.27	0.64
1:F:67:ALA:HB1	1:F:356:ILE:CD1	2.16	0.64
1:A:78:LYS:NZ	1:A:359:GLU:OE1	2.30	0.64
1:A:96:LYS:HG3	1:A:96:LYS:O	1.96	0.64
2:D:197:LYS:HG3	2:D:198:PRO:HD2	1.77	0.64
1:F:65:THR:HG23	1:F:66:HIS:N	2.11	0.64
1:F:111:MET:HE3	1:F:111:MET:N	2.12	0.64
2:G:220:LEU:H	2:G:221:PRO:HD2	1.61	0.64
2:D:207:LEU:HD22	2:D:229:PHE:HB2	1.80	0.64
2:G:207:LEU:CD1	2:G:208:ARG:H	1.99	0.64
1:C:101:PHE:HE2	1:C:357:TYR:CG	2.16	0.64
1:A:30:LYS:HD3	4:A:406:HOH:O	1.98	0.64
1:C:61:PHE:CZ	1:C:353:LYS:HB2	2.33	0.63
1:F:22:VAL:HG11	1:F:26:TYR:HB2	1.78	0.63
1:C:63:ASN:CB	1:C:65:THR:CG2	2.65	0.63
2:B:202:PRO:HG2	2:B:205:HIS:CG	2.33	0.63
2:G:202:PRO:HG2	2:G:205:HIS:CG	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:VAL:CG1	1:F:26:TYR:HB2	2.29	0.63
1:A:194:PRO:HA	1:A:197:ILE:HD12	1.81	0.63
2:G:177:LYS:O	2:G:181:GLN:HG2	1.98	0.63
2:H:190:ASN:ND2	2:H:195:CYS:O	2.31	0.63
1:F:15:ILE:HB	1:F:18:SER:OG	1.98	0.62
2:B:281:ILE:HG13	2:B:281:ILE:O	1.98	0.62
1:E:100:GLU:O	1:E:102:GLN:HG2	2.00	0.62
1:E:354:GLU:O	1:E:358:LYS:HG3	1.99	0.62
1:E:8:ASN:OD1	1:E:96:LYS:NZ	2.28	0.62
1:A:115:LEU:HD23	1:A:154:PRO:HA	1.82	0.62
1:E:355:LEU:O	1:E:358:LYS:HB2	1.99	0.62
2:B:207:LEU:HD22	2:B:229:PHE:HB2	1.81	0.62
1:F:60:PRO:HD2	1:F:61:PHE:CE1	2.35	0.62
1:C:83:LYS:NZ	1:C:329:GLU:OE2	2.33	0.61
2:B:202:PRO:HG2	2:B:205:HIS:CB	2.29	0.61
1:C:12:SER:C	1:C:13:VAL:CG2	2.71	0.61
1:E:64:GLN:O	1:E:68:LYS:HG2	2.00	0.61
1:C:61:PHE:HZ	1:C:353:LYS:HB2	1.66	0.61
1:C:63:ASN:HB2	1:C:66:HIS:CE1	2.36	0.61
1:C:22:VAL:HG11	1:C:26:TYR:HB2	1.81	0.61
2:D:202:PRO:HG2	2:D:205:HIS:HB2	1.83	0.61
2:B:202:PRO:O	2:B:205:HIS:N	2.29	0.60
2:B:259:ILE:HG23	2:B:263:MET:HE3	1.84	0.60
1:C:301:MET:HG2	1:C:310:ILE:HD11	1.82	0.60
2:G:206:PHE:CG	2:G:207:LEU:N	2.69	0.60
1:E:150:ARG:NH2	1:E:202:TYR:OH	2.34	0.60
1:E:74:LEU:O	1:E:78:LYS:HG3	2.02	0.60
1:E:329:GLU:HG3	1:E:330:ALA:H	1.66	0.60
1:F:92:PHE:CE1	1:F:105:TYR:CD1	2.90	0.60
1:E:86:ILE:HA	1:E:166:LYS:HD3	1.84	0.60
1:E:13:VAL:CG2	1:E:15:ILE:HD11	2.32	0.59
1:E:63:ASN:CG	1:E:65:THR:HG22	2.26	0.59
1:E:226:PRO:O	1:E:236:LYS:CE	2.48	0.59
1:E:329:GLU:HG3	1:E:330:ALA:N	2.17	0.59
2:B:207:LEU:HD22	2:B:229:PHE:CB	2.32	0.59
1:C:39:ILE:C	1:C:40:VAL:HG23	2.26	0.59
1:C:66:HIS:O	1:C:70:ALA:HB2	2.02	0.59
1:A:208:ILE:HD11	1:A:312:VAL:HA	1.85	0.59
2:G:174:VAL:CG1	2:G:198:PRO:HG3	2.31	0.59
1:C:101:PHE:CD1	1:C:101:PHE:O	2.56	0.59
1:F:354:GLU:O	1:F:357:TYR:N	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:220:LEU:N	2:G:221:PRO:CD	2.66	0.59
1:C:188:THR:CA	4:C:401:HOH:O	2.51	0.59
1:C:63:ASN:C	1:C:65:THR:H	2.10	0.59
1:F:110:LEU:O	1:F:111:MET:HE3	2.01	0.59
1:E:65:THR:HG23	1:E:66:HIS:N	2.16	0.59
2:G:202:PRO:HG2	2:G:205:HIS:CB	2.32	0.58
2:H:267:LEU:HD23	2:H:292:LEU:HD13	1.84	0.58
1:C:39:ILE:HG13	1:C:39:ILE:O	2.02	0.58
1:F:74:LEU:HD23	1:F:359:GLU:HB3	1.85	0.58
1:E:278:VAL:HG12	1:E:278:VAL:O	2.04	0.58
2:G:275:LYS:HB2	2:G:281:ILE:HD11	1.84	0.58
1:A:72:ARG:NH1	1:A:171:GLY:O	2.37	0.58
2:H:294:TYR:CE2	2:H:298:ILE:HD11	2.38	0.58
1:E:72:ARG:HH12	1:E:172:LEU:C	2.11	0.58
