



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:24 AM UTC

PDB ID : 5AYX / pdb_00005ayx
Title : Crystal structure of Human Quinolate Phosphoribosyltransferase
Authors : Kang, G.B.; Kim, M.-K.; Im, Y.J.; Lee, J.H.; Youn, H.-S.; An, J.Y.; Lee, J.-G.; Fukuoka, S.-I.; Eom, S.H.
Deposited on : 2015-09-14
Resolution : 2.80 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

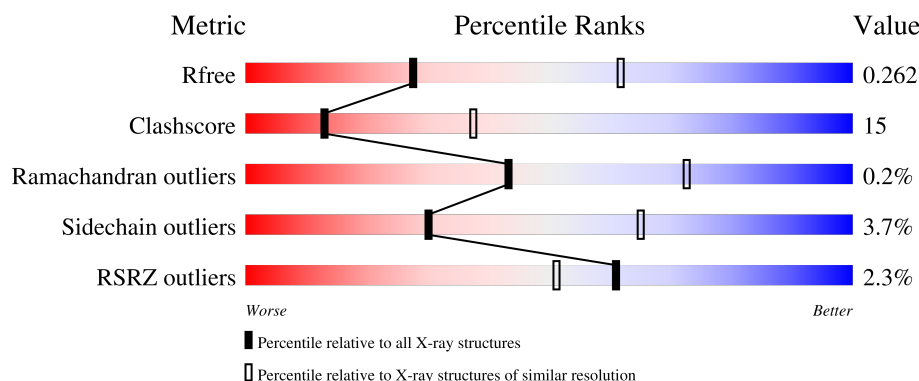
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	305	
1	B	305	
1	C	305	
1	D	305	
1	E	305	

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Mol	Chain	Length	Quality of chain
1	F	305	71% 19% 5%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 12499 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 Nicotinate-nucleotide pyrophosphorylase [carboxylating].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	B	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	C	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	D	276	Total	C	N	O	S	0	0	0
			2003	1276	346	371	10			
1	E	281	Total	C	N	O	S	0	0	0
			2045	1305	352	378	10			
1	F	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	LEU	-	expression tag	UNP Q15274
A	299	GLU	-	expression tag	UNP Q15274
A	300	HIS	-	expression tag	UNP Q15274
A	301	HIS	-	expression tag	UNP Q15274
A	302	HIS	-	expression tag	UNP Q15274
A	303	HIS	-	expression tag	UNP Q15274
A	304	HIS	-	expression tag	UNP Q15274
A	305	HIS	-	expression tag	UNP Q15274
B	298	LEU	-	expression tag	UNP Q15274
B	299	GLU	-	expression tag	UNP Q15274
B	300	HIS	-	expression tag	UNP Q15274
B	301	HIS	-	expression tag	UNP Q15274
B	302	HIS	-	expression tag	UNP Q15274
B	303	HIS	-	expression tag	UNP Q15274
B	304	HIS	-	expression tag	UNP Q15274
B	305	HIS	-	expression tag	UNP Q15274
C	298	LEU	-	expression tag	UNP Q15274

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Chain	Residue	Modelled	Actual	Comment	Reference
C	299	GLU	-	expression tag	UNP Q15274
C	300	HIS	-	expression tag	UNP Q15274
C	301	HIS	-	expression tag	UNP Q15274
C	302	HIS	-	expression tag	UNP Q15274
C	303	HIS	-	expression tag	UNP Q15274
C	304	HIS	-	expression tag	UNP Q15274
C	305	HIS	-	expression tag	UNP Q15274
D	298	LEU	-	expression tag	UNP Q15274
D	299	GLU	-	expression tag	UNP Q15274
D	300	HIS	-	expression tag	UNP Q15274
D	301	HIS	-	expression tag	UNP Q15274
D	302	HIS	-	expression tag	UNP Q15274
D	303	HIS	-	expression tag	UNP Q15274
D	304	HIS	-	expression tag	UNP Q15274
D	305	HIS	-	expression tag	UNP Q15274
E	298	LEU	-	expression tag	UNP Q15274
E	299	GLU	-	expression tag	UNP Q15274
E	300	HIS	-	expression tag	UNP Q15274
E	301	HIS	-	expression tag	UNP Q15274
E	302	HIS	-	expression tag	UNP Q15274
E	303	HIS	-	expression tag	UNP Q15274
E	304	HIS	-	expression tag	UNP Q15274
E	305	HIS	-	expression tag	UNP Q15274
F	298	LEU	-	expression tag	UNP Q15274
F	299	GLU	-	expression tag	UNP Q15274
F	300	HIS	-	expression tag	UNP Q15274
F	301	HIS	-	expression tag	UNP Q15274
F	302	HIS	-	expression tag	UNP Q15274
F	303	HIS	-	expression tag	UNP Q15274
F	304	HIS	-	expression tag	UNP Q15274
F	305	HIS	-	expression tag	UNP Q15274

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total O 9 9	0	0
2	B	3	Total O 3 3	0	0
2	D	1	Total O 1 1	0	0
2	E	1	Total O 1 1	0	0

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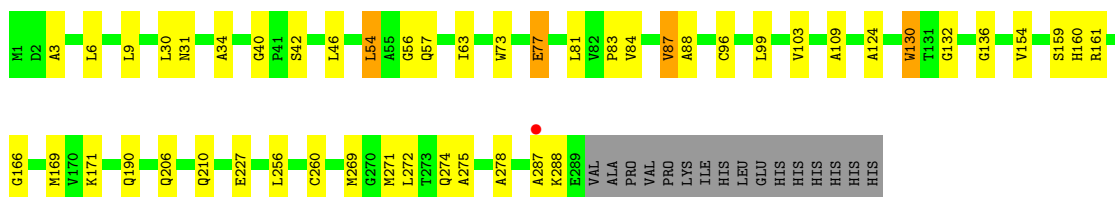
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	5	Total	O	0	0
			5	5		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

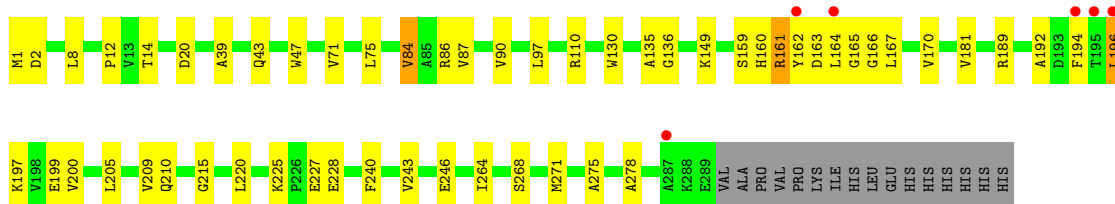
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain A: 



