



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:49 PM UTC

PDB ID : 4KNG / pdb_00004kng
Title : Crystal structure of human LGR5-RSPO1-RNF43
Authors : Chen, P.H.; He, X.
Deposited on : 2013-05-09
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 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

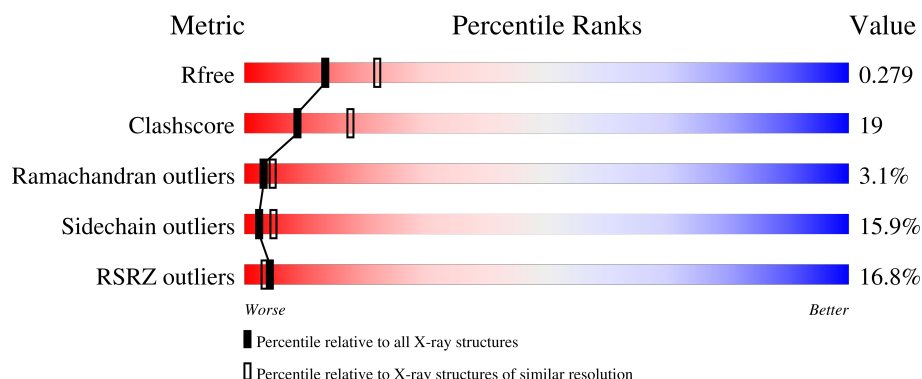
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	531	
1	B	531	
2	M	115	
2	P	115	
3	E	160	

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Mol	Chain	Length	Quality of chain
3	F	160	43% 54% 26% 9% • 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11252 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 Leucine-rich repeat-containing G-protein coupled receptor 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	1	0
			3622	2307	626	673	16			
1	B	463	Total	C	N	O	S	0	0	0
			3629	2312	627	674	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	expression tag	UNP O75473
A	31	PRO	-	expression tag	UNP O75473
A	558	ALA	-	expression tag	UNP O75473
A	559	ALA	-	expression tag	UNP O75473
A	560	ALA	-	expression tag	UNP O75473
B	30	GLY	-	expression tag	UNP O75473
B	31	PRO	-	expression tag	UNP O75473
B	558	ALA	-	expression tag	UNP O75473
B	559	ALA	-	expression tag	UNP O75473
B	560	ALA	-	expression tag	UNP O75473

- Molecule 2 is a protein called R-spondin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	98	Total	C	N	O	S	0	0	0
			750	465	131	136	18			
2	P	94	Total	C	N	O	S	0	0	0
			720	448	127	128	17			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	33	GLY	-	expression tag	UNP Q2MKA7
M	34	PRO	-	expression tag	UNP Q2MKA7

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Chain	Residue	Modelled	Actual	Comment	Reference
M	145	ALA	-	expression tag	UNP Q2MKA7
M	146	ALA	-	expression tag	UNP Q2MKA7
M	147	ALA	-	expression tag	UNP Q2MKA7
P	33	GLY	-	expression tag	UNP Q2MKA7
P	34	PRO	-	expression tag	UNP Q2MKA7
P	145	ALA	-	expression tag	UNP Q2MKA7
P	146	ALA	-	expression tag	UNP Q2MKA7
P	147	ALA	-	expression tag	UNP Q2MKA7

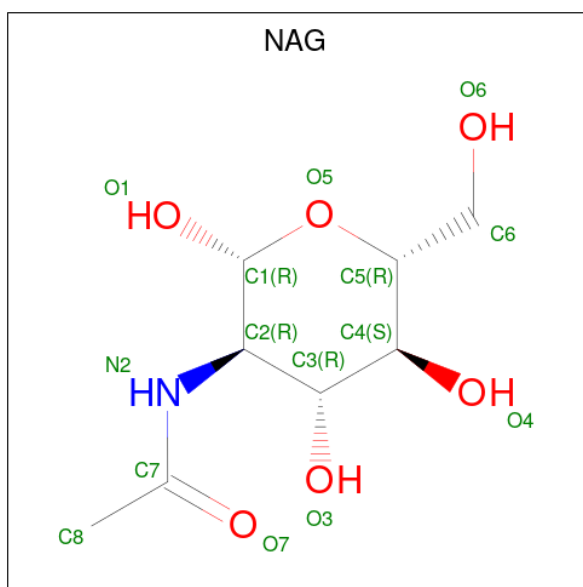
- Molecule 3 is a protein called E3 ubiquitin-protein ligase RNF43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	149	Total	C	N	O	S	0	0	0
			1152	734	200	212	6			
3	F	148	Total	C	N	O	S	0	0	0
			1145	729	199	211	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	42	GLY	-	expression tag	UNP Q68DV7
E	43	PRO	-	expression tag	UNP Q68DV7
E	199	ALA	-	expression tag	UNP Q68DV7
E	200	ALA	-	expression tag	UNP Q68DV7
E	201	ALA	-	expression tag	UNP Q68DV7
F	42	GLY	-	expression tag	UNP Q68DV7
F	43	PRO	-	expression tag	UNP Q68DV7
F	199	ALA	-	expression tag	UNP Q68DV7
F	200	ALA	-	expression tag	UNP Q68DV7
F	201	ALA	-	expression tag	UNP Q68DV7