1:E:111:MET:HG3	1:E:158:VAL:HG23	1.85	0.58
1:C:208:ILE:HD11	1:C:312:VAL:N	2.19	0.58
2:G:174:VAL:HG22	2:G:241:LEU:HD23	1.86	0.58
2:G:197:LYS:HE2	2:G:201:ILE:O	2.03	0.58
2:D:189:LEU:HD21	2:D:209:VAL:CG2	2.34	0.58
1:E:86:ILE:HD12	1:E:166:LYS:HD3	1.86	0.57
1:E:128:MET:HA	1:E:218:MET:HE1	1.86	0.57
1:E:98:LEU:C	1:E:98:LEU:HD23	2.29	0.57
1:C:208:ILE:HD11	1:C:312:VAL:HG12	1.86	0.57
1:C:188:THR:HA	4:C:401:HOH:O	2.03	0.57
1:F:22:VAL:HG12	1:F:23:LEU:O	2.03	0.57
1:F:65:THR:CG2	1:F:66:HIS:N	2.67	0.57
1:A:74:LEU:O	1:A:78:LYS:HG3	2.04	0.57
1:F:111:MET:HE3	1:F:111:MET:HA	1.83	0.57
1:A:78:LYS:NZ	1:A:359:GLU:HG3	2.19	0.57
1:E:229:ASP:CB	2:G:282:SER:HB2	2.35	0.57
1:A:63:ASN:HD21	1:A:65:THR:H	1.52	0.57
1:C:10:PHE:HE1	1:C:94:PRO:HB3	1.70	0.57
1:C:66:HIS:O	1:C:70:ALA:N	2.37	0.57
1:F:272:GLU:HA	1:F:295:ARG:HD2	1.86	0.57
1:E:32:ILE:HG12	1:E:40:VAL:O	2.04	0.57
1:C:254:PRO:O	1:C:258:THR:HG23	2.05	0.56
2:D:197:LYS:HG3	2:D:206:PHE:CE2	2.39	0.56
2:D:197:LYS:HG2	2:D:198:PRO:CD	2.34	0.56
2:H:209:VAL:O	2:H:211:VAL:HG22	2.05	0.56
1:A:229:ASP:CB	2:B:282:SER:HB2	2.36	0.56
1:E:115:LEU:O	1:E:119:ILE:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:ASN:OD1	1:C:284:SER:HA	2.06	0.56
1:F:83:LYS:NZ	1:F:329:GLU:OE2	2.28	0.56
2:G:164:PRO:O	2:G:165:ASN:HB2	2.06	0.56
1:E:284:SER:O	1:E:287:ASN:ND2	2.34	0.55
2:G:198:PRO:HG2	2:G:201:ILE:CG1	2.36	0.55
1:A:272:GLU:HA	1:A:295:ARG:HD2	1.87	0.55
1:A:215:MET:HA	1:A:218:MET:HE2	1.88	0.55
1:C:67:ALA:HB1	1:C:352:TRP:CD2	2.41	0.55
1:C:351:GLU:CG	1:C:352:TRP:H	2.20	0.55
2:H:220:LEU:HD12	2:H:223:LEU:HD12	1.89	0.55
2:D:189:LEU:HD21	2:D:209:VAL:HG21	1.88	0.55
2:D:191:ALA:CA	2:D:209:VAL:HB	2.30	0.55
1:F:22:VAL:HG22	1:F:92:PHE:HZ	1.72	0.55
1:E:56:LYS:HE3	1:E:105:TYR:OH	2.07	0.54
1:C:54:ILE:HG12	1:C:107:VAL:HG22	1.89	0.54
1:C:59:ARG:HG2	1:C:62:GLN:NE2	2.22	0.54
1:F:92:PHE:CD1	1:F:92:PHE:C	2.85	0.54
2:H:163:LEU:HD21	2:H:263:MET:HE2	1.88	0.54
2:G:161:ARG:NH1	4:G:502:HOH:O	2.35	0.54
1:C:10:PHE:HD1	1:C:10:PHE:O	1.90	0.54
1:C:92:PHE:CD1	1:C:92:PHE:C	2.85	0.54
1:F:18:SER:O	1:F:20:PHE:CE1	2.61	0.54
1:E:72:ARG:NH1	1:E:172:LEU:O	2.34	0.54
1:F:145:ALA:HB1	1:F:337:ILE:HD11	1.89	0.54
1:C:45:ASP:O	1:C:49:GLU:N	2.40	0.54
2:D:220:LEU:HD12	2:D:223:LEU:HD12	1.89	0.54
1:F:111:MET:CA	1:F:111:MET:CE	2.85	0.54
1:E:69:ARG:HH22	1:E:172:LEU:HD22	1.73	0.53
1:C:246:PRO:O	1:C:250:LYS:HG3	2.08	0.53
1:C:300:LYS:HB3	1:C:310:ILE:HG23	1.91	0.53
1:F:16:GLY:C	1:F:18:SER:N	2.58	0.53
2:H:198:PRO:HG2	2:H:201:ILE:HB	1.91	0.53
2:G:164:PRO:O	2:G:234:LYS:NZ	2.40	0.53
1:F:55:LYS:NZ	1:F:73:GLU:OE1	2.41	0.53
1:F:354:GLU:O	1:F:355:LEU:C	2.51	0.53
1:E:300:LYS:HB3	1:E:310:ILE:HG23	1.90	0.53
1:C:13:VAL:HG12	1:C:13:VAL:O	2.08	0.53
2:H:174:VAL:HG11	2:H:243:HIS:CD2	2.43	0.53
2:H:207:LEU:HD22	2:H:229:PHE:CB	2.39	0.53
1:C:351:GLU:HG2	1:C:352:TRP:H	1.74	0.53
1:E:65:THR:CG2	1:E:66:HIS:N	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:207:LEU:HD22	2:D:229:PHE:CB	2.38	0.52
1:C:100:GLU:O	1:C:100:GLU:HG3	2.08	0.52
1:E:278:VAL:O	1:E:278:VAL:CG1	2.58	0.52