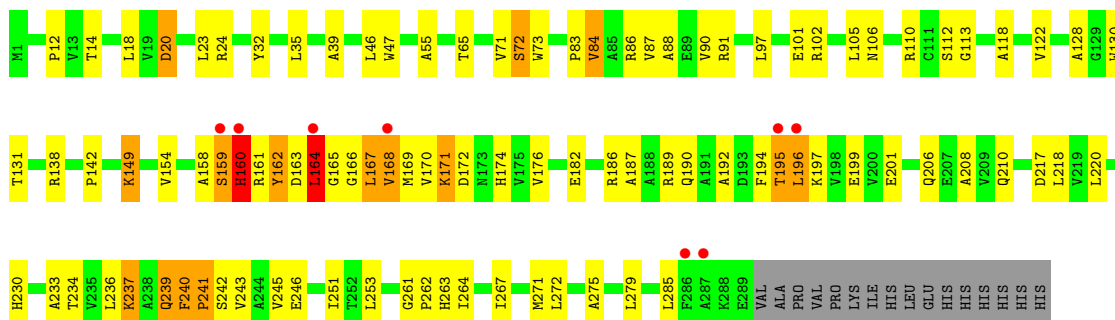
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain B: 

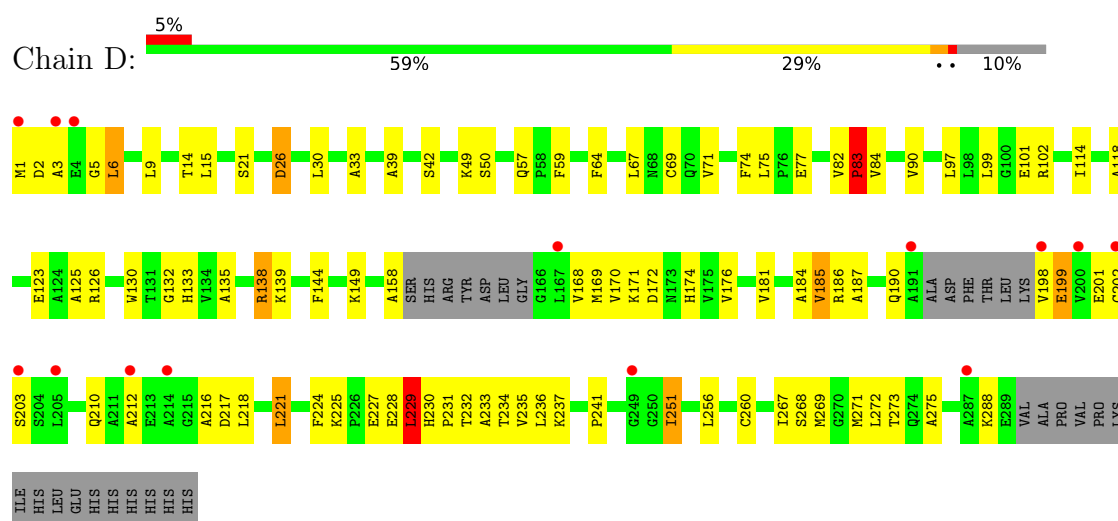


• Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

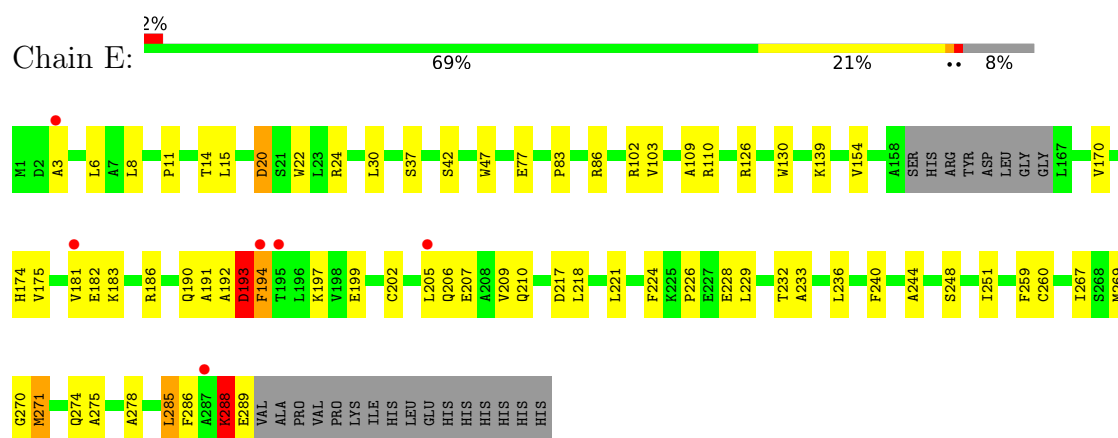
Chain C: 



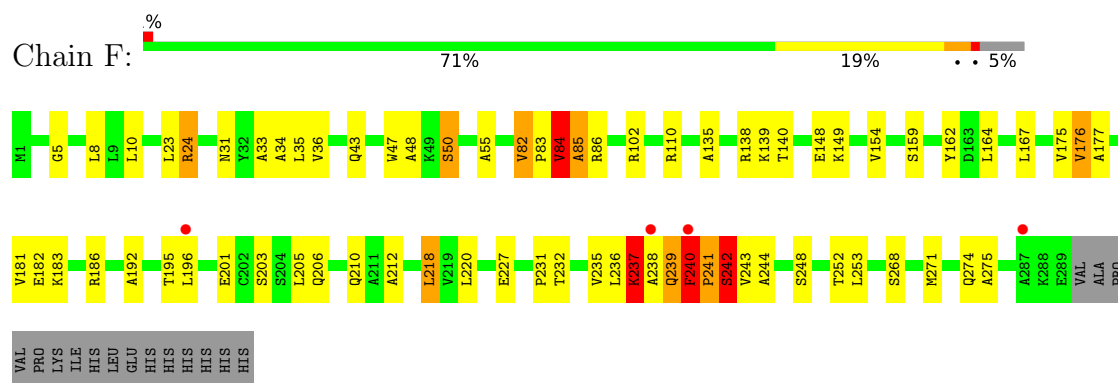
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]



● Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]



● Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.18Å 137.12Å 92.65Å 90.00° 103.76° 90.00°	Depositor
Resolution (Å)	48.00 – 2.80 48.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.00-2.80) 97.1 (48.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.51 (at 2.81Å)	Xtriage
Refinement program	REFMAC 6.5.0	Depositor
R, R_{free}	0.201 , 0.259 0.201 , 0.262	Depositor DCC
R_{free} test set	2227 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12499	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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