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ni	0	0
			1	1		

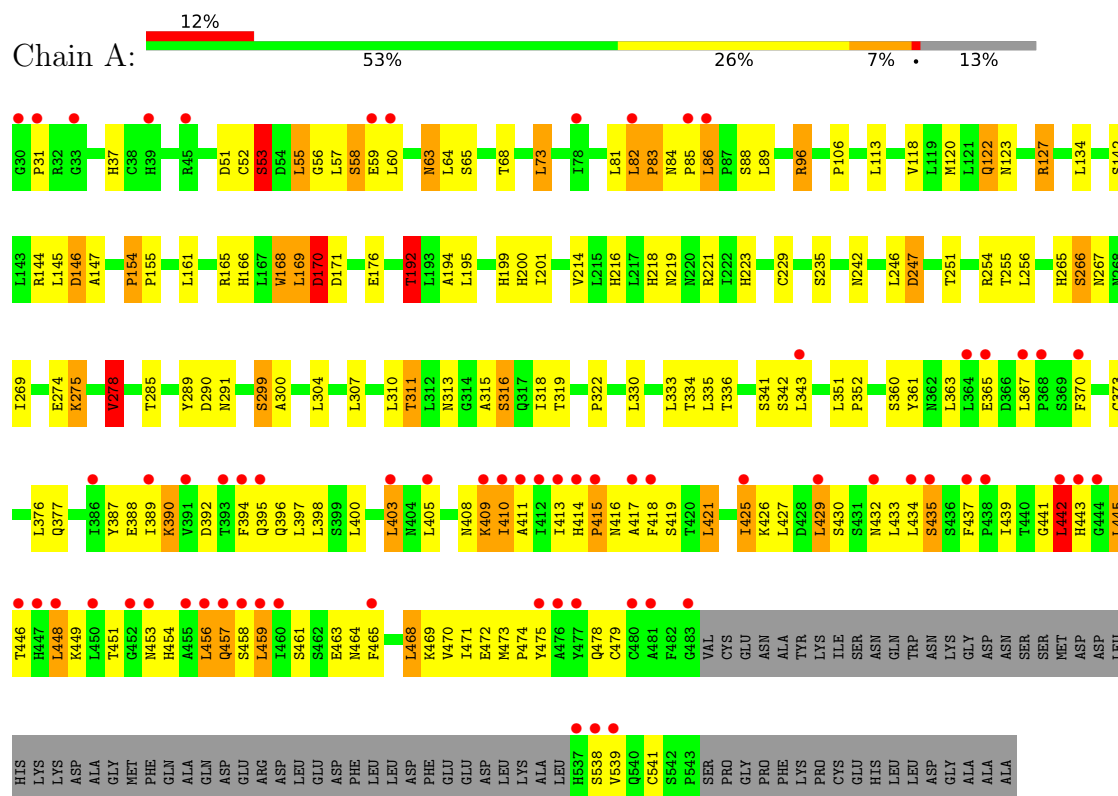
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	70	Total	O	0	0
			70	70		
6	B	85	Total	O	0	0
			85	85		
6	M	21	Total	O	0	0
			21	21		
6	P	7	Total	O	0	0
			7	7		
6	E	18	Total	O	0	0
			18	18		
6	F	4	Total	O	0	0
			4	4		

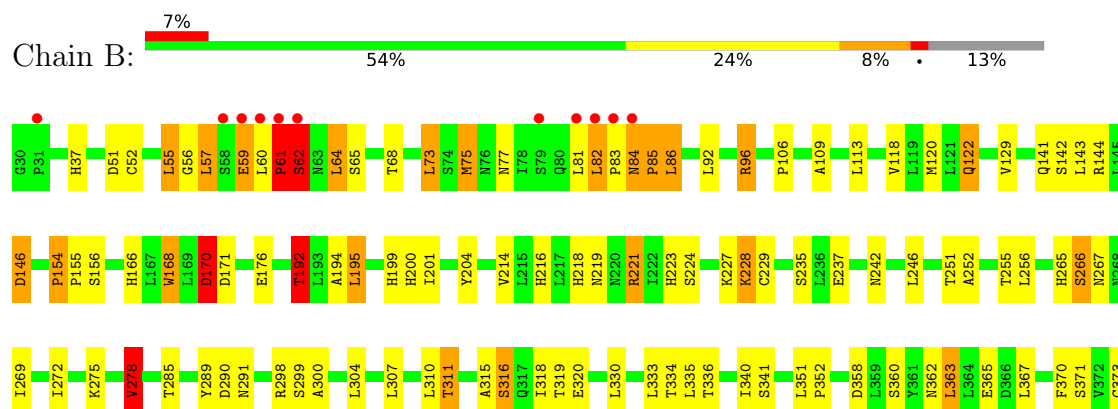
3 Residue-property plots [i](#)

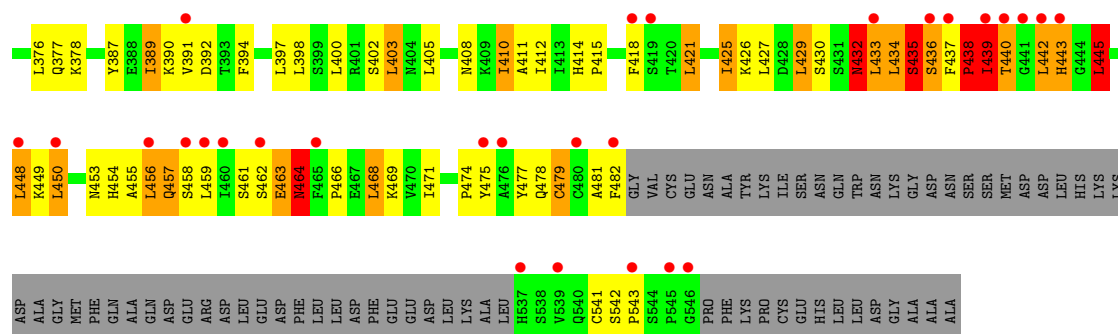
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Leucine-rich repeat-containing G-protein coupled receptor 5