1:C:11:TYR:HE2	1:C:13:VAL:CG2	2.22	0.52
2:B:165:ASN:HB3	2:B:239:CYS:HA	1.92	0.52
1:C:11:TYR:CE2	1:C:13:VAL:CG2	2.92	0.52
1:E:14:GLU:C	1:E:15:ILE:HD12	2.35	0.52
2:G:231:GLU:OE1	2:G:262:ARG:HD3	2.09	0.52
1:F:144:SER:HB3	1:F:334:PRO:HB3	1.90	0.52
2:D:163:LEU:HD21	2:D:263:MET:HE2	1.91	0.52
1:E:123:LEU:O	1:E:281:PRO:HG2	2.10	0.51
1:C:22:VAL:HG22	1:C:92:PHE:HZ	1.75	0.51
1:C:152:LEU:HD22	1:C:157:ILE:HD11	1.92	0.51
1:F:310:ILE:HD12	1:F:315:ALA:HB2	1.92	0.51
1:C:162:ASP:OD1	1:C:164:THR:OG1	2.28	0.51
1:F:152:LEU:HD22	1:F:157:ILE:HD11	1.92	0.51
2:G:192:SER:OG	2:G:195:CYS:HB2	2.11	0.51
1:C:336:LYS:O	1:C:338:PRO:HD3	2.10	0.51
2:G:259:ILE:HG23	2:G:263:MET:HE3	1.93	0.51
1:A:127:ARG:HG2	1:A:163:CYS:SG	2.51	0.51
1:C:39:ILE:CG2	1:C:40:VAL:HG23	2.37	0.51
1:E:64:GLN:O	1:E:68:LYS:HE2	2.11	0.51
2:G:174:VAL:CG1	2:G:198:PRO:HB3	2.34	0.51
1:E:162:ASP:O	1:E:163:CYS:HB2	2.10	0.51
2:H:259:ILE:HD12	2:H:263:MET:HE3	1.93	0.51
2:G:209:VAL:HG12	2:G:211:VAL:HG22	1.93	0.51
2:G:187:TYR:HD1	2:G:187:TYR:N	2.09	0.50
1:C:18:SER:HB3	1:C:56:LYS:NZ	2.26	0.50
1:E:15:ILE:HD13	1:E:20:PHE:HB2	1.92	0.50
1:F:162:ASP:O	1:F:163:CYS:HB2	2.12	0.50
1:E:250:LYS:O	2:B:218:LYS:NZ	2.38	0.50
1:A:67:ALA:HB1	1:A:352:TRP:CG	2.45	0.50
1:A:111:MET:SD	1:A:160:LYS:HG3	2.50	0.50
2:G:193:ASN:HD21	2:G:210:PRO:HB2	1.77	0.50
2:G:281:ILE:HG13	2:G:281:ILE:O	2.10	0.50
1:E:110:LEU:HA	4:E:426:HOH:O	2.11	0.50
1:C:67:ALA:O	1:C:71:TYR:N	2.45	0.50
2:D:198:PRO:HG2	2:D:201:ILE:HB	1.94	0.50
2:D:203:GLU:O	2:D:203:GLU:HG3	2.12	0.50
2:H:207:LEU:HD11	2:H:225:LYS:HD3	1.93	0.50
1:C:66:HIS:ND1	1:C:66:HIS:N	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:NH1	4:A:402:HOH:O	2.23	0.49
2:D:285:PHE:N	4:D:501:HOH:O	2.27	0.49
2:D:206:PHE:CD1	2:D:206:PHE:C	2.90	0.49
1:A:220:LYS:HD3	1:A:222:GLY:O	2.11	0.49
1:C:249:MET:HE1	1:C:260:VAL:HG12	1.94	0.49
1:A:65:THR:O	1:A:66:HIS:C	2.52	0.49
2:G:198:PRO:HG2	2:G:201:ILE:HG12	1.94	0.49
2:B:171:GLN:HA	2:B:174:VAL:HG12	1.94	0.49
1:C:39:ILE:C	1:C:40:VAL:CG2	2.86	0.49
1:C:216:GLY:HA3	1:C:224:LEU:HD11	1.94	0.49
1:F:300:LYS:HB3	1:F:310:ILE:HG23	1.94	0.49
1:E:300:LYS:HB3	1:E:310:ILE:CG2	2.43	0.49
2:G:197:LYS:CG	2:G:198:PRO:HD2	2.42	0.49
1:C:145:ALA:CB	1:C:335:PRO:CG	2.68	0.49
1:C:79:CYS:SG	1:C:337:ILE:HG13	2.53	0.49
2:G:174:VAL:CG1	2:G:198:PRO:CG	2.90	0.49
1:C:59:ARG:HG2	1:C:62:GLN:CD	2.38	0.49
2:G:294:TYR:CE2	2:G:298:ILE:HD11	2.48	0.49
1:A:98:LEU:HD11	1:A:354:GLU:HG3	1.95	0.49
2:D:209:VAL:O	2:D:211:VAL:HG22	2.12	0.49
1:F:15:ILE:HG13	1:F:20:PHE:CE1	2.48	0.49
1:F:67:ALA:HA	1:F:70:ALA:CB	2.43	0.49
2:G:207:LEU:HD12	2:G:208:ARG:C	2.38	0.48
1:C:56:LYS:CG	1:C:58:SER:OG	2.61	0.48
1:E:71:TYR:CE1	1:E:355:LEU:HD22	2.48	0.48
1:E:150:ARG:NE	1:E:202:TYR:CZ	2.80	0.48
2:G:190:ASN:O	2:G:209:VAL:N	2.43	0.48
2:D:197:LYS:CG	2:D:198:PRO:CD	2.86	0.48
2:D:263:MET:HE1	2:D:273:PHE:CZ	2.48	0.48
1:E:70:ALA:O	1:E:74:LEU:HB2	2.13	0.48
2:G:174:VAL:HG21	2:G:243:HIS:CD2	2.48	0.48
2:B:164:PRO:HD3	4:B:520:HOH:O	2.13	0.48
1:C:115:LEU:HD21	1:C:214:ILE:CG2	2.44	0.48