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	0.60	1/2151 (0.0%)	0.74	5/2931 (0.2%)
1	B	0.57	2/2151 (0.1%)	0.74	2/2931 (0.1%)
1	C	0.65	0/2151	0.91	14/2931 (0.5%)
1	D	0.62	0/2041	0.91	10/2780 (0.4%)
1	E	0.51	0/2085	0.79	5/2841 (0.2%)
1	F	0.61	0/2151	0.81	11/2931 (0.4%)
All	All	0.59	3/12730 (0.0%)	0.82	47/17345 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	LEU	C-N	-7.21	1.24	1.33
1	B	20	ASP	C-O	5.88	1.30	1.24
1	B	20	ASP	CA-C	-5.12	1.46	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	82	VAL	N-CA-C	-9.28	97.78	107.89
1	E	37	SER	N-CA-C	8.52	120.65	111.36
1	F	176	VAL	N-CA-C	8.48	120.28	110.62
1	C	159	SER	CB-CA-C	7.50	122.06	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	26	ASP	N-CA-C	7.40	119.13	111.14
1	C	164	LEU	N-CA-C	-7.25	103.69	112.54
1	B	196	LEU	CB-CA-C	-7.13	102.45	111.22
1	E	83	PRO	N-CA-C	6.92	121.23	111.33
1	D	83	PRO	N-CA-C	6.87	122.03	111.11
1	A	30	LEU	N-CA-C	6.85	119.14	110.24
1	F	241	PRO	CB-CA-C	6.83	121.92	111.40
1	D	199	GLU	N-CA-C	6.79	120.61	111.24
1	D	251	ILE	N-CA-C	-6.65	100.11	108.89
1	D	229	LEU	N-CA-C	6.44	121.42	113.50
1	C	162	TYR	N-CA-C	-6.30	104.33	111.07
1	C	158	ALA	N-CA-C	6.27	119.72	109.06
1	F	237	LYS	CB-CA-C	6.23	122.16	110.63
1	C	195	THR	N-CA-C	-6.08	97.84	110.80
1	D	251	ILE	CB-CA-C	6.06	119.03	111.15
1	A	54	LEU	N-CA-C	6.02	118.95	107.75
1	F	82	VAL	CB-CA-C	6.00	116.79	110.37
1	F	239	GLN	N-CA-C	-5.99	104.67	111.14
1	B	84	VAL	N-CA-C	5.90	121.62	109.34
1	A	54	LEU	CB-CA-C	-5.87	101.45	111.31
1	C	167	LEU	N-CA-C	5.74	121.03	112.94
1	C	171	LYS	N-CA-C	-5.70	102.03	110.46
1	C	83	PRO	N-CA-C	5.68	124.16	112.47
1	E	193	ASP	N-CA-C	5.63	119.44	112.24
1	A	130	TRP	CB-CA-C	5.61	118.99	109.80
1	D	82	VAL	CA-C-N	5.49	125.49	119.89
1	D	82	VAL	C-N-CA	5.49	125.49	119.89
1	C	72	SER	N-CA-C	5.48	117.61	108.02
1	C	72	SER	CB-CA-C	-5.43	102.00	110.74
1	C	84	VAL	N-CA-C	5.42	120.62	109.34
1	F	85	ALA	N-CA-C	5.42	118.45	109.46
1	D	185	VAL	N-CA-C	-5.41	105.10	110.62
1	F	242	SER	N-CA-C	-5.39	99.33	110.80
1	F	82	VAL	CA-C-N	-5.38	114.70	120.03
1	F	82	VAL	C-N-CA	-5.38	114.70	120.03
1	C	196	LEU	CB-CA-C	5.36	118.64	109.80
1	C	160	HIS	N-CA-CB	5.25	119.36	110.49
1	C	18	LEU	N-CA-C	5.18	117.00	111.36
1	A	83	PRO	N-CA-C	5.17	119.32	111.15
1	E	288	LYS	N-CA-C	5.16	117.72	110.23
1	F	176	VAL	CB-CA-C	-5.11	105.34	112.04
1	D	184	ALA	N-CA-C	5.06	116.88	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	102	ARG	N-CA-C	5.02	116.75	111.28

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	161	ARG	Sidechain
1	C	102	ARG	Sidechain
1	C	237	LYS	Peptide
1	D	138	ARG	Sidechain

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	2108	0	2128	30	0
1	B	2108	0	2128	57	0
1	C	2108	0	2128	101	0
1	D	2003	0	2030	86	0
1	E	2045	0	2072	60	0
1	F	2108	0	2128	78	0
2	A	9	0	0	2	0
2	B	3	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	5	0	0	0	0
All	All	12499	0	12614	377	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 15.

