



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:25 PM UTC

PDB ID : 4Z32 / pdb_00004z32
Title : Crystal Structure of the FERM-SH2 Domains of Jak2
Authors : McNally, R.; Eck, M.J.
Deposited on : 2015-03-30
Resolution : 3.04 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

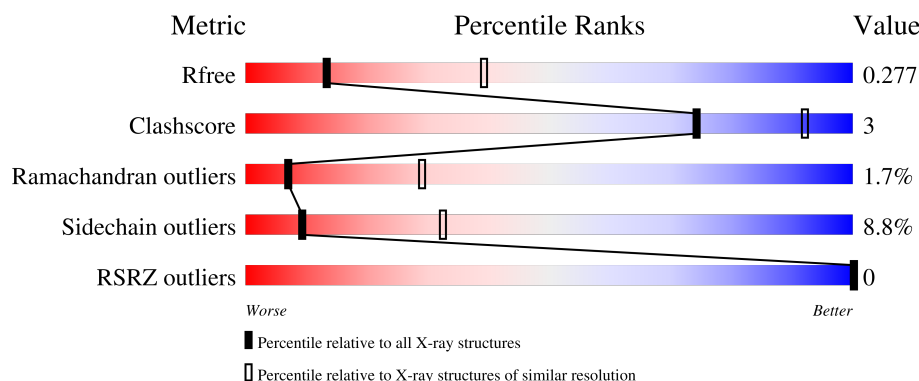
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

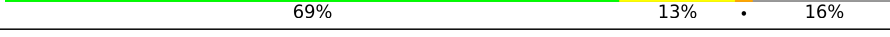
The reported resolution of this entry is 3.04 Å.

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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	497	 73% 14% • 11%
1	B	497	 72% 15% • 11%
1	C	497	 69% 14% • 16%
1	D	497	 69% 13% • 16%
1	E	497	 71% 13% • 14%

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Mol	Chain	Length	Quality of chain
1	F	497	 72%14% • 12%
1	G	497	 72%10%17%
1	H	497	 70%10% • 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27929 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 Tyrosine-protein kinase JAK2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3624	2334	622	646	22			
1	B	441	Total	C	N	O	S	0	0	0
			3624	2334	622	646	22			
1	C	418	Total	C	N	O	S	0	0	0
			3433	2211	588	612	22			
1	D	417	Total	C	N	O	S	0	0	0
			3423	2208	587	606	22			
1	E	427	Total	C	N	O	S	0	0	0
			3516	2271	602	622	21			
1	F	436	Total	C	N	O	S	0	0	0
			3586	2311	616	637	22			
1	G	411	Total	C	N	O	S	0	0	0
			3375	2179	578	597	21			
1	H	405	Total	C	N	O	S	0	0	0
			3336	2154	573	588	21			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	expression tag	UNP O60674
A	517	LEU	-	expression tag	UNP O60674
A	518	GLU	-	expression tag	UNP O60674
A	519	HIS	-	expression tag	UNP O60674
A	520	HIS	-	expression tag	UNP O60674
A	521	HIS	-	expression tag	UNP O60674
A	522	HIS	-	expression tag	UNP O60674
A	523	HIS	-	expression tag	UNP O60674
A	524	HIS	-	expression tag	UNP O60674
A	525	HIS	-	expression tag	UNP O60674
A	526	HIS	-	expression tag	UNP O60674
B	30	GLY	-	expression tag	UNP O60674
B	517	LEU	-	expression tag	UNP O60674

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Chain	Residue	Modelled	Actual	Comment	Reference
B	518	GLU	-	expression tag	UNP O60674
B	519	HIS	-	expression tag	UNP O60674
B	520	HIS	-	expression tag	UNP O60674
B	521	HIS	-	expression tag	UNP O60674
B	522	HIS	-	expression tag	UNP O60674
B	523	HIS	-	expression tag	UNP O60674
B	524	HIS	-	expression tag	UNP O60674
B	525	HIS	-	expression tag	UNP O60674
B	526	HIS	-	expression tag	UNP O60674
C	30	GLY	-	expression tag	UNP O60674
C	517	LEU	-	expression tag	UNP O60674
C	518	GLU	-	expression tag	UNP O60674
C	519	HIS	-	expression tag	UNP O60674
C	520	HIS	-	expression tag	UNP O60674
C	521	HIS	-	expression tag	UNP O60674
C	522	HIS	-	expression tag	UNP O60674
C	523	HIS	-	expression tag	UNP O60674
C	524	HIS	-	expression tag	UNP O60674
C	525	HIS	-	expression tag	UNP O60674
C	526	HIS	-	expression tag	UNP O60674
D	30	GLY	-	expression tag	UNP O60674
D	517	LEU	-	expression tag	UNP O60674
D	518	GLU	-	expression tag	UNP O60674
D	519	HIS	-	expression tag	UNP O60674
D	520	HIS	-	expression tag	UNP O60674
D	521	HIS	-	expression tag	UNP O60674
D	522	HIS	-	expression tag	UNP O60674
D	523	HIS	-	expression tag	UNP O60674
D	524	HIS	-	expression tag	UNP O60674
D	525	HIS	-	expression tag	UNP O60674
D	526	HIS	-	expression tag	UNP O60674
E	30	GLY	-	expression tag	UNP O60674
E	517	LEU	-	expression tag	UNP O60674
E	518	GLU	-	expression tag	UNP O60674
E	519	HIS	-	expression tag	UNP O60674
E	520	HIS	-	expression tag	UNP O60674
E	521	HIS	-	expression tag	UNP O60674
E	522	HIS	-	expression tag	UNP O60674
E	523	HIS	-	expression tag	UNP O60674
E	524	HIS	-	expression tag	UNP O60674
E	525	HIS	-	expression tag	UNP O60674
E	526	HIS	-	expression tag	UNP O60674