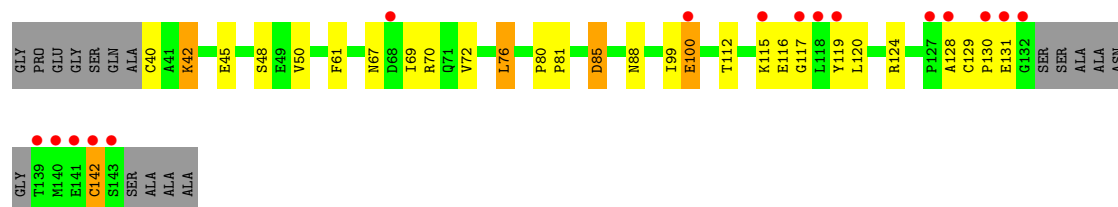


- Molecule 1: Leucine-rich repeat-containing G-protein coupled receptor 5

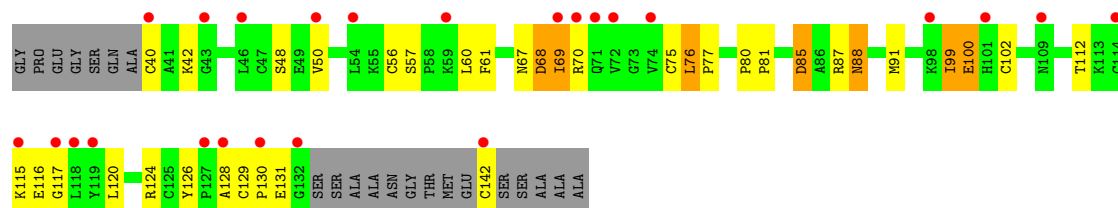




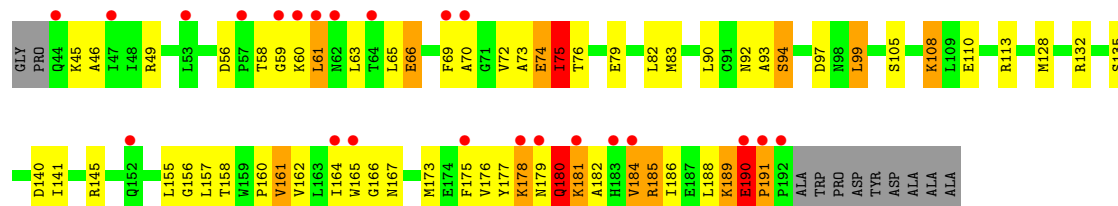
• Molecule 2: R-spondin-1



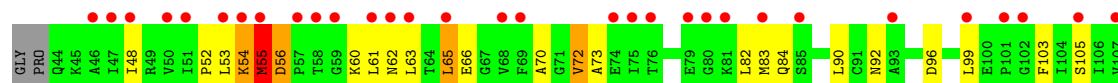
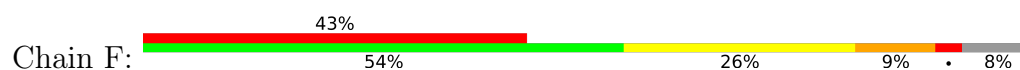
• Molecule 2: R-spondin-1

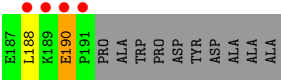
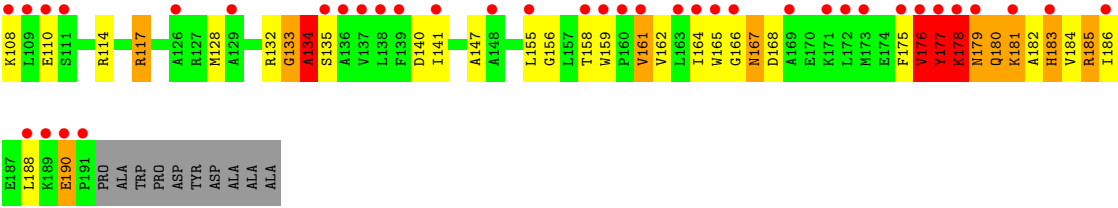


• Molecule 3: E3 ubiquitin-protein ligase RNF43



• Molecule 3: E3 ubiquitin-protein ligase RNF43





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.58Å 120.97Å 181.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.51 – 2.50 39.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (39.51-2.50) 97.1 (39.51-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.232 , 0.276 0.232 , 0.279	Depositor DCC
R_{free} test set	3894 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.6	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	0.93	EDS
Total number of atoms	11252	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.19% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.87	0/3704	1.11	15/5043 (0.3%)
1	B	1.00	2/3712 (0.1%)	1.18	18/5055 (0.4%)
2	M	0.92	0/765	1.22	7/1025 (0.7%)
2	P	0.87	0/735	1.20	6/985 (0.6%)
3	E	0.76	0/1175	1.04	4/1593 (0.3%)
3	F	0.67	0/1167	1.18	10/1581 (0.6%)
All	All	0.89	2/11258 (0.0%)	1.15	60/15282 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	8
2	P	0	1
3	E	0	3
3	F	0	3
All	All	0	16

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	440	THR	N-CA	6.68	1.54	1.46
1	B	272	ILE	N-CA	-5.83	1.41	1.46