All (377) 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:F:239:GLN:C	1:F:241:PRO:HD3	1.16	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:GLN:C	1:F:241:PRO:CD	2.13	1.20
1:F:240:PHE:N	1:F:241:PRO:HD3	1.43	1.15
1:F:240:PHE:N	1:F:241:PRO:CD	2.12	1.12
1:D:225:LYS:NZ	1:D:228:GLU:OE1	1.80	1.11
1:F:241:PRO:HB2	1:F:243:VAL:HG23	1.34	1.09
1:F:239:GLN:HB3	1:F:241:PRO:CD	1.82	1.09
1:E:192:ALA:C	1:E:193:ASP:OD2	1.97	1.07
1:F:218:LEU:HD22	1:F:244:ALA:HB3	1.40	1.04
1:B:165:GLY:O	1:C:165:GLY:HA2	1.63	0.99
1:C:163:ASP:OD1	1:C:163:ASP:O	1.83	0.96
1:F:239:GLN:HB3	1:F:241:PRO:HD2	1.53	0.88
1:C:112:SER:HB3	1:C:279:LEU:HD22	1.54	0.86
1:C:160:HIS:NE2	1:C:246:GLU:OE1	2.09	0.85
1:E:42:SER:HB3	1:E:288:LYS:HE2	1.56	0.85
1:F:239:GLN:CA	1:F:241:PRO:HD3	2.07	0.84
1:C:161:ARG:O	1:C:165:GLY:C	2.21	0.83
1:F:252:THR:HG22	1:F:271:MET:HG3	1.60	0.83
1:E:191:ALA:O	1:E:193:ASP:OD2	1.97	0.82
1:D:67:LEU:HD22	1:D:99:LEU:HD23	1.62	0.82
1:F:239:GLN:O	1:F:241:PRO:HD3	1.80	0.81
1:D:171:LYS:HG2	1:D:201:GLU:OE1	1.81	0.81
1:C:240:PHE:HB3	1:C:243:VAL:HG23	1.62	0.80
1:C:164:LEU:HD13	1:C:164:LEU:O	1.83	0.77
1:C:32:TYR:HB2	1:D:168:VAL:HG21	1.67	0.76
1:A:96:CYS:SG	2:A:409:HOH:O	2.42	0.76
1:B:136:GLY:O	1:B:160:HIS:NE2	2.17	0.76
1:B:162:TYR:HD1	1:B:163:ASP:N	1.83	0.76
1:E:192:ALA:C	1:E:193:ASP:CG	2.54	0.75
1:C:240:PHE:CD1	1:C:241:PRO:HD2	2.22	0.75
1:D:6:LEU:HD23	1:D:9:LEU:HD12	1.69	0.75
1:F:239:GLN:CB	1:F:241:PRO:CD	2.62	0.74
1:C:160:HIS:HB3	1:C:162:TYR:CD2	2.24	0.72
1:B:162:TYR:CE1	1:B:163:ASP:HB3	2.24	0.72
1:C:192:ALA:HB3	1:C:196:LEU:HD22	1.71	0.71
1:C:240:PHE:HD1	1:C:241:PRO:HD2	1.55	0.71
1:D:181:VAL:HG13	1:D:210:GLN:HG3	1.72	0.71
1:C:230:HIS:O	1:C:234:THR:HG23	1.91	0.71
1:F:82:VAL:O	1:F:85:ALA:HB2	1.89	0.71
1:F:83:PRO:C	1:F:84:VAL:HG13	2.16	0.70
1:D:1:MET:HB2	1:E:190:GLN:HB3	1.74	0.70
1:B:162:TYR:CD1	1:B:163:ASP:HB3	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:TYR:CD1	1:B:163:ASP:N	2.60	0.69
1:C:168:VAL:HG21	1:C:196:LEU:HD21	1.74	0.69
1:D:67:LEU:CD2	1:D:99:LEU:HD23	2.22	0.69
1:B:164:LEU:O	1:C:166:GLY:HA3	1.92	0.69
1:D:224:PHE:HD2	1:D:229:LEU:HD23	1.57	0.69
1:A:227:GLU:N	1:A:227:GLU:OE1	2.24	0.68
1:E:205:LEU:HD11	1:E:232:THR:HG22	1.76	0.68
1:F:84:VAL:HG23	1:F:84:VAL:O	1.94	0.68
1:F:192:ALA:HB3	1:F:196:LEU:HD23	1.76	0.68
1:B:162:TYR:O	1:B:164:LEU:N	2.23	0.67
1:F:218:LEU:CD2	1:F:244:ALA:HB3	2.23	0.67
1:C:149:LYS:HE3	1:C:163:ASP:HB3	1.76	0.67
1:D:272:LEU:HD12	1:D:272:LEU:H	1.59	0.67
1:B:162:TYR:CD1	1:B:162:TYR:C	2.73	0.67
1:E:182:GLU:HB3	1:E:186:ARG:NH2	2.10	0.67
1:E:229:LEU:O	1:E:232:THR:OG1	2.13	0.66
1:F:231:PRO:O	1:F:235:VAL:HG23	1.94	0.66
1:C:101:GLU:OE1	1:D:171:LYS:NZ	2.28	0.66
1:F:83:PRO:O	1:F:84:VAL:HG13	1.96	0.66
1:E:6:LEU:CD1	1:E:154:VAL:HG22	2.25	0.66
1:D:3:ALA:O	1:D:77:GLU:O	2.14	0.65
1:B:271:MET:HG2	1:B:275:ALA:HB3	1.77	0.65
1:F:83:PRO:O	1:F:84:VAL:HG22	1.96	0.65
1:F:241:PRO:HB2	1:F:243:VAL:CG2	2.21	0.65
1:C:167:LEU:HD22	1:C:197:LYS:HB2	1.80	0.64
1:E:6:LEU:HD11	1:E:154:VAL:HG22	1.78	0.64
1:D:185:VAL:HG13	1:D:186:ARG:N	2.12	0.64
1:C:169:MET:HE1	1:C:220:LEU:HD23	1.79	0.64
1:B:12:PRO:HD2	1:D:99:LEU:HD21	1.79	0.64
1:C:194:PHE:HD2	1:C:195:THR:O	1.81	0.64
1:C:72:SER:OG	1:C:91:ARG:NH1	2.31	0.64
1:D:202:CYS:SG	1:D:221:LEU:HD13	2.38	0.64
1:F:239:GLN:CB	1:F:241:PRO:HD3	2.26	0.63
1:C:163:ASP:OD1	1:C:163:ASP:C	2.42	0.63
1:A:6:LEU:HD23	1:A:154:VAL:HG22	1.80	0.63
1:E:181:VAL:HG21	1:E:207:GLU:HG2	1.80	0.63
1:C:159:SER:O	1:C:164:LEU:HG	1.99	0.62
1:C:167:LEU:HD22	1:C:197:LYS:CB	2.28	0.62
1:E:109:ALA:HB1	1:E:278:ALA:HB1	1.81	0.62
1:E:3:ALA:O	1:E:6:LEU:HD22	1.99	0.62
1:F:240:PHE:O	1:F:240:PHE:CD2	2.52	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:GLY:O	1:B:197:LYS:HB2	2.00	0.62
1:D:6:LEU:HD23	1:D:9:LEU:CD1	2.30	0.62
1:E:271:MET:HG3	1:E:275:ALA:HB3	1.81	0.61
1:B:163:ASP:OD2	1:B:164:LEU:N	2.33	0.61
1:D:126:ARG:HG3	1:D:126:ARG:HH11	1.66	0.61
1:F:241:PRO:CB	1:F:243:VAL:HG23	2.21	0.61
1:D:123:GLU:OE1	1:D:126:ARG:NH2	2.34	0.61
1:C:239:GLN:HG3	1:C:240:PHE:N	2.16	0.61
1:B:75:LEU:HD12	1:B:87:VAL:HG22	1.82	0.60
1:F:237:LYS:O	1:F:240:PHE:N	2.34	0.60
1:C:84:VAL:HG12	1:C:84:VAL:O	2.00	0.60
1:A:56:GLY:N	1:A:77:GLU:OE2	2.34	0.60
1:B:110:ARG:HG2	1:B:110:ARG:HH11	1.65	0.60
1:E:199:GLU:HG3	1:E:218:LEU:HB2	1.83	0.60
1:B:167:LEU:HD12	1:B:197:LYS:HB3	1.83	0.60
1:C:237:LYS:HE3	1:C:263:HIS:HD2	1.66	0.60
1:D:212:ALA:HA	1:D:216:ALA:HB3	1.83	0.60
1:E:110:ARG:HH12	1:F:274:GLN:HE21	1.48	0.60
1:E:170:VAL:HG13	1:E:174:HIS:HB2	1.84	0.60
1:E:192:ALA:O	1:E:193:ASP:CG	2.44	0.60
1:E:233:ALA:HA	1:E:236:LEU:HD12	1.84	0.60
1:F:50:SER:C	1:F:83:PRO:HG3	2.27	0.60
1:C:71:VAL:HG22	1:C:90:VAL:HG22	1.84	0.60
1:B:84:VAL:HG12	1:B:84:VAL:O	2.00	0.59
1:C:199:GLU:HG3	1:C:218:LEU:HB2	1.84	0.59
1:F:241:PRO:C	1:F:243:VAL:N	2.59	0.59
1:E:193:ASP:OD2	1:E:193:ASP:N	2.34	0.59
1:A:287:ALA:HB2	2:A:403:HOH:O	2.03	0.59
1:E:228:GLU:O	1:E:232:THR:HG23	2.03	0.59
1:F:239:GLN:HB3	1:F:241:PRO:CG	2.31	0.59
1:A:169:MET:HE2	1:A:171:LYS:HD2	1.85	0.58
1:F:241:PRO:C	1:F:243:VAL:H	2.10	0.58
1:C:271:MET:HB2	1:C:275:ALA:HB3	1.84	0.58
1:B:162:TYR:C	1:B:164:LEU:H	2.11	0.58
1:D:251:ILE:HG22	1:D:269:MET:HE3	1.85	0.58
1:C:113:GLY:HA2	1:C:279:LEU:HD13	1.86	0.58
1:C:187:ALA:HA	1:C:190:GLN:HG3	1.84	0.58
1:C:262:PRO:HG2	1:C:263:HIS:ND1	2.19	0.58
1:C:169:MET:HE3	1:C:201:GLU:HB2	1.86	0.58
1:C:55:ALA:HB2	1:C:154:VAL:HG11	1.85	0.57
1:F:55:ALA:HB2	1:F:154:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLN:HB3	1:B:278:ALA:HB3	1.85	0.57
1:C:161:ARG:H	1:C:164:LEU:HB3	1.67	0.57
1:C:39:ALA:HB2	1:E:8:LEU:HD11	1.87	0.57