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Chain	Residue	Modelled	Actual	Comment	Reference
F	30	GLY	-	expression tag	UNP O60674
F	517	LEU	-	expression tag	UNP O60674
F	518	GLU	-	expression tag	UNP O60674
F	519	HIS	-	expression tag	UNP O60674
F	520	HIS	-	expression tag	UNP O60674
F	521	HIS	-	expression tag	UNP O60674
F	522	HIS	-	expression tag	UNP O60674
F	523	HIS	-	expression tag	UNP O60674
F	524	HIS	-	expression tag	UNP O60674
F	525	HIS	-	expression tag	UNP O60674
F	526	HIS	-	expression tag	UNP O60674
G	30	GLY	-	expression tag	UNP O60674
G	517	LEU	-	expression tag	UNP O60674
G	518	GLU	-	expression tag	UNP O60674
G	519	HIS	-	expression tag	UNP O60674
G	520	HIS	-	expression tag	UNP O60674
G	521	HIS	-	expression tag	UNP O60674
G	522	HIS	-	expression tag	UNP O60674
G	523	HIS	-	expression tag	UNP O60674
G	524	HIS	-	expression tag	UNP O60674
G	525	HIS	-	expression tag	UNP O60674
G	526	HIS	-	expression tag	UNP O60674
H	30	GLY	-	expression tag	UNP O60674
H	517	LEU	-	expression tag	UNP O60674
H	518	GLU	-	expression tag	UNP O60674
H	519	HIS	-	expression tag	UNP O60674
H	520	HIS	-	expression tag	UNP O60674
H	521	HIS	-	expression tag	UNP O60674
H	522	HIS	-	expression tag	UNP O60674
H	523	HIS	-	expression tag	UNP O60674
H	524	HIS	-	expression tag	UNP O60674
H	525	HIS	-	expression tag	UNP O60674
H	526	HIS	-	expression tag	UNP O60674

- Molecule 2 is water.

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

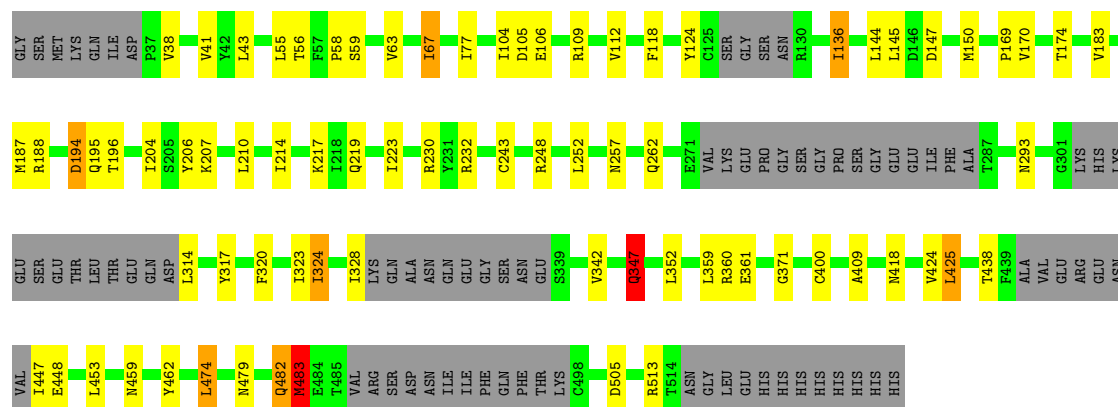
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	O	0	0
			1	1		
2	F	1	Total	O	0	0
			1	1		

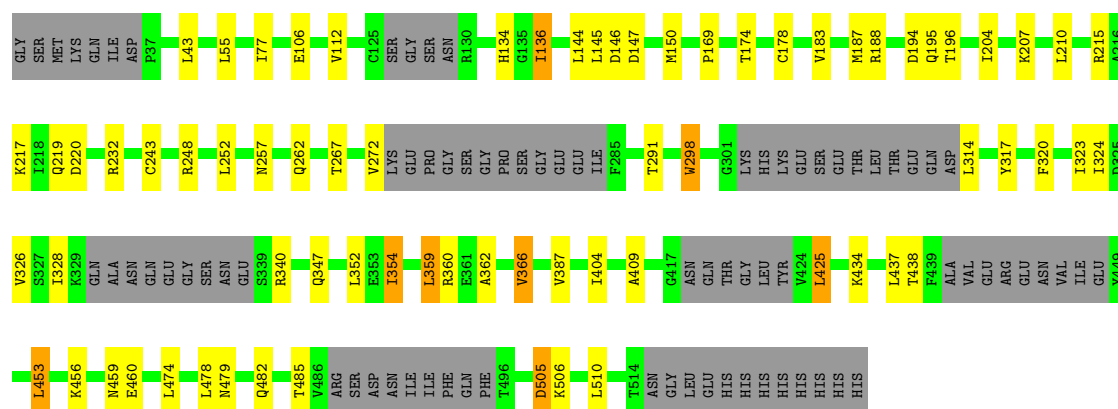
- Molecule 1: Tyrosine-protein kinase JAK2





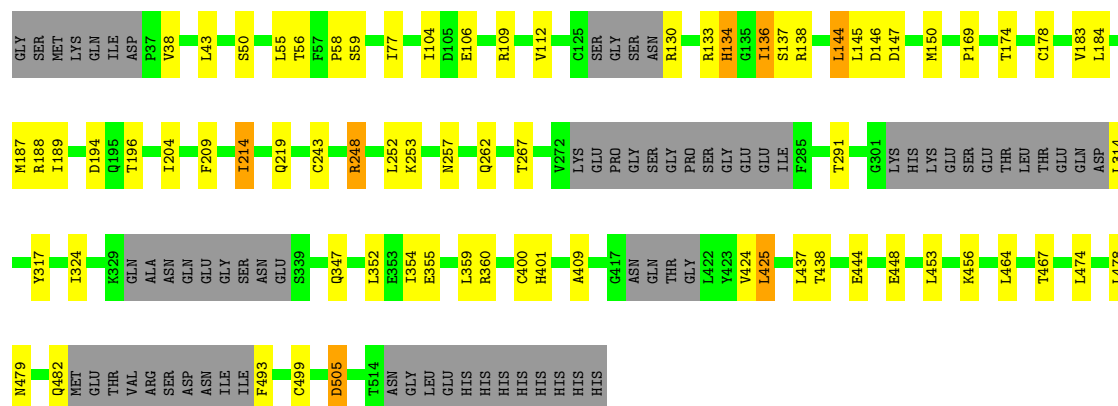
• Molecule 1: Tyrosine-protein kinase JAK2