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	PRO	N-CA-C	9.32	124.26	111.22
3	F	62	ASN	N-CA-C	9.30	122.41	111.71
3	F	134	ALA	N-CA-C	8.87	122.01	108.52
1	B	440	THR	N-CA-C	8.62	121.69	108.42
3	F	177	TYR	N-CA-C	-8.51	97.28	109.96
1	A	192	THR	CB-CA-C	-8.21	95.51	109.72
2	M	80	PRO	CA-C-N	8.15	130.03	119.84
2	M	80	PRO	C-N-CA	8.15	130.03	119.84
2	P	80	PRO	CA-C-N	8.13	130.00	119.84
2	P	80	PRO	C-N-CA	8.13	130.00	119.84
1	B	192	THR	CB-CA-C	-7.52	95.85	109.38
3	F	180	GLN	N-CA-C	-7.50	99.11	110.14
1	A	214	VAL	CB-CA-C	-7.32	99.71	110.62
1	B	214	VAL	CB-CA-C	-7.28	99.85	110.63
1	B	439	ILE	N-CA-C	7.23	124.38	109.34
1	B	445	LEU	N-CA-C	7.08	120.22	110.24
1	A	86	LEU	CA-C-N	6.99	128.91	120.94
1	A	86	LEU	C-N-CA	6.99	128.91	120.94
3	F	178	LYS	N-CA-C	6.88	125.46	110.80
1	B	154	PRO	CA-C-N	6.72	128.24	119.84
1	B	154	PRO	C-N-CA	6.72	128.24	119.84
1	A	154	PRO	CA-C-N	6.69	128.20	119.84
1	A	154	PRO	C-N-CA	6.69	128.20	119.84
1	A	170	ASP	N-CA-CB	-6.48	99.54	110.49
1	B	410	ILE	N-CA-C	6.47	116.80	108.12
1	B	316	SER	N-CA-C	6.38	120.17	112.38
1	B	170	ASP	N-CA-CB	-6.32	99.81	110.49
1	B	62	SER	N-CA-C	-6.29	97.41	110.80
1	B	443	HIS	N-CA-C	6.24	124.08	110.80
1	A	278	VAL	CB-CA-C	-6.00	103.29	112.05
3	E	190	GLU	CA-C-N	-5.84	114.37	120.38
3	E	190	GLU	C-N-CA	-5.84	114.37	120.38
1	B	129	VAL	N-CA-C	-5.77	103.30	108.95
1	A	442	LEU	N-CA-C	-5.72	100.57	109.72
1	B	278	VAL	CB-CA-C	-5.64	104.52	112.14
3	F	176	VAL	N-CA-C	5.64	119.17	113.47
1	A	316	SER	N-CA-C	5.64	119.67	112.34
3	E	141	ILE	N-CA-C	5.59	117.55	112.29
1	B	433	LEU	CB-CA-C	5.57	120.38	111.91
1	B	464	ASN	N-CA-C	-5.57	104.91	110.97
3	F	190	GLU	N-CA-C	5.41	117.42	110.39
1	A	421	LEU	CA-C-N	5.31	124.77	119.24
1	A	421	LEU	C-N-CA	5.31	124.77	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	PHE	CA-C-N	5.31	124.64	118.85
1	A	465	PHE	C-N-CA	5.31	124.64	118.85
1	A	168	TRP	CA-CB-CG	5.22	123.52	113.60
2	M	99	ILE	N-CA-C	5.18	115.73	108.89
3	F	167	ASN	N-CA-C	5.13	118.00	111.69
3	F	177	TYR	N-CA-CB	5.12	117.61	109.51
2	M	129	CYS	CA-C-N	-5.11	114.53	119.90
2	M	129	CYS	C-N-CA	-5.11	114.53	119.90
3	F	72	VAL	CB-CA-C	-5.09	105.27	112.14
3	E	74	GLU	N-CA-C	5.08	120.48	113.97
2	M	67	ASN	CA-C-N	5.07	130.82	121.70
2	M	67	ASN	C-N-CA	5.07	130.82	121.70
1	B	86	LEU	CA-CB-CG	-5.03	98.69	116.30
2	P	129	CYS	CA-C-N	-5.02	114.63	119.90
2	P	129	CYS	C-N-CA	-5.02	114.63	119.90
2	P	57	SER	CA-C-N	5.01	126.10	119.84
2	P	57	SER	C-N-CA	5.01	126.10	119.84

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	409	LYS	Peptide
1	B	432	ASN	Peptide
1	B	434	LEU	Peptide
1	B	435	SER	Peptide
1	B	438	PRO	Peptide
1	B	466	PRO	Peptide
1	B	57	LEU	Peptide
1	B	59	GLU	Peptide
1	B	61	PRO	Peptide
3	E	180	GLN	Peptide
3	E	61	LEU	Peptide
3	E	92	ASN	Peptide
3	F	134	ALA	Peptide
3	F	177	TYR	Peptide
3	F	179	ASN	Peptide
2	P	67	ASN	Peptide