1:C:90:VAL:HG12	1:C:97:LEU:HD21	1.86	0.57
1:A:166:GLY:HA3	1:F:164:LEU:HA	1.85	0.56
1:D:185:VAL:CG1	1:D:186:ARG:N	2.68	0.56
1:C:159:SER:O	1:C:164:LEU:CB	2.53	0.56
1:D:74:PHE:O	1:D:75:LEU:HD23	2.05	0.56
1:E:181:VAL:HG21	1:E:207:GLU:CG	2.36	0.56
1:E:182:GLU:HB3	1:E:186:ARG:HH22	1.69	0.56
1:A:46:LEU:HG	1:A:87:VAL:HG22	1.88	0.56
1:B:160:HIS:HB2	1:B:162:TYR:CD2	2.41	0.56
1:D:198:VAL:N	1:D:218:LEU:HD13	2.21	0.56
1:A:109:ALA:HB1	1:A:278:ALA:HB1	1.87	0.56
1:F:212:ALA:HB1	1:F:239:GLN:HG2	1.87	0.55
1:C:160:HIS:O	1:C:161:ARG:CB	2.53	0.55
1:D:217:ASP:HB2	1:D:218:LEU:HD12	1.87	0.55
1:C:194:PHE:HD2	1:C:195:THR:C	2.13	0.55
1:B:194:PHE:HZ	1:C:164:LEU:HG	1.71	0.55
1:D:221:LEU:HG	1:D:229:LEU:HD21	1.88	0.55
1:C:236:LEU:HA	1:C:239:GLN:HB3	1.88	0.55
1:E:286:PHE:CD1	1:E:286:PHE:C	2.84	0.55
1:B:225:LYS:NZ	1:B:228:GLU:OE1	2.37	0.55
1:D:171:LYS:HG2	1:D:172:ASP:H	1.72	0.54
1:E:285:LEU:HB3	1:F:176:VAL:HG11	1.89	0.54
1:A:130:TRP:CZ2	1:A:132:GLY:HA3	2.42	0.54
1:F:149:LYS:HD2	1:F:159:SER:HB2	1.89	0.54
1:B:194:PHE:HZ	1:C:159:SER:O	1.90	0.54
1:E:42:SER:CB	1:E:288:LYS:HE2	2.33	0.54
1:E:193:ASP:O	1:E:194:PHE:HB2	2.08	0.54
1:E:22:TRP:HB3	1:E:103:VAL:HG11	1.89	0.54
1:D:9:LEU:HD21	1:F:35:LEU:HG	1.89	0.54
1:D:132:GLY:C	1:D:133:HIS:CD2	2.86	0.53
1:D:170:VAL:HG13	1:D:174:HIS:HB2	1.90	0.53
1:E:270:GLY:O	1:E:274:GLN:HB2	2.08	0.53
1:B:189:ARG:NH2	1:B:215:GLY:O	2.41	0.53
1:C:142:PRO:HG2	1:D:144:PHE:CE1	2.44	0.53
1:D:14:THR:HG23	1:F:24:ARG:CZ	2.38	0.53
1:F:206:GLN:O	1:F:210:GLN:HG3	2.09	0.53
1:C:161:ARG:HG2	1:C:167:LEU:HG	1.91	0.53
1:C:245:VAL:HG12	1:C:264:ILE:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLN:O	1:A:210:GLN:HG3	2.08	0.53
1:C:90:VAL:CG1	1:C:97:LEU:HD21	2.38	0.53
1:C:131:THR:O	1:C:131:THR:OG1	2.27	0.53
1:D:237:LYS:O	1:D:241:PRO:HG3	2.09	0.53
1:A:136:GLY:O	1:A:160:HIS:HE1	1.90	0.53
1:D:102:ARG:CZ	1:D:102:ARG:HB3	2.36	0.52
1:D:225:LYS:H	1:D:225:LYS:HD2	1.74	0.52
1:C:194:PHE:CD2	1:C:195:THR:O	2.63	0.52
1:C:161:ARG:O	1:C:165:GLY:O	2.27	0.52
1:B:194:PHE:CZ	1:C:164:LEU:HG	2.44	0.52
1:D:118:ALA:HA	1:D:272:LEU:HD23	1.92	0.52
1:B:162:TYR:C	1:B:164:LEU:N	2.64	0.52
1:A:3:ALA:O	1:A:6:LEU:HB2	2.10	0.51
1:E:226:PRO:HD3	1:E:259:PHE:CZ	2.45	0.51
1:C:106:ASN:O	1:C:110:ARG:HG3	2.10	0.51
1:E:232:THR:O	1:E:236:LEU:HG	2.10	0.51
1:D:224:PHE:CD2	1:D:229:LEU:HD23	2.43	0.51
1:E:192:ALA:CA	1:E:193:ASP:OD2	2.59	0.51
1:B:8:LEU:HD21	1:D:39:ALA:HB2	1.92	0.51
1:C:189:ARG:NH2	1:C:217:ASP:OD2	2.43	0.51
1:C:241:PRO:HG2	1:C:242:SER:N	2.24	0.51
1:C:253:LEU:H	1:C:253:LEU:HD23	1.76	0.51
1:B:205:LEU:O	1:B:209:VAL:HG23	2.11	0.51
1:D:221:LEU:N	1:D:221:LEU:CD2	2.73	0.51
1:D:251:ILE:HD13	1:D:267:ILE:HG23	1.91	0.51
1:F:237:LYS:O	1:F:238:ALA:C	2.53	0.51
1:D:225:LYS:HD3	1:D:228:GLU:OE1	2.09	0.51
1:B:194:PHE:HD1	1:B:194:PHE:H	1.59	0.51
1:C:285:LEU:HD22	1:D:176:VAL:HG12	1.92	0.51
1:D:90:VAL:HG12	1:D:97:LEU:HD21	1.93	0.51
1:E:205:LEU:CD1	1:E:232:THR:HG22	2.41	0.51
1:B:130:TRP:HZ2	1:B:264:ILE:HG22	1.77	0.50
1:E:42:SER:HB2	1:E:285:LEU:HD21	1.93	0.50
1:D:130:TRP:CD1	1:D:260:CYS:HB3	2.46	0.50
1:D:221:LEU:N	1:D:221:LEU:HD22	2.25	0.50
1:F:31:ASN:ND2	1:F:34:ALA:HB2	2.26	0.50
1:D:2:ASP:HB2	1:D:5:GLY:H	1.75	0.50
1:A:130:TRP:CE2	1:A:132:GLY:HA3	2.47	0.50
1:E:110:ARG:NH1	1:F:274:GLN:HE21	2.10	0.50
1:A:63:ILE:HD13	1:A:103:VAL:HG12	1.93	0.50
1:C:20:ASP:OD2	1:C:24:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLY:C	1:C:165:GLY:HA2	2.36	0.50
1:D:181:VAL:CG1	1:D:210:GLN:HG3	2.42	0.50
1:B:161:ARG:HA	1:B:164:LEU:HD12	1.94	0.49
1:D:14:THR:HG23	1:F:24:ARG:NH1	2.27	0.49
1:F:84:VAL:O	1:F:84:VAL:CG2	2.60	0.49
1:D:227:GLU:OE1	1:D:227:GLU:N	2.45	0.49
1:E:221:LEU:HB3	1:E:224:PHE:CE1	2.47	0.49
1:D:15:LEU:HD11	1:D:59:PHE:CD2	2.48	0.49
1:F:192:ALA:CB	1:F:196:LEU:HD23	2.42	0.49
1:B:227:GLU:H	1:B:227:GLU:CD	2.19	0.49
1:E:217:ASP:HB2	1:E:218:LEU:HD12	1.94	0.49
1:C:160:HIS:NE2	1:C:246:GLU:CD	2.70	0.49
1:D:169:MET:HA	1:D:198:VAL:O	2.13	0.49
1:E:6:LEU:HD12	1:E:154:VAL:HG22	1.95	0.49
1:C:208:ALA:HB1	1:C:236:LEU:HD11	1.94	0.48
1:C:261:GLY:C	1:C:263:HIS:H	2.19	0.48
1:D:269:MET:HB2	1:D:272:LEU:HD11	1.95	0.48
1:A:42:SER:OG	1:A:288:LYS:HG2	2.12	0.48
1:F:48:ALA:HB3	1:F:85:ALA:HB3	1.96	0.48
1:F:47:TRP:CZ3	1:F:86:ARG:HB2	2.49	0.48
1:C:167:LEU:CD2	1:C:197:LYS:HB2	2.43	0.48
1:D:114:ILE:HD13	1:D:273:THR:HG22	1.95	0.48
1:F:33:ALA:O	1:F:36:VAL:HG22	2.14	0.48
1:F:242:SER:O	1:F:242:SER:OG	2.27	0.48
1:A:40:GLY:H	1:A:288:LYS:HZ1	1.61	0.48
1:B:240:PHE:O	1:B:243:VAL:HG12	2.14	0.48
1:C:237:LYS:HE3	1:C:263:HIS:CD2	2.49	0.48
1:D:199:GLU:HG2	1:D:218:LEU:HB2	1.95	0.48
1:E:175:VAL:HG22	1:E:181:VAL:HA	1.96	0.48
1:F:241:PRO:O	1:F:243:VAL:N	2.45	0.48
1:F:239:GLN:CG	1:F:241:PRO:HG2	2.44	0.48
1:C:130:TRP:CH2	1:C:267:ILE:HD12	2.49	0.47
1:D:272:LEU:HD12	1:D:272:LEU:N	2.27	0.47
1:F:240:PHE:O	1:F:240:PHE:CG	2.66	0.47
1:B:39:ALA:HB2	1:F:8:LEU:HD21	1.94	0.47
1:B:110:ARG:HH11	1:B:110:ARG:CG	2.26	0.47
1:B:160:HIS:HB2	1:B:162:TYR:CE2	2.50	0.47
1:D:232:THR:O	1:D:236:LEU:HD22	2.14	0.47
1:F:135:ALA:O	1:F:268:SER:HA	2.14	0.47
1:C:170:VAL:HG13	1:C:174:HIS:HB2	1.95	0.47
1:A:9:LEU:HB3	1:E:30:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:LEU:HD22	1:C:197:LYS:HB3	1.95	0.47
1:D:187:ALA:O	1:D:190:GLN:HG2	2.14	0.47
1:D:225:LYS:HD3	1:D:228:GLU:HG3	1.96	0.47
1:D:30:LEU:HD12	1:D:30:LEU:H	1.79	0.47
1:D:230:HIS:N	1:D:231:PRO:HD2	2.30	0.47
1:E:130:TRP:CG	1:E:260:CYS:HG	2.33	0.47
1:C:167:LEU:O	1:C:168:VAL:HG23	2.15	0.47
1:C:47:TRP:CH2	1:C:86:ARG:HG3	2.50	0.47
1:C:194:PHE:CD2	1:C:194:PHE:C	2.92	0.47
1:C:35:LEU:HD23	1:C:35:LEU:HA	1.61	0.46
1:C:168:VAL:CG2	1:C:196:LEU:HD21	2.42	0.46