Chain D: 69% 13% 16%



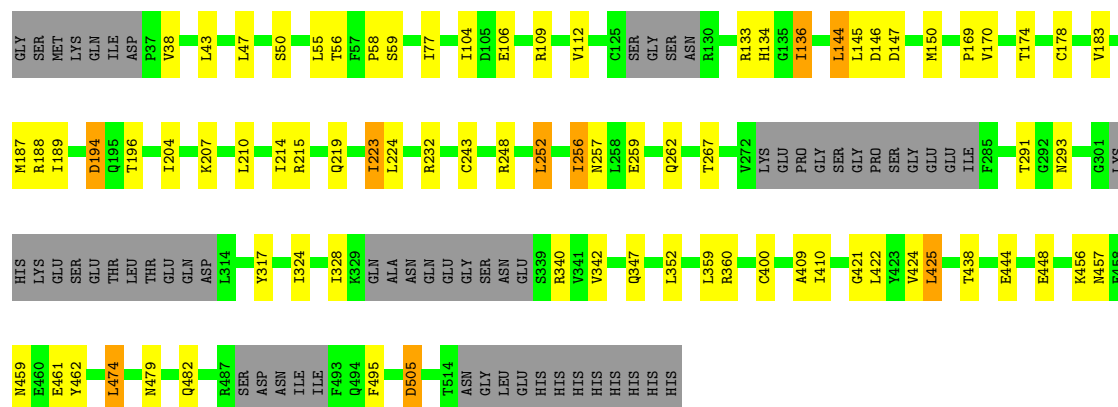
• Molecule 1: Tyrosine-protein kinase JAK2

Chain E: 71% 13% 14%



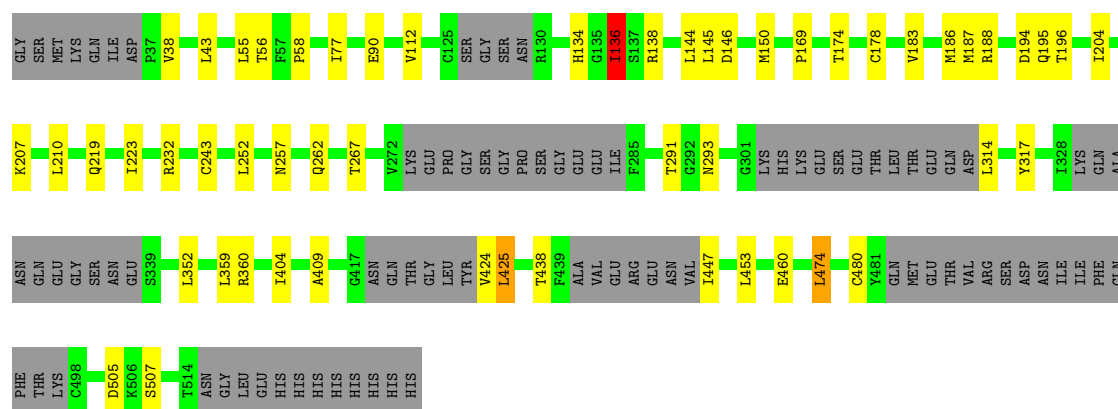
• Molecule 1: Tyrosine-protein kinase JAK2

Chain F: 72% 14% 12%



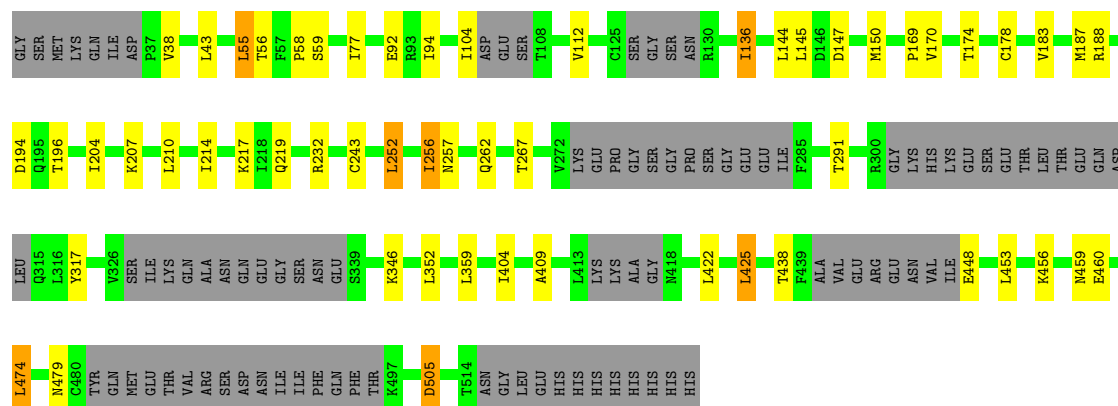
• Molecule 1: Tyrosine-protein kinase JAK2