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	3622	0	3626	136	0
1	B	3629	0	3634	152	0
2	M	750	0	719	17	0
2	P	720	0	692	26	0
3	E	1152	0	1182	46	0
3	F	1145	0	1175	50	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	B	1	0	0	0	0
6	A	70	0	0	9	0
6	B	85	0	0	7	0
6	E	18	0	0	4	0
6	F	4	0	0	1	0
6	M	21	0	0	2	0
6	P	7	0	0	8	0
All	All	11252	0	11054	413	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 (413) 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)
3:F:177:TYR:O	3:F:179:ASN:HA	1.44	1.17
1:B:450:LEU:HD12	1:B:453:ASN:HD22	0.98	1.15
1:B:459:LEU:HD21	1:B:478:GLN:CB	1.76	1.14
1:B:459:LEU:CD2	1:B:478:GLN:HB2	1.78	1.14
1:B:459:LEU:HD21	1:B:478:GLN:HB2	1.22	1.08
1:B:450:LEU:HD12	1:B:453:ASN:ND2	1.72	1.04
3:F:54:LYS:HA	3:F:55:MET:HB2	1.48	0.95
1:B:84:ASN:HB3	1:B:85:PRO:HA	1.48	0.93
1:A:414:HIS:HB3	1:A:415:PRO:HD2	1.52	0.91
1:B:60:LEU:HB3	1:B:61:PRO:HD3	1.50	0.91
3:F:181:LYS:HA	3:F:182:ALA:HB3	1.54	0.90
1:B:410:ILE:HB	1:B:432:ASN:OD1	1.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:PRO:HB2	1:B:439:ILE:HG22	1.53	0.87
3:E:173:MET:HA	3:E:176:VAL:HG12	1.58	0.85
3:E:179:ASN:N	3:E:180:GLN:HA	1.95	0.81
2:P:75:CYS:HB3	6:P:203:HOH:O	1.80	0.80
1:B:363:LEU:HD13	3:E:113:ARG:HG2	1.64	0.80
1:B:84:ASN:HB3	1:B:85:PRO:CA	2.12	0.79
1:B:192:THR:HG23	1:B:216:HIS:HB2	1.65	0.79
1:B:450:LEU:CD1	1:B:453:ASN:HD22	1.89	0.78
1:B:389:ILE:HD11	1:B:418:PHE:HE1	1.48	0.78
1:A:468:LEU:HD11	1:A:471:ILE:HG12	1.64	0.78
3:E:113:ARG:HD2	6:E:312:HOH:O	1.84	0.78
1:B:55:LEU:O	1:B:57:LEU:HG	1.85	0.77
1:B:65:SER:O	1:B:68:THR:HG22	1.86	0.76
3:E:162:VAL:HG21	3:E:188:LEU:HD11	1.68	0.76
3:F:70:ALA:HB3	3:F:161:VAL:HG22	1.68	0.76
3:F:103:PHE:O	3:F:134:ALA:CB	2.33	0.76
1:A:55:LEU:O	1:A:57:LEU:HG	1.85	0.76
1:B:394:PHE:O	1:B:421:LEU:HD11	1.86	0.76
1:B:192:THR:HG22	1:B:194:ALA:H	1.51	0.75
3:F:177:TYR:C	3:F:179:ASN:HA	2.10	0.74
1:A:192:THR:HG23	1:A:216:HIS:HB2	1.69	0.74
1:B:61:PRO:HG2	1:B:86:LEU:CD1	2.17	0.74
3:E:128:MET:HE3	3:E:132:ARG:CZ	2.16	0.74
3:E:73:ALA:HB3	6:E:311:HOH:O	1.87	0.74
1:B:459:LEU:HD21	1:B:478:GLN:HB3	1.68	0.73
2:M:61:PHE:CZ	2:M:85:ASP:HB3	2.22	0.73
1:A:435:SER:CB	1:A:456:LEU:HD12	2.17	0.73
1:A:410:ILE:HG23	1:A:432:ASN:HB2	1.69	0.73
1:B:408:ASN:O	1:B:432:ASN:HB3	1.89	0.72
1:A:65:SER:O	1:A:68:THR:HG22	1.89	0.72
2:P:60:LEU:HD12	6:P:203:HOH:O	1.90	0.72
3:F:162:VAL:HG21	3:F:188:LEU:HD11	1.70	0.72
1:B:237:GLU:OE1	2:P:124:ARG:NH2	2.24	0.71
1:B:311:THR:CG2	6:B:739:HOH:O	2.38	0.71
2:P:61:PHE:CZ	2:P:85:ASP:HB3	2.25	0.71
1:B:52:CYS:SG	1:B:60:LEU:HD11	2.32	0.70
1:B:459:LEU:O	1:B:459:LEU:HD23	1.92	0.70
1:B:61:PRO:HG2	1:B:86:LEU:HD13	1.73	0.69
1:A:468:LEU:HD21	1:A:471:ILE:HD11	1.75	0.68
1:A:218:HIS:HD2	1:A:219:ASN:HD22	1.41	0.68
1:A:192:THR:HG22	1:A:194:ALA:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ASP:OD1	1:B:221:ARG:HD3	1.94	0.67
1:B:85:PRO:O	1:B:86:LEU:HG	1.93	0.67
1:B:200:HIS:N	6:B:767:HOH:O	2.26	0.67