1:C:18:SER:HB3	1:C:56:LYS:HZ3	1.77	0.48
1:F:79:CYS:SG	1:F:337:ILE:HG12	2.53	0.48
1:E:86:ILE:HD12	1:E:166:LYS:CD	2.44	0.48
1:A:254:PRO:O	1:A:258:THR:HG23	2.14	0.48
1:E:208:ILE:HD11	1:E:312:VAL:N	2.29	0.48
2:G:187:TYR:CD1	2:G:187:TYR:N	2.77	0.48
1:E:13:VAL:HG23	1:E:15:ILE:CD1	2.39	0.47
1:C:63:ASN:C	1:C:65:THR:N	2.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:ILE:HG21	1:E:168:LEU:HD23	1.96	0.47
1:E:305:ASP:OD2	1:E:308:LYS:HE3	2.14	0.47
2:B:198:PRO:C	2:B:200:PHE:N	2.71	0.47
1:C:78:LYS:NZ	1:C:362:ASP:OD1	2.47	0.47
1:F:111:MET:HG3	1:F:160:LYS:HG3	1.96	0.47
1:F:114:ASN:HD22	1:F:155:SER:HA	1.79	0.47
1:C:61:PHE:HZ	1:C:353:LYS:CB	2.27	0.47
1:A:30:LYS:CD	4:A:406:HOH:O	2.58	0.47
2:B:209:VAL:O	2:B:211:VAL:HG22	2.15	0.47
1:C:13:VAL:C	1:C:19:THR:HG22	2.40	0.47
1:C:57:LEU:HD23	1:C:57:LEU:HA	1.68	0.47
1:F:149:HIS:O	1:F:150:ARG:HB2	2.15	0.47
1:C:11:TYR:CD2	1:C:12:SER:O	2.65	0.47
1:E:124:ASP:OD1	1:E:127:ARG:HB2	2.15	0.47
1:C:58:SER:O	1:C:59:ARG:C	2.57	0.47
1:A:132:LEU:HA	1:A:135:MET:HE3	1.97	0.47
2:G:209:VAL:HG12	2:G:209:VAL:O	2.15	0.46
2:D:278:ARG:O	2:D:281:ILE:HG23	2.14	0.46
1:C:111:MET:SD	1:C:160:LYS:HG3	2.55	0.46
1:C:165:LEU:C	1:C:165:LEU:HD23	2.39	0.46
2:H:174:VAL:HG12	2:H:241:LEU:HD23	1.96	0.46
1:E:47:ILE:O	1:E:47:ILE:HG22	2.16	0.46
1:C:22:VAL:HG13	1:C:26:TYR:CD2	2.46	0.46
1:C:39:ILE:HG23	1:C:40:VAL:CG2	2.39	0.46
1:E:76:LEU:HD23	1:E:76:LEU:HA	1.75	0.46
1:E:173:ALA:O	1:E:174:ARG:CB	2.64	0.46
2:G:174:VAL:HG13	2:G:198:PRO:HG3	1.97	0.46
1:F:145:ALA:HB3	1:F:147:ILE:CD1	2.37	0.46
1:F:156:ASN:HA	1:F:168:LEU:HD12	1.98	0.46
2:H:189:LEU:HD21	2:H:209:VAL:HG21	1.97	0.46
1:A:352:TRP:O	1:A:353:LYS:C	2.59	0.46
1:C:45:ASP:CG	1:C:48:LEU:CB	2.89	0.46
1:C:208:ILE:CD1	1:C:312:VAL:HG12	2.45	0.46
1:F:83:LYS:HE3	4:F:442:HOH:O	2.16	0.46
1:F:332:ALA:HB1	1:F:333:PRO:HD2	1.96	0.46
1:E:263:ARG:O	1:E:264:PRO:C	2.58	0.46
1:C:11:TYR:OH	1:C:26:TYR:O	2.26	0.46
1:C:95:GLN:CB	1:C:101:PHE:HA	2.45	0.46
1:F:61:PHE:CD1	1:F:61:PHE:N	2.80	0.46
1:E:61:PHE:C	1:E:63:ASN:N	2.72	0.46
1:E:250:LYS:HD3	1:A:254:PRO:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:263:MET:HE1	2:H:273:PHE:CZ	2.51	0.46
2:G:174:VAL:HG12	2:G:198:PRO:CB	2.39	0.45
1:E:119:ILE:HD12	1:E:218:MET:HG2	1.98	0.45
2:G:167:TYR:OH	2:G:183:ASN:ND2	2.49	0.45
1:C:64:GLN:O	1:C:68:LYS:HG3	2.16	0.45
2:G:218:LYS:HE3	4:G:517:HOH:O	2.16	0.45
1:F:151:ASP:OD2	1:F:153:LYS:NZ	2.45	0.45
2:D:191:ALA:HB2	2:D:254:ILE:HD12	1.98	0.45
1:F:29:LEU:HA	1:F:42:ALA:O	2.17	0.45
1:E:229:ASP:HB2	2:G:282:SER:HB2	1.98	0.45
2:B:201:ILE:HG13	2:B:202:PRO:HD2	1.99	0.45
1:E:329:GLU:CG	1:E:330:ALA:H	2.30	0.45
2:G:277:LYS:NZ	1:F:220:LYS:O	2.47	0.45
2:G:197:LYS:HB2	2:G:206:PHE:CE2	2.52	0.45
1:C:86:ILE:HG21	1:C:108:MET:HE3	1.99	0.45
1:F:149:HIS:O	1:F:171:GLY:HA3	2.16	0.45
2:B:198:PRO:O	2:B:200:PHE:N	2.49	0.45
1:F:18:SER:HB2	1:F:20:PHE:CE1	2.52	0.45
1:E:124:ASP:CG	1:E:127:ARG:HE	2.25	0.44
1:A:296:ASP:OD2	1:A:318:HIS:NE2	2.27	0.44
2:B:163:LEU:HD21	2:B:263:MET:HE2	1.99	0.44
2:B:185:ILE:HG21	2:B:241:LEU:HB2	2.00	0.44