Chain G: 72% 10% 17%



• Molecule 1: Tyrosine-protein kinase JAK2

Chain H: 70% 10% 19%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.19Å 188.74Å 118.58Å 90.00° 113.87° 90.00°	Depositor
Resolution (Å)	42.95 – 3.04 42.95 – 3.04	Depositor EDS
% Data completeness (in resolution range)	96.2 (42.95-3.04) 95.2 (42.95-3.04)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.257 , 0.276 0.259 , 0.277	Depositor DCC
R_{free} test set	4470 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	67.8	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.116 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27929	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.1980e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.71	0/3713	1.26	3/5015 (0.1%)
1	B	0.73	0/3713	1.28	4/5015 (0.1%)
1	C	0.72	0/3517	1.28	4/4748 (0.1%)
1	D	0.71	0/3506	1.27	2/4730 (0.0%)
1	E	0.71	1/3603 (0.0%)	1.25	2/4863 (0.0%)
1	F	0.72	0/3674	1.27	3/4960 (0.1%)
1	G	0.72	0/3458	1.28	1/4667 (0.0%)
1	H	0.71	0/3418	1.26	3/4613 (0.1%)
All	All	0.72	1/28602 (0.0%)	1.27	22/38611 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	214	ILE	CG1-CD1	-6.57	1.26	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	TYR	CA-C-N	5.38	131.39	121.70
1	C	124	TYR	C-N-CA	5.38	131.39	121.70
1	C	347	GLN	CA-C-N	5.37	127.74	120.38
1	C	347	GLN	C-N-CA	5.37	127.74	120.38
1	B	356	LEU	CA-C-N	5.27	128.07	120.38
1	B	356	LEU	C-N-CA	5.27	128.07	120.38
1	A	124	TYR	CA-C-N	5.23	131.11	121.70
1	A	124	TYR	C-N-CA	5.23	131.11	121.70
1	E	505	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	247	ALA	CA-C-N	5.14	127.17	120.28
1	B	247	ALA	C-N-CA	5.14	127.17	120.28
1	H	346	LYS	CA-C-N	5.14	127.16	120.28
1	H	346	LYS	C-N-CA	5.14	127.16	120.28
1	D	505	ASP	CA-CB-CG	5.13	117.73	112.60
1	F	146	ASP	CA-CB-CG	5.12	117.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	146	ASP	CA-CB-CG	5.10	117.70	112.60
1	E	146	ASP	CA-CB-CG	5.09	117.69	112.60
1	F	495	PHE	CA-CB-CG	5.09	118.89	113.80
1	D	146	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	505	ASP	CA-CB-CG	5.06	117.66	112.60
1	F	505	ASP	CA-CB-CG	5.06	117.66	112.60
1	H	505	ASP	CA-CB-CG	5.00	117.61	112.60

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	3624	0	3603	25	0
1	B	3624	0	3603	29	0
1	C	3433	0	3406	30	0
1	D	3423	0	3409	25	0
1	E	3516	0	3496	23	0
1	F	3586	0	3565	29	0
1	G	3375	0	3354	13	0
1	H	3336	0	3311	14	0
2	A	5	0	0	0	0
2	B	4	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
All	All	27929	0	27747	175	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 3.