1:C:174:HIS:HE2	1:D:33:ALA:HB1	1.80	0.46
1:E:139:LYS:O	1:F:110:ARG:NH2	2.42	0.46
1:F:139:LYS:HB3	1:F:274:GLN:NE2	2.30	0.46
1:F:162:TYR:CE2	1:F:167:LEU:HD23	2.51	0.46
1:F:5:GLY:O	1:F:8:LEU:HD12	2.16	0.46
1:B:71:VAL:HG22	1:B:90:VAL:HG13	1.98	0.46
1:C:159:SER:O	1:C:164:LEU:HB3	2.15	0.46
1:C:206:GLN:O	1:C:210:GLN:HG3	2.16	0.46
1:D:132:GLY:O	1:D:133:HIS:CD2	2.69	0.46
1:D:203:SER:HA	1:D:224:PHE:HE1	1.81	0.46
1:A:54:LEU:HB2	1:A:81:LEU:HD11	1.98	0.45
1:D:125:ALA:HB2	1:D:256:LEU:HD21	1.98	0.45
1:E:205:LEU:H	1:E:205:LEU:HD12	1.82	0.45
1:D:232:THR:O	1:D:235:VAL:HG22	2.15	0.45
1:F:201:GLU:HA	1:F:220:LEU:HB3	1.98	0.45
1:A:31:ASN:OD1	1:A:34:ALA:HB2	2.16	0.45
1:D:230:HIS:O	1:D:234:THR:HG23	2.15	0.45
1:F:218:LEU:HD22	1:F:244:ALA:CB	2.30	0.45
1:F:271:MET:HB3	1:F:275:ALA:HB3	1.99	0.45
1:C:73:TRP:CE3	1:C:88:ALA:HB2	2.52	0.45
1:C:171:LYS:HE2	1:D:101:GLU:OE1	2.17	0.45
1:B:90:VAL:HG12	1:B:97:LEU:HD11	1.98	0.45
1:E:47:TRP:CZ3	1:E:86:ARG:HB2	2.51	0.45
1:E:248:SER:HA	1:E:251:ILE:HD12	1.98	0.45
1:D:230:HIS:HA	1:D:233:ALA:HB3	1.99	0.45
1:A:130:TRP:CG	1:A:260:CYS:HG	2.35	0.44
1:B:110:ARG:CG	1:B:110:ARG:NH1	2.80	0.44
1:C:160:HIS:O	1:C:161:ARG:HB3	2.16	0.44
1:D:198:VAL:N	1:D:218:LEU:CD1	2.80	0.44
1:F:138:ARG:HA	1:F:149:LYS:HZ1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:PHE:HB3	1:D:69:CYS:HB2	1.99	0.44
1:F:239:GLN:O	1:F:241:PRO:CD	2.52	0.44
1:E:20:ASP:O	1:E:24:ARG:HG3	2.18	0.44
1:A:271:MET:HG2	1:A:275:ALA:HB3	1.99	0.44
1:B:181:VAL:HG11	1:B:210:GLN:HB3	2.00	0.44
1:C:128:ALA:O	1:C:130:TRP:N	2.51	0.44
1:E:209:VAL:HG23	1:E:240:PHE:HE2	1.81	0.44
1:B:192:ALA:HB1	1:B:194:PHE:HE1	1.83	0.44
1:C:164:LEU:HD13	1:C:164:LEU:C	2.42	0.44
1:F:182:GLU:OE2	1:F:186:ARG:NH2	2.33	0.44
1:C:118:ALA:HA	1:C:272:LEU:HD22	2.00	0.44
1:C:182:GLU:HG3	1:C:186:ARG:HH12	1.83	0.44
1:D:50:SER:C	1:D:83:PRO:HG3	2.43	0.43
1:E:218:LEU:HA	1:E:244:ALA:O	2.18	0.43
1:F:236:LEU:HD23	1:F:236:LEU:HA	1.89	0.43
1:A:161:ARG:NH2	1:F:195:THR:O	2.51	0.43
1:E:139:LYS:HD3	1:F:102:ARG:NH2	2.34	0.43
1:F:23:LEU:HD23	1:F:23:LEU:HA	1.75	0.43
1:D:271:MET:HB2	1:D:275:ALA:HB3	2.00	0.43
1:A:6:LEU:HD23	1:A:154:VAL:CG2	2.47	0.43
1:B:47:TRP:CZ3	1:B:86:ARG:HB2	2.53	0.43
1:B:161:ARG:O	1:B:164:LEU:HB2	2.19	0.43
1:B:192:ALA:HB1	1:B:194:PHE:CE1	2.53	0.43
1:E:186:ARG:O	1:E:190:GLN:HG3	2.18	0.43
1:B:170:VAL:CG1	1:B:200:VAL:HG22	2.49	0.43
1:B:227:GLU:OE2	1:B:227:GLU:N	2.29	0.43
1:C:241:PRO:CG	1:C:242:SER:N	2.82	0.43
1:A:57:GLN:HG2	1:A:73:TRP:CZ2	2.53	0.43
1:A:269:MET:HB2	1:A:272:LEU:HG	2.01	0.43
1:C:167:LEU:C	1:C:168:VAL:CG2	2.92	0.43
1:D:6:LEU:CD2	1:D:9:LEU:CD1	2.95	0.43
1:E:251:ILE:HD13	1:E:267:ILE:HG23	2.00	0.43
1:C:233:ALA:HB1	1:C:263:HIS:O	2.19	0.43
1:B:162:TYR:HE1	1:B:163:ASP:HB3	1.81	0.42
1:D:57:GLN:HG3	1:D:77:GLU:OE1	2.19	0.42
1:D:135:ALA:HB2	1:D:158:ALA:HB3	2.01	0.42
1:D:198:VAL:HG22	1:D:217:ASP:H	1.84	0.42
1:E:197:LYS:HB3	1:E:217:ASP:OD2	2.18	0.42
1:E:206:GLN:O	1:E:210:GLN:HG3	2.19	0.42
1:F:183:LYS:HD2	1:F:183:LYS:O	2.19	0.42
1:C:23:LEU:HA	1:C:23:LEU:HD23	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:GLU:H	1:F:227:GLU:HG3	1.54	0.42
1:F:239:GLN:CB	1:F:241:PRO:CG	2.95	0.42
1:C:46:LEU:O	1:C:87:VAL:HG22	2.20	0.42
1:C:110:ARG:NH2	1:D:139:LYS:O	2.53	0.42
1:B:1:MET:SD	1:B:2:ASP:N	2.93	0.41
1:F:10:LEU:HD23	1:F:10:LEU:HA	1.85	0.41
1:C:159:SER:O	1:C:164:LEU:CG	2.65	0.41
1:D:225:LYS:H	1:D:225:LYS:CD	2.33	0.41
1:D:6:LEU:CD2	1:D:9:LEU:HD11	2.50	0.41
1:D:135:ALA:O	1:D:268:SER:HA	2.20	0.41
1:D:185:VAL:O	1:D:186:ARG:C	2.61	0.41
1:E:6:LEU:HD21	1:E:77:GLU:HG2	2.02	0.41
1:A:73:TRP:CE3	1:A:88:ALA:HB2	2.56	0.41
1:B:135:ALA:O	1:B:268:SER:HA	2.21	0.41
1:C:118:ALA:O	1:C:122:VAL:HG13	2.20	0.41
1:C:161:ARG:NH2	1:C:167:LEU:HD21	2.36	0.41
1:D:203:SER:HA	1:D:224:PHE:CE1	2.55	0.41
1:F:140:THR:OG1	1:F:148:GLU:OE1	2.30	0.41
1:B:149:LYS:HD3	1:B:149:LYS:HA	1.84	0.41
1:C:194:PHE:CE2	1:C:196:LEU:HB2	2.56	0.41
1:C:240:PHE:HB3	1:C:243:VAL:CG2	2.42	0.41
1:F:175:VAL:HG13	1:F:181:VAL:N	2.35	0.41
1:B:164:LEU:HD11	1:C:194:PHE:CZ	2.56	0.41
1:B:194:PHE:CZ	1:C:159:SER:O	2.72	0.41
1:D:42:SER:OG	1:D:288:LYS:HG2	2.20	0.41
1:D:71:VAL:HG22	1:D:90:VAL:HG13	2.02	0.41
1:E:288:LYS:HD2	1:F:177:ALA:HA	2.03	0.41
1:E:288:LYS:O	1:E:289:GLU:C	2.63	0.41
1:F:205:LEU:CD2	1:F:232:THR:HG23	2.51	0.41
1:C:172:ASP:O	1:C:176:VAL:HG23	2.21	0.41
1:B:189:ARG:HH11	1:B:196:LEU:HD22	1.85	0.40
1:D:1:MET:SD	1:D:1:MET:O	2.79	0.40
1:E:205:LEU:HD12	1:E:205:LEU:N	2.36	0.40
1:C:105:LEU:HD23	1:C:105:LEU:HA	1.92	0.40
1:D:15:LEU:HD12	1:D:15:LEU:HA	1.90	0.40
1:F:220:LEU:HD11	1:F:248:SER:HB2	2.03	0.40
1:A:99:LEU:HD21	1:C:12:PRO:HD2	2.02	0.40
1:B:220:LEU:HD13	1:B:246:GLU:HG2	2.03	0.40
1:D:138:ARG:HH22	1:D:149:LYS:HE2	1.87	0.40
1:E:11:PRO:HG2	1:E:14:THR:HB	2.03	0.40
1:E:202:CYS:HB3	1:E:207:GLU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:LYS:HD3	1:F:237:LYS:N	2.36	0.40
1:B:164:LEU:HD11	1:C:194:PHE:CE1	2.56	0.40
1:B:167:LEU:HD11	1:B:199:GLU:HB2	2.03	0.40
1:C:172:ASP:OD1	1:C:172:ASP:N	2.54	0.40
1:C:251:ILE:HD13	1:C:267:ILE:HG23	2.04	0.40
1:F:236:LEU:O	1:F:239:GLN:HB2	2.22	0.40
1:A:124:ALA:HB3	1:A:256:LEU:HD23	2.04	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	287/305 (94%)	278 (97%)	9 (3%)	0	100	100
1	B	287/305 (94%)	274 (96%)	13 (4%)	0	100	100
1	C	287/305 (94%)	269 (94%)	17 (6%)	1 (0%)	36	66
1	D	270/305 (88%)	253 (94%)	17 (6%)	0	100	100
1	E	277/305 (91%)	264 (95%)	13 (5%)	0	100	100
1	F	287/305 (94%)	273 (95%)	12 (4%)	2 (1%)	18	47
All	All	1695/1830 (93%)	1611 (95%)	81 (5%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	240	PHE
1	F	84	VAL
1	C	160	HIS