2:H:232:LYS:HB2	2:H:232:LYS:HE3	1.81	0.44
1:E:124:ASP:CG	1:E:127:ARG:HH21	2.19	0.44
1:E:310:ILE:HD13	1:E:315:ALA:HB2	1.98	0.44
1:C:92:PHE:CD1	1:C:105:TYR:HD2	2.34	0.44
1:F:15:ILE:HG22	1:F:15:ILE:O	2.17	0.44
1:F:20:PHE:CD1	1:F:20:PHE:N	2.86	0.44
1:A:122:GLU:CD	1:A:122:GLU:N	2.72	0.44
1:C:65:THR:CG2	1:C:66:HIS:HE1	2.24	0.44
2:D:292:LEU:HD12	2:D:292:LEU:HA	1.88	0.44
1:F:114:ASN:HA	1:F:158:VAL:HA	1.99	0.44
1:F:205:ASN:O	1:F:208:ILE:HB	2.17	0.44
1:C:56:LYS:HG2	1:C:58:SER:HG	1.77	0.44
1:E:15:ILE:N	1:E:15:ILE:CD1	2.79	0.44
1:E:119:ILE:CD1	1:E:218:MET:HG2	2.48	0.44
1:A:226:PRO:O	1:A:236:LYS:HG3	2.17	0.44
1:C:45:ASP:CG	1:C:48:LEU:HB2	2.43	0.44
1:F:74:LEU:O	1:F:78:LYS:HB2	2.17	0.44
1:E:329:GLU:CG	1:E:330:ALA:N	2.80	0.44
1:A:232:ASP:O	1:A:236:LYS:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:GLN:HA	1:C:120:GLN:HE21	1.81	0.44
1:F:133:TYR:HB2	1:F:321:ILE:HG23	1.99	0.44
1:E:60:PRO:O	1:E:66:HIS:HB2	2.18	0.43
2:D:190:ASN:ND2	2:D:243:HIS:CE1	2.86	0.43
1:F:254:PRO:O	1:F:258:THR:HG23	2.17	0.43
1:C:23:LEU:HD23	1:C:24:LYS:HG2	1.99	0.43
1:C:290:LYS:HA	1:C:290:LYS:HD3	1.77	0.43
1:F:25:ARG:O	1:F:45:ASP:HB3	2.18	0.43
2:B:263:MET:HE1	2:B:273:PHE:CZ	2.54	0.43
1:F:40:VAL:HG22	1:F:55:LYS:HD2	2.00	0.43
1:A:63:ASN:OD1	1:A:66:HIS:ND1	2.41	0.43
1:E:60:PRO:O	1:E:66:HIS:CB	2.67	0.43
1:E:72:ARG:HE	1:E:76:LEU:HD11	1.83	0.43
2:B:198:PRO:O	2:B:199:ASP:C	2.60	0.43
1:C:124:ASP:CG	1:C:127:ARG:HH21	2.26	0.43
1:C:40:VAL:HG22	1:C:55:LYS:HG3	2.01	0.43
1:E:151:ASP:HB2	1:E:172:LEU:HG	2.00	0.43
1:A:211:VAL:CG1	1:A:301:MET:HE1	2.49	0.43
1:A:96:LYS:O	1:A:96:LYS:CG	2.67	0.43
2:D:223:LEU:HD23	2:D:223:LEU:HA	1.84	0.43
1:E:29:LEU:C	1:E:30:LYS:HG2	2.43	0.43
1:E:229:ASP:HB2	2:G:282:SER:CB	2.48	0.43
1:C:351:GLU:HG2	1:C:352:TRP:N	2.34	0.43
2:D:243:HIS:C	2:D:251:SER:HB3	2.44	0.43
1:F:123:LEU:O	1:F:281:PRO:HG2	2.19	0.43
1:E:276:PRO:HG2	1:E:279:LEU:HG	2.01	0.42
1:E:278:VAL:CG2	2:H:262:ARG:NH1	2.80	0.42
1:C:20:PHE:CE2	1:C:56:LYS:HB2	2.54	0.42
1:E:63:ASN:ND2	1:E:63:ASN:C	2.77	0.42
1:A:160:LYS:HB3	1:A:162:ASP:OD1	2.19	0.42
1:F:275:PHE:HA	1:F:279:LEU:HD12	2.01	0.42
2:H:300:ASN:OD1	2:H:300:ASN:N	2.52	0.42
1:A:229:ASP:HB3	2:B:282:SER:HB2	2.01	0.42
1:C:92:PHE:HE1	1:C:105:TYR:CE2	2.37	0.42
1:F:28:ASN:OD1	1:F:30:LYS:HE2	2.19	0.42
1:A:72:ARG:HH12	1:A:171:GLY:C	2.27	0.42
1:A:290:LYS:HD3	1:A:293:GLN:OE1	2.19	0.42
2:D:209:VAL:HG11	2:D:254:ILE:HD11	2.00	0.42
1:E:200:MET:HE2	1:E:200:MET:HB3	1.87	0.42
1:E:216:GLY:HA3	1:E:224:LEU:HD11	2.02	0.42
1:A:191:TYR:OH	1:A:217:GLU:OE1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:THR:CG2	1:E:66:HIS:CD2	3.01	0.42
1:E:232:ASP:O	1:E:236:LYS:HG2	2.20	0.42
2:G:164:PRO:O	2:G:165:ASN:CB	2.68	0.42
1:C:63:ASN:HB2	1:C:66:HIS:ND1	2.34	0.42
1:C:332:ALA:HB1	1:C:333:PRO:CD	2.37	0.42
2:D:195:CYS:C	2:D:208:ARG:HH22	2.27	0.42
1:F:62:GLN:HB2	1:F:63:ASN:OD1	2.19	0.42
1:E:301:MET:HG2	1:E:310:ILE:HD11	2.02	0.42
1:A:38:GLY:O	4:A:401:HOH:O	2.22	0.42
1:F:111:MET:SD	1:F:166:LYS:HD2	2.60	0.42