All (175) 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:C:41:VAL:HG21	1:C:67:ILE:HD11	1.42	1.01
1:H:252:LEU:O	1:H:256:ILE:HD13	1.75	0.87
1:F:252:LEU:O	1:F:256:ILE:HD13	1.76	0.86
1:B:147:ASP:HB3	1:B:248:ARG:HH12	1.42	0.84
1:F:207:LYS:HA	1:F:210:LEU:HD12	1.61	0.83
1:A:207:LYS:HA	1:A:210:LEU:HD12	1.62	0.81
1:G:207:LYS:HA	1:G:210:LEU:HD12	1.66	0.76
1:C:248:ARG:HH12	1:D:195:GLN:HG2	1.51	0.74
1:H:207:LYS:HA	1:H:210:LEU:HD12	1.68	0.74
1:F:147:ASP:HB3	1:F:248:ARG:HH22	1.53	0.72
1:C:41:VAL:HG21	1:C:67:ILE:CD1	2.19	0.71
1:B:267:THR:HG22	1:B:291:THR:HG22	1.72	0.71
1:D:267:THR:HG22	1:D:291:THR:HG22	1.72	0.70
1:A:267:THR:HG22	1:A:291:THR:HG22	1.74	0.70
1:F:267:THR:HG22	1:F:291:THR:HG22	1.73	0.70
1:C:147:ASP:HB3	1:C:248:ARG:HH22	1.58	0.69
1:E:267:THR:HG22	1:E:291:THR:HG22	1.73	0.69
1:F:147:ASP:HB3	1:F:248:ARG:NH2	2.08	0.68
1:F:133:ARG:HG3	1:F:144:LEU:HA	1.77	0.67
1:G:267:THR:HG22	1:G:291:THR:HG22	1.77	0.66
1:B:147:ASP:HB3	1:B:248:ARG:NH1	2.11	0.65
1:D:328:ILE:HD11	1:D:366:VAL:HG21	1.78	0.65
1:D:326:VAL:HG11	1:D:366:VAL:HG12	1.80	0.64
1:B:147:ASP:CB	1:B:248:ARG:HH12	2.09	0.63
1:C:147:ASP:HB3	1:C:248:ARG:NH2	2.13	0.63
1:E:400:CYS:HA	1:E:425:LEU:HB3	1.81	0.62
1:D:425:LEU:HD21	1:D:478:LEU:HD11	1.83	0.60
1:G:195:GLN:HE22	1:H:147:ASP:HB2	1.65	0.60
1:C:195:GLN:HE22	1:D:147:ASP:HB2	1.66	0.60
1:D:362:ALA:O	1:D:366:VAL:HG22	2.02	0.60
1:E:178:CYS:SG	1:E:214:ILE:HD13	2.41	0.60
1:E:204:ILE:HD13	1:F:47:LEU:HB3	1.83	0.60
1:H:409:ALA:HB1	1:H:438:THR:HG21	1.83	0.59
1:E:50:SER:HB2	1:F:189:ILE:HG12	1.85	0.59
1:H:183:VAL:HG12	1:H:187:MET:HE2	1.85	0.58
1:E:183:VAL:HG12	1:E:187:MET:HE2	1.86	0.58
1:G:425:LEU:HD11	1:G:474:LEU:HD22	1.85	0.58
1:A:183:VAL:HG12	1:A:187:MET:HE2	1.86	0.58
1:B:147:ASP:CB	1:B:248:ARG:NH1	2.66	0.57
1:F:183:VAL:HG12	1:F:187:MET:HE2	1.86	0.57
1:B:441:VAL:HG11	1:B:491:ILE:HG21	1.86	0.57
1:E:133:ARG:HG3	1:E:144:LEU:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:VAL:HG12	1:G:187:MET:HE2	1.88	0.56
1:B:434:LYS:HD3	1:B:453:LEU:HD11	1.88	0.56
1:D:409:ALA:HB1	1:D:438:THR:HG21	1.87	0.56
1:D:183:VAL:HG12	1:D:187:MET:HE2	1.88	0.56
1:F:409:ALA:HB1	1:F:438:THR:HG21	1.89	0.55
1:C:183:VAL:HG12	1:C:187:MET:HE2	1.88	0.55
1:B:183:VAL:HG12	1:B:187:MET:HE2	1.87	0.55
1:D:207:LYS:HA	1:D:210:LEU:HD12	1.89	0.54
1:E:189:ILE:HG12	1:F:50:SER:HB2	1.89	0.54
1:B:147:ASP:CG	1:B:248:ARG:NH1	2.67	0.53
1:F:178:CYS:HB3	1:F:210:LEU:HD23	1.91	0.53
1:A:272:VAL:HG21	1:A:354:ILE:HG23	1.89	0.53
1:A:194:ASP:O	1:B:248:ARG:NH2	2.35	0.53
1:A:50:SER:HB3	1:B:189:ILE:HG12	1.91	0.52
1:F:207:LYS:HB3	1:F:215:ARG:HG3	1.91	0.52
1:B:409:ALA:HB1	1:B:438:THR:HG21	1.91	0.52
1:E:409:ALA:HB1	1:E:438:THR:HG21	1.90	0.52
1:H:169:PRO:HG2	1:H:174:THR:HG21	1.92	0.52
1:D:169:PRO:HG2	1:D:174:THR:HG21	1.92	0.51
1:C:206:TYR:HE1	1:C:230:ARG:HG2	1.75	0.51
1:C:409:ALA:HB1	1:C:438:THR:HG21	1.92	0.51
1:A:419:GLN:HB3	1:A:422:LEU:HD12	1.92	0.51
1:D:366:VAL:HG23	1:D:387:VAL:HG11	1.92	0.51
1:C:169:PRO:HG2	1:C:174:THR:HG21	1.93	0.51
1:A:147:ASP:HB2	1:B:195:GLN:HE22	1.75	0.51
1:G:169:PRO:HG2	1:G:174:THR:HG21	1.92	0.51
1:B:356:LEU:HD13	1:B:362:ALA:HA	1.92	0.50
1:C:425:LEU:HD11	1:C:474:LEU:HD22	1.92	0.50
1:B:169:PRO:HG2	1:B:174:THR:HG21	1.93	0.50
1:E:38:VAL:HG12	1:E:109:ARG:HG2	1.94	0.50
1:A:178:CYS:HB3	1:A:210:LEU:HD23	1.92	0.50
1:G:409:ALA:HB1	1:G:438:THR:HG21	1.93	0.50
1:C:43:LEU:HD11	1:C:55:LEU:HD13	1.94	0.50
1:B:435:TYR:HE1	1:B:456:LYS:HG3	1.77	0.50
1:G:178:CYS:HB3	1:G:210:LEU:HD23	1.94	0.50
1:D:43:LEU:HD11	1:D:55:LEU:HD13	1.94	0.49
1:E:425:LEU:HD21	1:E:478:LEU:HD21	1.93	0.49
1:A:169:PRO:HG2	1:A:174:THR:HG21	1.93	0.49
1:B:38:VAL:HG23	1:B:109:ARG:HG2	1.94	0.49
1:F:43:LEU:HD11	1:F:55:LEU:HD13	1.94	0.49
1:F:169:PRO:HG2	1:F:174:THR:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:LEU:HD11	1:G:55:LEU:HD13	1.94	0.49
1:H:178:CYS:HB3	1:H:210:LEU:HD23	1.94	0.49
1:C:293:ASN:HA	1:C:513:ARG:HD2	1.95	0.49
1:A:409:ALA:HB1	1:A:438:THR:HG21	1.93	0.49
1:E:169:PRO:HG2	1:E:174:THR:HG21	1.93	0.49
1:H:43:LEU:HD11	1:H:55:LEU:HD23	1.93	0.49
1:A:400:CYS:HB2	1:A:425:LEU:HD13	1.96	0.48
1:B:170:VAL:HG12	1:B:217:LYS:HD2	1.96	0.48
1:C:38:VAL:HG12	1:C:109:ARG:HG2	1.95	0.48