1:A:146:ASP:HB3	1:A:170:ASP:HB3	1.76	0.67
2:M:45:GLU:OE2	6:M:205:HOH:O	2.13	0.67
3:F:141:ILE:CG2	3:F:165:TRP:HB3	2.25	0.67
1:B:218:HIS:HD2	1:B:219:ASN:HD22	1.43	0.66
1:A:435:SER:HB2	1:A:456:LEU:HD12	1.78	0.66
1:B:433:LEU:O	1:B:433:LEU:HD12	1.95	0.66
1:A:416:ASN:C	1:A:418:PHE:H	2.04	0.66
1:A:468:LEU:O	1:A:539:VAL:HG11	1.95	0.66
1:B:468:LEU:HD21	1:B:471:ILE:HB	1.78	0.65
1:B:432:ASN:O	1:B:434:LEU:N	2.21	0.65
1:B:335:LEU:C	1:B:335:LEU:HD23	2.21	0.65
3:F:176:VAL:O	3:F:178:LYS:HA	1.97	0.65
1:B:442:LEU:HG	1:B:443:HIS:H	1.60	0.65
1:B:146:ASP:HB3	1:B:170:ASP:HB3	1.79	0.65
1:A:64:LEU:HD12	1:A:86:LEU:HD23	1.79	0.64
1:A:85:PRO:O	1:A:86:LEU:HD22	1.97	0.64
1:B:333:LEU:C	1:B:333:LEU:HD23	2.22	0.64
3:F:103:PHE:O	3:F:134:ALA:HB1	1.96	0.64
1:B:168:TRP:CZ3	6:P:204:HOH:O	2.50	0.64
3:E:190:GLU:HB2	3:E:191:PRO:CD	2.27	0.64
1:B:52:CYS:SG	1:B:60:LEU:CD1	2.86	0.64
1:B:61:PRO:HG3	1:B:64:LEU:HD13	1.78	0.64
2:M:48:SER:OG	3:E:110:GLU:OE2	2.11	0.64
2:P:87:ARG:CZ	6:P:201:HOH:O	2.46	0.64
1:A:59:GLU:HG2	1:A:83:PRO:HD2	1.80	0.64
3:F:70:ALA:HB3	3:F:161:VAL:CG2	2.28	0.63
1:B:429:LEU:O	1:B:432:ASN:ND2	2.32	0.63
1:B:471:ILE:CG2	1:B:541:CYS:SG	2.87	0.63
3:F:141:ILE:HG22	3:F:165:TRP:HB3	1.81	0.63
3:E:83:MET:O	3:E:105:SER:HA	1.99	0.62
1:B:142:SER:OG	1:B:166:HIS:HD2	1.80	0.62
2:M:70:ARG:HG2	3:E:181:LYS:HB3	1.82	0.62
1:A:218:HIS:CD2	1:A:219:ASN:HD22	2.17	0.61
3:F:83:MET:O	3:F:105:SER:HA	1.99	0.61
3:F:103:PHE:CZ	3:F:133:GLY:HA3	2.35	0.61
1:B:168:TRP:HZ3	6:P:204:HOH:O	1.83	0.61
1:B:351:LEU:N	1:B:352:PRO:CD	2.63	0.61
1:A:85:PRO:C	1:A:86:LEU:HD22	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LEU:C	1:A:442:LEU:HD22	2.26	0.61
2:P:88:ASN:HD22	2:P:91:MET:H	1.48	0.61
1:A:333:LEU:HD23	1:A:333:LEU:C	2.26	0.61
1:A:199:HIS:HB2	1:A:223:HIS:CE1	2.36	0.60
1:B:60:LEU:HD23	1:B:60:LEU:C	2.27	0.60
1:B:218:HIS:CD2	1:B:219:ASN:HD22	2.20	0.60
1:A:351:LEU:N	1:A:352:PRO:CD	2.65	0.60
1:A:274:GLU:O	1:A:299:SER:HB2	2.02	0.60
2:M:88:ASN:HB3	6:M:209:HOH:O	2.02	0.60
1:A:315:ALA:HB3	1:A:318:ILE:HD12	1.84	0.60
1:A:377:GLN:HA	1:A:400:LEU:HA	1.82	0.60
3:F:73:ALA:HB2	3:F:161:VAL:HG13	1.82	0.60
3:F:184:VAL:HG12	3:F:185:ARG:N	2.16	0.60
1:B:298:ARG:NH1	6:B:758:HOH:O	2.35	0.60
3:F:54:LYS:HA	3:F:55:MET:CB	2.28	0.60
3:F:182:ALA:O	3:F:183:HIS:HB2	2.02	0.60
1:B:315:ALA:HB3	1:B:318:ILE:HD12	1.84	0.59
1:B:438:PRO:C	1:B:439:ILE:HG22	2.27	0.59
3:E:46:ALA:HB2	3:E:69:PHE:CE1	2.37	0.59
1:B:267:ASN:HB2	1:B:291:ASN:HD21	1.68	0.59
1:A:63:ASN:H	1:A:63:ASN:HD22	1.50	0.58
1:B:377:GLN:HA	1:B:400:LEU:HA	1.84	0.58
1:B:141:GLN:HB2	6:B:713:HOH:O	2.02	0.58
2:P:85:ASP:N	2:P:85:ASP:OD1	2.37	0.58
1:B:144:ARG:HG2	1:B:168:TRP:CD1	2.38	0.58
3:F:180:GLN:O	3:F:181:LYS:C	2.46	0.58
1:A:86:LEU:HD12	1:A:88:SER:OG	2.03	0.58
1:A:267:ASN:HB2	1:A:291:ASN:HD21	1.68	0.58
1:A:142:SER:OG	1:A:166:HIS:HD2	1.86	0.58
1:B:435:SER:HB3	1:B:455:ALA:HB3	1.86	0.58
1:A:387:TYR:HA	1:A:410:ILE:N	2.18	0.57