1:E:277:ASP:HB2	4:E:402:HOH:O	2.18	0.42
1:C:11:TYR:HE2	1:C:13:VAL:HG21	1.84	0.42
1:C:93:THR:HG22	1:C:360:VAL:CG1	2.44	0.42
1:E:8:ASN:O	1:E:8:ASN:CG	2.63	0.42
2:G:247:GLY:HA2	2:G:251:SER:OG	2.19	0.42
1:C:82:HIS:HB3	1:C:85:ILE:HG12	2.02	0.42
1:C:277:ASP:HB3	1:C:286:HIS:NE2	2.35	0.42
2:B:174:VAL:HG11	2:B:243:HIS:CE1	2.55	0.41
1:C:10:PHE:O	1:C:10:PHE:CD1	2.70	0.41
1:E:61:PHE:C	1:E:63:ASN:H	2.27	0.41
2:G:174:VAL:HG11	2:G:198:PRO:HD3	2.01	0.41
1:C:29:LEU:HA	1:C:42:ALA:O	2.20	0.41
2:D:172:ARG:NE	4:D:503:HOH:O	2.50	0.41
1:C:53:ALA:HB2	1:C:110:LEU:HD13	2.03	0.41
2:D:174:VAL:CG1	2:D:241:LEU:HD23	2.45	0.41
1:F:18:SER:O	1:F:20:PHE:CD1	2.74	0.41
1:F:141:HIS:CE1	1:F:335:PRO:HG3	2.55	0.41
1:E:110:LEU:C	1:E:111:MET:HE2	2.45	0.41
1:A:124:ASP:CG	1:A:127:ARG:HH21	2.28	0.41
1:A:352:TRP:O	1:A:355:LEU:N	2.50	0.41
2:B:207:LEU:HD22	2:B:229:PHE:CG	2.55	0.41
1:C:337:ILE:HG23	1:C:339:ASP:H	1.85	0.41
1:E:310:ILE:HD12	1:E:310:ILE:C	2.46	0.41
2:G:198:PRO:C	2:G:200:PHE:N	2.78	0.41
2:B:174:VAL:HG11	2:B:243:HIS:NE2	2.36	0.41
1:F:20:PHE:HZ	1:F:39:ILE:HD13	1.86	0.41
2:D:275:LYS:NZ	2:D:279:PRO:O	2.50	0.41
1:E:158:VAL:CG1	1:E:168:LEU:HD11	2.51	0.41
2:G:167:TYR:CZ	2:G:183:ASN:ND2	2.89	0.41
2:G:267:LEU:HD22	2:G:292:LEU:HG	2.02	0.41
2:G:284:ASN:OD1	2:G:286:ASN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ALA:HA	1:A:209:TRP:CD1	2.56	0.41
2:B:198:PRO:HG2	2:B:201:ILE:CG2	2.48	0.41
2:D:189:LEU:HD21	2:D:209:VAL:HG23	2.01	0.41
1:F:22:VAL:HG13	1:F:26:TYR:CD2	2.45	0.41
2:G:223:LEU:HD23	2:G:223:LEU:HA	1.88	0.41
2:D:191:ALA:HA	2:D:209:VAL:CB	2.36	0.41
2:H:189:LEU:HD21	2:H:209:VAL:CG2	2.50	0.41
1:E:278:VAL:HG23	4:E:402:HOH:O	2.21	0.41
1:C:226:PRO:O	1:C:236:LYS:HG3	2.20	0.41
1:C:280:PHE:HA	1:C:281:PRO:HD3	1.84	0.41
2:D:220:LEU:HB3	2:D:221:PRO:HD3	2.02	0.41
1:F:283:ASP:OD1	1:F:283:ASP:N	2.53	0.41
1:F:290:LYS:HD2	1:F:290:LYS:HA	1.51	0.41
2:H:197:LYS:CG	2:H:198:PRO:HD2	2.51	0.41
2:B:190:ASN:OD1	2:B:190:ASN:C	2.64	0.40
1:C:252:LEU:HB2	1:C:257:ARG:HB2	2.02	0.40
1:F:312:VAL:HG13	4:F:441:HOH:O	2.21	0.40
1:A:56:LYS:HE3	1:A:105:TYR:OH	2.21	0.40
1:F:92:PHE:CE1	1:F:105:TYR:CG	3.09	0.40
2:G:207:LEU:HD12	2:G:208:ARG:O	2.08	0.40
1:C:92:PHE:CZ	1:C:105:TYR:CD2	3.06	0.40
1:E:195:GLU:HG3	4:E:462:HOH:O	2.20	0.40
1:F:92:PHE:CE1	1:F:105:TYR:HB2	2.56	0.40
1:F:92:PHE:HE1	1:F:105:TYR:CD1	2.39	0.40
1:F:280:PHE:HA	1:F:281:PRO:HD3	1.86	0.40
1:E:124:ASP:OD1	1:E:127:ARG:NE	2.55	0.40
1:A:246:PRO:O	1:A:250:LYS:HG3	2.21	0.40
1:C:45:ASP:CG	1:C:48:LEU:HB3	2.47	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	312/371 (84%)	306 (98%)	6 (2%)	0	100	100
1	C	308/371 (83%)	299 (97%)	9 (3%)	0	100	100
1	E	309/371 (83%)	294 (95%)	15 (5%)	0	100	100
1	F	285/371 (77%)	276 (97%)	9 (3%)	0	100	100
2	B	140/167 (84%)	132 (94%)	8 (6%)	0	100	100
2	D	140/167 (84%)	135 (96%)	5 (4%)	0	100	100
2	G	139/167 (83%)	131 (94%)	8 (6%)	0	100	100
2	H	141/167 (84%)	137 (97%)	4 (3%)	0	100	100
All	All	1774/2152 (82%)	1710 (96%)	64 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	285/333 (86%)	272 (95%)	13 (5%)	24	41