1:D:506:LYS:HA	1:D:510:LEU:HD12	1.96	0.48
1:A:43:LEU:HD11	1:A:55:LEU:HD13	1.96	0.48
1:F:400:CYS:HB2	1:F:425:LEU:HD13	1.95	0.48
1:F:457:ASN:HB2	1:F:461:GLU:H	1.79	0.47
1:E:43:LEU:HD11	1:E:55:LEU:HD13	1.95	0.47
1:D:317:TYR:CZ	1:D:352:LEU:HB2	2.50	0.47
1:B:43:LEU:HD11	1:B:55:LEU:HD13	1.97	0.47
1:B:207:LYS:HZ1	1:B:226:ARG:HH11	1.62	0.47
1:B:400:CYS:HB2	1:B:425:LEU:HD13	1.97	0.47
1:F:317:TYR:CZ	1:F:352:LEU:HB2	2.49	0.47
1:B:42:TYR:HB3	1:B:113:LEU:HD23	1.97	0.47
1:C:207:LYS:HA	1:C:210:LEU:HD12	1.97	0.47
1:E:317:TYR:CZ	1:E:352:LEU:HB2	2.50	0.47
1:H:267:THR:HG22	1:H:291:THR:HG22	1.95	0.47
1:B:461:GLU:HG3	1:B:470:ASN:HB3	1.97	0.47
1:C:400:CYS:HB2	1:C:425:LEU:HD13	1.96	0.47
1:C:482:GLN:O	1:C:483:MET:HB2	2.15	0.47
1:H:425:LEU:HD11	1:H:474:LEU:HD22	1.97	0.47
1:A:441:VAL:HG21	1:A:491:ILE:HG12	1.96	0.46
1:C:324:ILE:HD11	1:C:347:GLN:HA	1.98	0.46
1:B:324:ILE:HD11	1:B:347:GLN:HA	1.97	0.46
1:D:324:ILE:HD11	1:D:347:GLN:HA	1.97	0.46
1:E:147:ASP:HB3	1:E:248:ARG:NH2	2.29	0.46
1:F:324:ILE:HD11	1:F:347:GLN:HA	1.96	0.46
1:G:317:TYR:CZ	1:G:352:LEU:HB2	2.50	0.46
1:A:317:TYR:CZ	1:A:352:LEU:HB2	2.50	0.46
1:A:324:ILE:HD11	1:A:347:GLN:HA	1.97	0.46
1:C:118:PHE:CZ	1:C:371:GLY:HA3	2.51	0.46
1:D:320:PHE:HA	1:D:323:ILE:HD12	1.98	0.46
1:G:136:ILE:C	1:G:138:ARG:H	2.24	0.46
1:E:324:ILE:HD11	1:E:347:GLN:HA	1.97	0.45
1:B:425:LEU:HD11	1:B:474:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ILE:HG12	1:B:50:SER:HB3	1.97	0.45
1:C:317:TYR:CZ	1:C:352:LEU:HB2	2.52	0.45
1:F:38:VAL:HG12	1:F:109:ARG:HG2	1.98	0.45
1:A:425:LEU:HD11	1:A:474:LEU:HD22	1.98	0.45
1:H:92:GLU:HB3	1:H:94:ILE:HD12	1.98	0.45
1:B:201:TYR:CE2	1:B:234:ARG:HD3	2.52	0.44
1:E:424:VAL:HB	1:E:438:THR:HG23	1.99	0.44
1:C:63:VAL:O	1:C:67:ILE:HG22	2.18	0.44
1:E:184:LEU:HD21	1:E:253:LYS:HZ2	1.83	0.44
1:F:425:LEU:HD11	1:F:474:LEU:HD22	2.00	0.44
1:A:461:GLU:O	1:A:462:TYR:HB2	2.18	0.43
1:B:435:TYR:HB2	1:B:454:ILE:HB	2.00	0.43
1:A:272:VAL:CG2	1:A:354:ILE:HG23	2.49	0.43
1:D:340:ARG:HD3	1:D:359:LEU:HB3	2.01	0.43
1:H:317:TYR:CZ	1:H:352:LEU:HB2	2.54	0.43
1:D:178:CYS:HB3	1:D:210:LEU:HD23	2.01	0.43
1:F:424:VAL:HB	1:F:438:THR:HG23	2.01	0.43
1:G:134:HIS:HB2	1:G:507:SER:O	2.19	0.43
1:G:424:VAL:HB	1:G:438:THR:HG23	2.01	0.42
1:F:400:CYS:HA	1:F:425:LEU:HB3	2.01	0.42
1:C:248:ARG:NH1	1:D:195:GLN:HG2	2.29	0.42
1:F:170:VAL:HG13	1:F:214:ILE:HD13	2.01	0.42
1:C:170:VAL:HG13	1:C:214:ILE:HD13	2.02	0.42
1:D:267:THR:HG22	1:D:291:THR:CG2	2.46	0.42
1:C:194:ASP:OD2	1:D:248:ARG:HG2	2.20	0.42
1:E:204:ILE:HD12	1:E:209:PHE:CZ	2.55	0.42
1:H:59:SER:HA	1:H:104:ILE:HG22	2.02	0.42
1:E:248:ARG:HD2	1:F:194:ASP:HB2	2.02	0.42
1:C:170:VAL:HG12	1:C:217:LYS:HD2	2.02	0.42
1:D:298:TRP:CD1	1:D:298:TRP:C	2.98	0.41
1:A:59:SER:HA	1:A:104:ILE:HG22	2.03	0.41
1:D:434:LYS:HE3	1:D:453:LEU:HD13	2.01	0.41
1:F:328:ILE:HG12	1:F:342:VAL:HG22	2.03	0.41
1:H:170:VAL:HG13	1:H:214:ILE:HD13	2.01	0.41
1:C:320:PHE:HA	1:C:323:ILE:HD12	2.02	0.41
1:A:170:VAL:HG13	1:A:214:ILE:HD13	2.02	0.41
1:F:59:SER:HA	1:F:104:ILE:HG22	2.02	0.41
1:F:223:ILE:HD13	1:F:224:LEU:HG	2.02	0.41
1:E:401:HIS:HE1	1:E:499:CYS:O	2.03	0.41
1:C:59:SER:HA	1:C:104:ILE:HG22	2.03	0.40
1:C:424:VAL:HB	1:C:438:THR:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ILE:HG12	1:C:342:VAL:HG22	2.02	0.40
1:E:267:THR:HG22	1:E:291:THR:CG2	2.48	0.40
1:A:328:ILE:HG12	1:A:342:VAL:HG22	2.02	0.40
1:B:59:SER:HA	1:B:104:ILE:HG22	2.03	0.40
1:D:272:VAL:HG21	1:D:354:ILE:HG12	2.04	0.40
1:F:267:THR:HG22	1:F:291:THR:CG2	2.48	0.40
1:A:400:CYS:HA	1:A:425:LEU:HB3	2.04	0.40
1:A:424:VAL:HB	1:A:438:THR:HG23	2.04	0.40
1:C:400:CYS:HA	1:C:425:LEU:HB3	2.03	0.40
1:E:59:SER:HA	1:E:104:ILE:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/497 (87%)	399 (93%)	23 (5%)	9 (2%)	5	24
1	B	431/497 (87%)	400 (93%)	20 (5%)	11 (3%)	4	20
1	C	404/497 (81%)	375 (93%)	21 (5%)	8 (2%)	6	25
1	D	401/497 (81%)	378 (94%)	20 (5%)	3 (1%)	18	49
1	E	413/497 (83%)	388 (94%)	18 (4%)	7 (2%)	7	29
1	F	424/497 (85%)	393 (93%)	22 (5%)	9 (2%)	5	24
1	G	395/497 (80%)	372 (94%)	19 (5%)	4 (1%)	12	41
1	H	387/497 (78%)	362 (94%)	21 (5%)	4 (1%)	12	41
All	All	3286/3976 (83%)	3067 (93%)	164 (5%)	55 (2%)	7	29