1:B:389:ILE:CD1	1:B:418:PHE:HE1	2.17	0.57
1:B:410:ILE:CB	1:B:432:ASN:OD1	2.48	0.57
1:B:459:LEU:CD2	1:B:478:GLN:CB	2.54	0.57
1:B:192:THR:HG21	6:B:779:HOH:O	2.04	0.57
1:B:200:HIS:HD2	1:B:224:SER:HB2	1.70	0.57
1:A:416:ASN:HB3	1:A:419:SER:HB3	1.87	0.57
2:M:85:ASP:OD1	2:M:85:ASP:N	2.37	0.57
1:B:408:ASN:O	1:B:432:ASN:CB	2.53	0.57
2:P:87:ARG:NH1	6:P:201:HOH:O	2.36	0.57
1:A:415:PRO:O	1:A:439:ILE:HD13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:54:LYS:CA	3:F:55:MET:HB2	2.30	0.56
3:F:175:PHE:HE2	3:F:184:VAL:HG21	1.71	0.56
1:A:82:LEU:HD23	1:A:106:PRO:HG2	1.86	0.56
1:A:165:ARG:HH22	2:M:120:LEU:HD23	1.70	0.56
1:A:413:ILE:HG22	1:A:439:ILE:HD12	1.88	0.56
1:A:373:CYS:HB3	1:A:376:LEU:HD22	1.86	0.56
1:A:82:LEU:HA	1:A:84:ASN:N	2.21	0.56
3:E:82:LEU:HB3	3:E:184:VAL:HG23	1.87	0.56
3:F:175:PHE:CE2	3:F:184:VAL:HG21	2.40	0.56
2:P:128:ALA:O	2:P:130:PRO:HD3	2.05	0.56
3:E:73:ALA:HB2	3:E:161:VAL:HG13	1.88	0.56
3:E:179:ASN:N	3:E:180:GLN:CA	2.69	0.56
1:B:373:CYS:HB3	1:B:376:LEU:HD22	1.86	0.55
2:M:76:LEU:HD23	2:M:76:LEU:N	2.21	0.55
1:B:55:LEU:O	1:B:56:GLY:C	2.49	0.55
1:B:389:ILE:HD11	1:B:418:PHE:CE1	2.35	0.55
1:B:387:TYR:O	1:B:410:ILE:HA	2.06	0.55
2:P:76:LEU:N	2:P:76:LEU:HD23	2.22	0.55
3:E:70:ALA:HB2	3:E:161:VAL:HG22	1.89	0.55
1:A:86:LEU:HB3	1:A:89:LEU:HG	1.88	0.55
1:B:199:HIS:HB2	1:B:223:HIS:CE1	2.42	0.55
1:B:61:PRO:CG	1:B:64:LEU:HD22	2.37	0.55
1:B:471:ILE:HG21	1:B:541:CYS:SG	2.46	0.55
3:E:162:VAL:HA	6:E:309:HOH:O	2.05	0.55
1:B:61:PRO:HG2	1:B:86:LEU:HD11	1.88	0.55
1:B:85:PRO:C	1:B:86:LEU:HG	2.33	0.54
3:F:82:LEU:HB2	3:F:186:ILE:HD13	1.89	0.54
3:F:141:ILE:HG13	3:F:147:ALA:HB3	1.89	0.54
1:A:254:ARG:HD3	6:A:754:HOH:O	2.06	0.54
2:M:128:ALA:O	2:M:130:PRO:HD3	2.06	0.54
1:A:442:LEU:HD21	1:A:445:LEU:HD13	1.88	0.54
1:A:446:THR:HA	1:A:468:LEU:HA	1.90	0.54
1:B:195:LEU:N	1:B:195:LEU:HD23	2.22	0.54
1:B:64:LEU:HD21	1:B:86:LEU:HD13	1.90	0.54
1:B:265:HIS:HD2	1:B:266:SER:OG	1.90	0.54
3:E:45:LYS:HB3	3:E:66:GLU:OE2	2.07	0.54
3:F:184:VAL:CG1	3:F:185:ARG:N	2.71	0.54
3:F:52:PRO:C	3:F:54:LYS:H	2.16	0.53
1:B:456:LEU:O	1:B:459:LEU:HB2	2.09	0.53
1:B:252:ALA:HB1	6:B:727:HOH:O	2.09	0.53
1:A:59:GLU:O	1:A:60:LEU:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:LEU:CD1	1:A:403:LEU:C	2.82	0.53
1:A:410:ILE:CG2	1:A:432:ASN:HB2	2.37	0.53
1:A:429:LEU:O	1:A:432:ASN:HB3	2.09	0.53
1:B:403:LEU:CD1	1:B:403:LEU:C	2.82	0.52
3:E:79:GLU:HB3	3:E:185:ARG:NH2	2.23	0.52
1:B:411:ALA:HB2	1:B:433:LEU:HD11	1.91	0.52
1:B:432:ASN:O	1:B:453:ASN:OD1	2.28	0.52
1:A:435:SER:HB3	1:A:456:LEU:HD12	1.90	0.52
1:A:58:SER:O	1:A:60:LEU:O	2.28	0.52
1:A:265:HIS:HD2	1:A:266:SER:OG	1.92	0.52
1:B:336:THR:HG22	1:B:360:SER:HB3	1.91	0.52
1:A:395:GLN:O	1:A:396:GLN:HB2	2.09	0.52
1:A:55:LEU:O	1:A:56:GLY:C	2.51	0.51
1:A:127:ARG:CD	6:A:744:HOH:O	2.58	0.51
1:A:411:ALA:O	1:A:434:LEU:HD23	2.09	0.51
1:A:468:LEU:CD2	1:A:471:ILE:HD11	2.38	0.51
1:B:400:LEU:C	1:B:400:LEU:HD23	2.35	0.51