1	C	283/333 (85%)	260 (92%)	23 (8%)	11	18
1	E	282/333 (85%)	254 (90%)	28 (10%)	7	11
1	F	266/333 (80%)	242 (91%)	24 (9%)	9	15
2	B	127/149 (85%)	119 (94%)	8 (6%)	16	29
2	D	127/149 (85%)	123 (97%)	4 (3%)	35	57
2	G	126/149 (85%)	121 (96%)	5 (4%)	28	47
2	H	128/149 (86%)	118 (92%)	10 (8%)	11	20
All	All	1624/1928 (84%)	1509 (93%)	115 (7%)	13	23

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	13	VAL
1	E	15	ILE

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Mol	Chain	Res	Type
1	E	17	ASP
1	E	18	SER
1	E	21	THR
1	E	30	LYS
1	E	39	ILE
1	E	57	LEU
1	E	62	GLN
1	E	63	ASN
1	E	77	MET
1	E	81	ASN
1	E	122	GLU
1	E	135	MET
1	E	148	ILE
1	E	159	VAL
1	E	208	ILE
1	E	220	LYS
1	E	247	GLU
1	E	258	THR
1	E	265	LYS
1	E	273	LYS
1	E	284	SER
1	E	288	LYS
1	E	289	LEU
1	E	312	VAL
1	E	355	LEU
1	E	358	LYS
2	G	197	LYS
2	G	206	PHE
2	G	207	LEU
2	G	209	VAL
2	G	227	VAL
1	A	59	ARG
1	A	78	LYS
1	A	99	GLU
1	A	122	GLU
1	A	159	VAL
1	A	161	SER
1	A	208	ILE
1	A	218	MET
1	A	273	LYS
1	A	285	GLU
1	A	288	LYS

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Mol	Chain	Res	Type
1	A	312	VAL
1	A	328	SER
2	B	174	VAL
2	B	197	LYS
2	B	201	ILE
2	B	227	VAL
2	B	236	SER
2	B	237	ASN
2	B	263	MET
2	B	268	ASP
1	C	17	ASP
1	C	18	SER
1	C	22	VAL
1	C	23	LEU
1	C	59	ARG
1	C	66	HIS
1	C	77	MET
1	C	93	THR
1	C	97	SER
1	C	100	GLU
1	C	101	PHE
1	C	104	VAL
1	C	120	GLN
1	C	159	VAL
1	C	164	THR
1	C	208	ILE
1	C	218	MET
1	C	278	VAL
1	C	285	GLU
1	C	312	VAL
1	C	336	LYS
1	C	337	ILE
1	C	353	LYS
2	D	206	PHE
2	D	208	ARG
2	D	227	VAL
2	D	293	ASP
1	F	17	ASP
1	F	22	VAL
1	F	62	GLN
1	F	63	ASN
1	F	64	GLN

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Mol	Chain	Res	Type
1	F	77	MET
1	F	78	LYS
1	F	91	VAL
1	F	111	MET
1	F	150	ARG
1	F	159	VAL
1	F	161	SER
1	F	208	ILE
1	F	218	MET
1	F	232	ASP
1	F	265	LYS
1	F	273	LYS
1	F	286	HIS
1	F	290	LYS
1	F	312	VAL
1	F	328	SER
1	F	329	GLU
1	F	358	LYS
1	F	361	MET
2	H	177	LYS
2	H	178	GLU
2	H	179	LEU
2	H	196	PRO
2	H	227	VAL
2	H	234	LYS
2	H	236	SER
2	H	245	LEU
2	H	296	LYS
2	H	300	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	62	GLN
1	E	63	ASN
1	E	66	HIS
1	E	233	GLN
2	G	165	ASN
2	G	183	ASN
2	G	193	ASN
1	A	230	HIS
1	A	233	GLN

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Mol	Chain	Res	Type
1	A	317	GLN
2	B	193	ASN
2	B	212	ASN
1	C	51	ASN
1	C	120	GLN
1	C	233	GLN
1	C	253	GLN
2	D	183	ASN
2	D	190	ASN
2	D	193	ASN
2	D	212	ASN
1	F	51	ASN
1	F	62	GLN
1	F	114	ASN
1	F	141	HIS
1	F	253	GLN
1	F	286	HIS
2	H	182	GLN
2	H	243	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	320/371 (86%)	0.25	22 (6%) 23 19	20, 33, 92, 159	0
1	C	318/371 (85%)	0.58	42 (13%) 7 5	22, 40, 106, 170	0
1	E	317/371 (85%)	0.28	22 (6%) 23 19	23, 34, 90, 159	0
1	F	300/371 (80%)	0.69	45 (15%) 5 4	10, 41, 100, 158	1 (0%)
2	B	141/167 (84%)	0.10	4 (2%) 55 51	14, 32, 73, 86	1 (0%)
2	D	142/167 (85%)	0.42	5 (3%) 47 43	24, 50, 80, 90	0
2	G	141/167 (84%)	0.43	9 (6%) 25 22	20, 47, 88, 98	0
2	H	143/167 (85%)	0.46	8 (5%) 30 26	24, 49, 82, 93	0