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	212/228 (93%)	207 (98%)	5 (2%)	43	77
1	B	212/228 (93%)	209 (99%)	3 (1%)	59	85
1	C	212/228 (93%)	201 (95%)	11 (5%)	21	53
1	D	202/228 (89%)	194 (96%)	8 (4%)	28	63
1	E	206/228 (90%)	196 (95%)	10 (5%)	22	55
1	F	212/228 (93%)	202 (95%)	10 (5%)	23	57
All	All	1256/1368 (92%)	1209 (96%)	47 (4%)	30	65

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLU
1	A	84	VAL
1	A	87	VAL
1	A	159	SER
1	A	190	GLN
1	B	14	THR
1	B	43	GLN
1	B	159	SER
1	C	14	THR
1	C	20	ASP
1	C	65	THR
1	C	138	ARG
1	C	149	LYS
1	C	160	HIS
1	C	164	LEU
1	C	168	VAL
1	C	239	GLN
1	C	240	PHE
1	C	241	PRO
1	D	6	LEU
1	D	21	SER
1	D	26	ASP

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Mol	Chain	Res	Type
1	D	49	LYS
1	D	83	PRO
1	D	84	VAL
1	D	221	LEU
1	D	229	LEU
1	E	15	LEU
1	E	20	ASP
1	E	126	ARG
1	E	183	LYS
1	E	193	ASP
1	E	194	PHE
1	E	269	MET
1	E	271	MET
1	E	285	LEU
1	E	288	LYS
1	F	24	ARG
1	F	43	GLN
1	F	50	SER
1	F	84	VAL
1	F	203	SER
1	F	218	LEU
1	F	237	LYS
1	F	240	PHE
1	F	242	SER
1	F	253	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	133	HIS
1	A	160	HIS
1	A	230	HIS
1	B	66	GLN
1	B	210	GLN
1	B	263	HIS
1	C	66	GLN
1	D	133	HIS
1	D	210	GLN
1	E	43	GLN
1	E	206	GLN
1	E	223	ASN