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ILE
1	B	106	GLU
1	B	136	ILE
1	C	106	GLU
1	C	136	ILE
1	C	483	MET
1	D	136	ILE
1	E	106	GLU
1	E	136	ILE
1	F	106	GLU
1	F	136	ILE
1	F	462	TYR
1	G	136	ILE
1	H	136	ILE
1	A	462	TYR
1	B	134	HIS
1	C	347	GLN
1	A	194	ASP
1	B	444	GLU
1	B	462	TYR
1	B	489	ASP
1	C	462	TYR
1	E	134	HIS
1	F	134	HIS
1	A	106	GLU
1	A	134	HIS
1	A	196	THR
1	A	444	GLU
1	A	489	ASP
1	B	194	ASP
1	B	196	THR
1	B	294	GLY
1	B	485	THR
1	C	196	THR
1	D	196	THR
1	E	194	ASP
1	E	196	THR
1	E	444	GLU
1	F	194	ASP
1	F	196	THR
1	F	421	GLY
1	F	444	GLU
1	G	196	THR

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Mol	Chain	Res	Type
1	H	196	THR
1	D	194	ASP
1	G	194	ASP
1	H	194	ASP
1	C	194	ASP
1	B	58	PRO
1	C	58	PRO
1	A	58	PRO
1	E	58	PRO
1	F	58	PRO
1	H	58	PRO
1	G	58	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/446 (89%)	365 (92%)	33 (8%)	10	34
1	B	398/446 (89%)	361 (91%)	37 (9%)	8	30
1	C	377/446 (84%)	343 (91%)	34 (9%)	9	31
1	D	376/446 (84%)	339 (90%)	37 (10%)	7	28
1	E	385/446 (86%)	350 (91%)	35 (9%)	9	31
1	F	393/446 (88%)	361 (92%)	32 (8%)	11	35
1	G	370/446 (83%)	339 (92%)	31 (8%)	10	34
1	H	366/446 (82%)	335 (92%)	31 (8%)	10	34
All	All	3063/3568 (86%)	2793 (91%)	270 (9%)	9	32

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	THR
1	A	77	ILE
1	A	112	VAL

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Mol	Chain	Res	Type
1	A	134	HIS
1	A	136	ILE
1	A	144	LEU
1	A	145	LEU
1	A	150	MET
1	A	188	ARG
1	A	200	ILE
1	A	204	ILE
1	A	219	GLN
1	A	223	ILE
1	A	232	ARG
1	A	243	CYS
1	A	252	LEU
1	A	257	ASN
1	A	262	GLN
1	A	271	GLU
1	A	285	PHE
1	A	314	LEU
1	A	359	LEU
1	A	360	ARG
1	A	425	LEU
1	A	448	GLU
1	A	453	LEU
1	A	459	ASN
1	A	460	GLU
1	A	474	LEU
1	A	479	ASN
1	A	482	GLN
1	A	493	PHE
1	A	505	ASP
1	B	38	VAL
1	B	66	GLU
1	B	77	ILE
1	B	78	THR
1	B	105	ASP
1	B	108	THR
1	B	109	ARG
1	B	112	VAL
1	B	136	ILE
1	B	144	LEU
1	B	145	LEU
1	B	150	MET

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Mol	Chain	Res	Type
1	B	188	ARG
1	B	204	ILE
1	B	219	GLN
1	B	232	ARG
1	B	234	ARG
1	B	252	LEU
1	B	257	ASN
1	B	262	GLN
1	B	290	ILE
1	B	314	LEU
1	B	316	LEU
1	B	339	SER
1	B	355	GLU
1	B	359	LEU
1	B	360	ARG
1	B	419	GLN
1	B	425	LEU
1	B	448	GLU
1	B	460	GLU
1	B	474	LEU
1	B	479	ASN
1	B	484	GLU
1	B	485	THR
1	B	505	ASP
1	B	506	LYS
1	C	56	THR
1	C	67	ILE
1	C	77	ILE
1	C	105	ASP
1	C	112	VAL
1	C	136	ILE
1	C	144	LEU
1	C	145	LEU
1	C	150	MET
1	C	188	ARG
1	C	204	ILE
1	C	219	GLN
1	C	223	ILE
1	C	232	ARG
1	C	243	CYS
1	C	252	LEU
1	C	257	ASN

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Mol	Chain	Res	Type
1	C	262	GLN
1	C	314	LEU
1	C	324	ILE
1	C	359	LEU
1	C	360	ARG
1	C	361	GLU
1	C	418	ASN
1	C	425	LEU
1	C	447	ILE
1	C	448	GLU
1	C	453	LEU
1	C	459	ASN
1	C	474	LEU
1	C	479	ASN
1	C	482	GLN
1	C	483	MET
1	C	505	ASP
1	D	77	ILE
1	D	106	GLU
1	D	112	VAL
1	D	134	HIS
1	D	136	ILE
1	D	144	LEU
1	D	145	LEU
1	D	150	MET
1	D	188	ARG
1	D	204	ILE
1	D	215	ARG
1	D	217	LYS
1	D	219	GLN
1	D	220	ASP
1	D	232	ARG
1	D	243	CYS
1	D	252	LEU
1	D	257	ASN
1	D	262	GLN
1	D	298	TRP
1	D	314	LEU
1	D	354	ILE
1	D	359	LEU
1	D	360	ARG
1	D	366	VAL