All	All	1822/2152 (84%)	0.42	157 (8%) 16 13	10, 39, 92, 170	2 (0%)

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	361	MET	6.9
1	F	33	GLY	6.6
1	F	357	TYR	6.6
1	F	362	ASP	6.2
1	F	356	ILE	5.9
1	C	338	PRO	5.4
1	F	358	LYS	5.3
1	C	336	LYS	5.3
1	F	354	GLU	5.2
1	E	122	GLU	4.9
1	C	99	GLU	4.8
1	C	60	PRO	4.5
1	F	355	LEU	4.3
1	C	17	ASP	4.3
1	C	102	GLN	4.2
1	E	60	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	62	GLN	4.0
1	A	61	PHE	4.0
1	F	359	GLU	4.0
1	F	57	LEU	3.9
1	F	93	THR	3.9
1	C	101	PHE	3.8
1	C	98	LEU	3.8
2	B	191	ALA	3.7
1	F	283	ASP	3.7
1	F	67	ALA	3.7
1	C	339	ASP	3.7
1	C	61	PHE	3.7
1	A	99	GLU	3.6
1	C	24	LYS	3.6
1	F	171	GLY	3.6
1	F	27	GLN	3.6
1	F	61	PHE	3.6
1	C	23	LEU	3.5
1	E	330	ALA	3.5
1	F	10	PHE	3.5
1	F	38	GLY	3.4
2	H	178	GLU	3.4
1	C	337	ILE	3.4
1	F	360	VAL	3.3
1	F	331	GLU	3.3
1	C	97	SER	3.3
1	F	338	PRO	3.3
1	E	173	ALA	3.3
1	C	21	THR	3.2
1	C	357	TYR	3.2
1	E	61	PHE	3.2
1	A	60	PRO	3.2
1	A	96	LYS	3.2
1	E	97	SER	3.1
1	F	60	PRO	3.1
1	F	108	MET	3.1
1	F	336	LYS	3.1
1	A	59	ARG	3.1
1	C	39	ILE	3.1
1	C	351	GLU	3.0
1	C	353	LYS	3.0
1	C	19	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	20	PHE	3.0
2	D	200	PHE	3.0
2	D	198	PRO	3.0
1	C	361	MET	2.9
1	C	100	GLU	2.9
1	C	197	ILE	2.9
1	F	15	ILE	2.9
2	H	179	LEU	2.9
1	E	102	GLN	2.9
1	E	15	ILE	2.9
1	E	150	ARG	2.9
1	C	62	GLN	2.8
1	A	68	LYS	2.8
1	C	59	ARG	2.8
1	C	171	GLY	2.8
1	F	65	THR	2.8
1	C	57	LEU	2.8
2	G	191	ALA	2.8
1	A	163	CYS	2.8
1	C	103	ASP	2.7
1	C	10	PHE	2.7
1	C	11	TYR	2.7
1	A	97	SER	2.7
2	G	199	ASP	2.7
2	H	195	CYS	2.7
1	F	104	VAL	2.6
1	C	93	THR	2.6
2	G	200	PHE	2.6
1	E	98	LEU	2.6
1	E	100	GLU	2.6
1	E	58	SER	2.6
1	A	330	ALA	2.6
1	F	41	CYS	2.6
2	G	298	ILE	2.6
2	G	178	GLU	2.6
1	A	65	THR	2.6
2	H	175	LEU	2.5
1	F	286	HIS	2.5
1	A	173	ALA	2.5
1	E	62	GLN	2.5
1	C	96	LYS	2.5
1	C	283	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	98	LEU	2.5
1	C	356	ILE	2.4
2	H	181	GLN	2.4
1	A	352	TRP	2.4
1	C	284	SER	2.4
2	D	181	GLN	2.4
1	F	40	VAL	2.4
1	E	67	ALA	2.4
1	C	68	LYS	2.4
1	F	32	ILE	2.3
1	E	283	ASP	2.3
1	F	28	ASN	2.3
1	A	282	ALA	2.3
1	A	102	GLN	2.3
1	C	48	LEU	2.3
1	A	100	GLU	2.3
2	H	236	SER	2.3
1	E	163	CYS	2.3
1	E	59	ARG	2.3
1	F	71	TYR	2.2
1	F	120	GLN	2.2
1	F	68	LYS	2.2
2	D	202	PRO	2.2
2	H	235	ALA	2.2
1	F	24	LYS	2.2
1	E	69	ARG	2.2
1	E	78	LYS	2.2
1	C	330	ALA	2.2
1	F	66	HIS	2.2
1	A	355	LEU	2.2
1	F	79	CYS	2.2
1	A	284	SER	2.2
1	C	12	SER	2.2
2	H	196	PRO	2.2
1	F	21	THR	2.1
1	A	69	ARG	2.1
1	E	7	ASP	2.1
2	G	196	PRO	2.1
1	C	22	VAL	2.1
2	B	183	ASN	2.1
1	C	169	ASP	2.1
1	E	96	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	283	ASP	2.1
2	B	181	GLN	2.1
1	A	67	ALA	2.1
1	C	67	ALA	2.1
1	F	63	ASN	2.0
2	B	179	LEU	2.0
1	F	17	ASP	2.0
1	E	327	PRO	2.0
1	F	18	SER	2.0
2	D	239	CYS	2.0
2	G	208	ARG	2.0
1	F	16	GLY	2.0
2	G	296	LYS	2.0
1	F	19	THR	2.0
2	G	202	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	B	401	1/1	0.92	0.11	30,30,30,30	0
3	CL	D	401	1/1	0.94	0.07	30,30,30,30	0
3	CL	H	401	1/1	0.95	0.06	30,30,30,30	0
3	CL	G	401	1/1	0.97	0.06	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.