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Mol	Chain	Res	Type
1	F	274	GLN

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

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	289/305 (94%)	-0.42	1 (0%) 90 86	25, 48, 71, 115	0
1	B	289/305 (94%)	-0.29	6 (2%) 63 54	28, 49, 101, 155	0
1	C	289/305 (94%)	0.04	8 (2%) 55 45	38, 71, 111, 156	0
1	D	276/305 (90%)	0.20	14 (5%) 33 25	36, 76, 143, 164	0
1	E	281/305 (92%)	0.03	6 (2%) 63 54	33, 59, 112, 169	0
1	F	289/305 (94%)	-0.27	4 (1%) 73 64	32, 53, 81, 110	0
All	All	1713/1830 (93%)	-0.12	39 (2%) 61 51	25, 56, 122, 169	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	287	ALA	4.8
1	F	287	ALA	4.7
1	D	167	LEU	3.9
1	C	164	LEU	3.9
1	B	287	ALA	3.6
1	A	287	ALA	3.5
1	B	195	THR	3.3
1	F	240	PHE	3.3
1	C	168	VAL	3.3
1	C	287	ALA	3.2
1	E	287	ALA	3.1
1	D	214	ALA	3.0
1	B	196	LEU	3.0
1	B	164	LEU	2.9
1	E	205	LEU	2.7
1	D	200	VAL	2.6
1	C	195	THR	2.6
1	C	160	HIS	2.5
1	C	196	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	194	PHE	2.5
1	D	202	CYS	2.5
1	D	198	VAL	2.4
1	E	3	ALA	2.4
1	E	181	VAL	2.4
1	B	162	TYR	2.3
1	E	195	THR	2.3
1	D	212	ALA	2.3
1	C	159	SER	2.2
1	D	205	LEU	2.2
1	F	196	LEU	2.2
1	D	191	ALA	2.2
1	F	238	ALA	2.2
1	D	1	MET	2.1
1	C	286	PHE	2.1
1	D	3	ALA	2.1
1	E	194	PHE	2.1
1	D	249	GLY	2.0
1	D	4	GLU	2.0
1	D	203	SER	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.