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Mol	Chain	Res	Type
1	D	404	ILE
1	D	425	LEU
1	D	437	LEU
1	D	453	LEU
1	D	456	LYS
1	D	459	ASN
1	D	460	GLU
1	D	474	LEU
1	D	479	ASN
1	D	482	GLN
1	D	485	THR
1	D	505	ASP
1	E	56	THR
1	E	77	ILE
1	E	112	VAL
1	E	130	ARG
1	E	134	HIS
1	E	136	ILE
1	E	137	SER
1	E	138	ARG
1	E	144	LEU
1	E	145	LEU
1	E	150	MET
1	E	188	ARG
1	E	219	GLN
1	E	243	CYS
1	E	248	ARG
1	E	252	LEU
1	E	257	ASN
1	E	262	GLN
1	E	314	LEU
1	E	354	ILE
1	E	355	GLU
1	E	359	LEU
1	E	360	ARG
1	E	425	LEU
1	E	437	LEU
1	E	448	GLU
1	E	453	LEU
1	E	456	LYS
1	E	464	LEU
1	E	467	THR

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Mol	Chain	Res	Type
1	E	474	LEU
1	E	479	ASN
1	E	482	GLN
1	E	493	PHE
1	E	505	ASP
1	F	56	THR
1	F	77	ILE
1	F	112	VAL
1	F	136	ILE
1	F	144	LEU
1	F	145	LEU
1	F	150	MET
1	F	188	ARG
1	F	204	ILE
1	F	219	GLN
1	F	223	ILE
1	F	232	ARG
1	F	243	CYS
1	F	252	LEU
1	F	256	ILE
1	F	257	ASN
1	F	259	GLU
1	F	262	GLN
1	F	293	ASN
1	F	340	ARG
1	F	359	LEU
1	F	360	ARG
1	F	410	ILE
1	F	422	LEU
1	F	425	LEU
1	F	448	GLU
1	F	456	LYS
1	F	459	ASN
1	F	474	LEU
1	F	479	ASN
1	F	482	GLN
1	F	505	ASP
1	G	38	VAL
1	G	56	THR
1	G	77	ILE
1	G	90	GLU
1	G	112	VAL

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Mol	Chain	Res	Type
1	G	136	ILE
1	G	144	LEU
1	G	145	LEU
1	G	150	MET
1	G	186	MET
1	G	188	ARG
1	G	204	ILE
1	G	219	GLN
1	G	223	ILE
1	G	232	ARG
1	G	243	CYS
1	G	252	LEU
1	G	257	ASN
1	G	262	GLN
1	G	293	ASN
1	G	314	LEU
1	G	359	LEU
1	G	360	ARG
1	G	404	ILE
1	G	425	LEU
1	G	447	ILE
1	G	453	LEU
1	G	460	GLU
1	G	474	LEU
1	G	480	CYS
1	G	505	ASP
1	H	38	VAL
1	H	55	LEU
1	H	56	THR
1	H	77	ILE
1	H	112	VAL
1	H	136	ILE
1	H	144	LEU
1	H	145	LEU
1	H	150	MET
1	H	188	ARG
1	H	204	ILE
1	H	217	LYS
1	H	219	GLN
1	H	232	ARG
1	H	243	CYS
1	H	252	LEU

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Mol	Chain	Res	Type
1	H	256	ILE
1	H	257	ASN
1	H	262	GLN
1	H	359	LEU
1	H	404	ILE
1	H	422	LEU
1	H	425	LEU
1	H	448	GLU
1	H	453	LEU
1	H	456	LYS
1	H	459	ASN
1	H	460	GLU
1	H	474	LEU
1	H	479	ASN
1	H	505	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	99	ASN
1	A	238	GLN
1	A	239	GLN
1	A	293	ASN
1	A	315	GLN
1	A	322	ASN
1	A	351	ASN
1	A	418	ASN
1	A	419	GLN
1	A	470	ASN
1	B	40	GLN
1	B	99	ASN
1	B	195	GLN
1	B	219	GLN
1	B	239	GLN
1	B	257	ASN
1	B	315	GLN
1	B	322	ASN
1	B	345	HIS
1	B	419	GLN
1	B	457	ASN
1	B	463	ASN

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Mol	Chain	Res	Type
1	B	470	ASN
1	C	99	ASN
1	C	195	GLN
1	C	239	GLN
1	C	315	GLN
1	C	322	ASN
1	C	457	ASN
1	D	99	ASN
1	D	193	ASN
1	D	238	GLN
1	D	239	GLN
1	D	293	ASN
1	D	315	GLN
1	D	322	ASN
1	D	395	ASN
1	D	463	ASN
1	D	482	GLN
1	E	99	ASN
1	E	193	ASN
1	E	238	GLN
1	E	239	GLN
1	E	293	ASN
1	E	315	GLN
1	E	322	ASN
1	E	399	ASN
1	E	433	ASN
1	E	463	ASN
1	F	99	ASN
1	F	193	ASN
1	F	195	GLN
1	F	239	GLN
1	F	315	GLN
1	F	322	ASN
1	F	418	ASN
1	F	482	GLN
1	G	99	ASN
1	G	172	HIS
1	G	175	GLN
1	G	195	GLN
1	G	239	GLN
1	G	315	GLN
1	G	322	ASN

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Mol	Chain	Res	Type
1	G	451	HIS
1	G	479	ASN
1	H	99	ASN
1	H	193	ASN
1	H	219	GLN
1	H	293	ASN
1	H	315	GLN
1	H	322	ASN
1	H	418	ASN
1	H	457	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	441/497 (88%)	-1.20	0 100 100	33, 64, 120, 158	0
1	B	441/497 (88%)	-1.22	0 100 100	32, 64, 116, 134	0
1	C	418/497 (84%)	-0.93	0 100 100	52, 104, 152, 167	0
1	D	417/497 (83%)	-1.10	0 100 100	44, 86, 149, 165	0
1	E	427/497 (85%)	-1.08	0 100 100	40, 77, 138, 183	0
1	F	436/497 (87%)	-1.17	0 100 100	34, 73, 127, 167	0
1	G	411/497 (82%)	-0.98	0 100 100	48, 99, 156, 181	0
1	H	405/497 (81%)	-0.80	0 100 100	56, 114, 160, 176	0
All	All	3396/3976 (85%)	-1.06	0 100 100	32, 82, 149, 183	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.