3:E:82:LEU:HB2	3:E:186:ILE:HD13	1.91	0.51
3:E:140:ASP:C	3:E:140:ASP:OD1	2.52	0.51
1:A:118:VAL:HG22	1:A:142:SER:HB2	1.92	0.51
2:M:119:TYR:HB3	2:M:142:CYS:HB2	1.92	0.51
1:A:435:SER:HB3	1:A:456:LEU:HA	1.93	0.51
3:F:65:LEU:HB2	3:F:168:ASP:HB3	1.93	0.51
1:A:414:HIS:CB	1:A:415:PRO:HD2	2.34	0.51
1:B:61:PRO:HB3	1:B:62:SER:C	2.35	0.51
3:F:96:ASP:OD2	3:F:132:ARG:HG3	2.11	0.51
1:A:459:LEU:HG	1:A:478:GLN:HB2	1.92	0.51
1:B:370:PHE:O	1:B:397:LEU:HD21	2.11	0.50
3:F:140:ASP:OD1	3:F:140:ASP:C	2.54	0.50
1:B:242:ASN:ND2	1:B:265:HIS:H	2.10	0.50
1:B:448:LEU:HB3	1:B:471:ILE:HD12	1.92	0.50
1:A:418:PHE:HA	1:A:421:LEU:HD23	1.92	0.50
1:A:59:GLU:HG2	1:A:83:PRO:CD	2.41	0.50
1:A:442:LEU:HD21	1:A:445:LEU:HD22	1.92	0.50
2:M:61:PHE:CE2	2:M:85:ASP:HB3	2.47	0.50
3:F:135:SER:HB3	3:F:159:TRP:HB3	1.93	0.50
1:B:201:ILE:HG22	1:B:229:CYS:HB2	1.93	0.50
3:E:58:THR:O	3:E:60:LYS:N	2.45	0.50
1:B:462:SER:O	1:B:464:ASN:N	2.41	0.50
3:F:177:TYR:C	3:F:177:TYR:CD1	2.90	0.50
1:A:311:THR:HB	1:A:334:THR:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ASN:C	1:A:418:PHE:N	2.69	0.49
1:A:370:PHE:O	1:A:397:LEU:HD21	2.12	0.49
1:B:60:LEU:HB3	1:B:61:PRO:CD	2.34	0.49
3:F:185:ARG:HD3	3:F:186:ILE:N	2.27	0.49
1:A:63:ASN:H	1:A:63:ASN:ND2	2.09	0.49
1:B:82:LEU:HG	1:B:106:PRO:HG3	1.94	0.49
1:B:242:ASN:HD22	1:B:265:HIS:H	1.61	0.48
1:B:311:THR:HB	1:B:334:THR:HB	1.94	0.48
2:P:56:CYS:HB3	6:P:203:HOH:O	2.13	0.48
1:A:469:LYS:C	1:A:539:VAL:HG13	2.38	0.48
2:P:69:ILE:CG2	3:F:82:LEU:O	2.62	0.48
1:A:59:GLU:HG2	1:A:83:PRO:HG2	1.96	0.48
1:A:247:ASP:HB2	6:A:721:HOH:O	2.13	0.48
1:A:432:ASN:OD1	1:A:453:ASN:HB3	2.14	0.48
2:P:61:PHE:CE2	2:P:85:ASP:HB3	2.47	0.48
3:E:190:GLU:O	3:E:191:PRO:O	2.30	0.48
1:A:201:ILE:HG22	1:A:229:CYS:HB2	1.94	0.48
1:A:96:ARG:HA	1:A:120:MET:HB2	1.95	0.48
1:B:450:LEU:CD1	1:B:453:ASN:ND2	2.61	0.48
2:P:75:CYS:CB	6:P:203:HOH:O	2.52	0.48
1:A:269:ILE:H	1:A:291:ASN:HD22	1.62	0.48
1:A:343:LEU:C	6:A:735:HOH:O	2.57	0.48
1:A:360:SER:HB3	1:A:361:TYR:CD1	2.48	0.48
1:B:459:LEU:HD13	1:B:475:TYR:HB2	1.95	0.48
1:A:171:ASP:HA	1:A:195:LEU:O	2.14	0.48
1:A:322:PRO:HB3	6:A:733:HOH:O	2.12	0.47
1:A:59:GLU:CG	1:A:83:PRO:HG2	2.44	0.47
3:E:97:ASP:HB3	3:E:99:LEU:CD1	2.44	0.47
3:F:177:TYR:C	3:F:177:TYR:HD1	2.22	0.47
1:B:403:LEU:HD11	1:B:405:LEU:HG	1.96	0.47
1:A:459:LEU:CD2	1:A:475:TYR:HD1	2.28	0.47
1:B:51:ASP:C	1:B:51:ASP:OD1	2.56	0.47
1:B:204:TYR:OH	1:B:228:LYS:HE2	2.15	0.47
1:B:436:SER:HA	1:B:437:PHE:HA	1.80	0.47
1:B:457:GLN:O	1:B:459:LEU:N	2.40	0.47
2:M:69:ILE:HB	3:E:181:LYS:HB2	1.97	0.47
2:P:120:LEU:O	2:P:142:CYS:HA	2.14	0.47
3:F:181:LYS:HA	3:F:182:ALA:CB	2.32	0.47
3:E:175:PHE:CZ	3:E:182:ALA:HB3	2.50	0.47
1:A:127:ARG:HD3	6:A:744:HOH:O	2.13	0.47
1:A:400:LEU:HD23	1:A:400:LEU:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:70:ALA:N	6:E:309:HOH:O	2.48	0.47
3:E:182:ALA:O	3:E:184:VAL:HG22	2.15	0.47
3:F:90:LEU:HA	3:F:128:MET:CE	2.45	0.47
1:B:122:GLN:HG3	1:B:144:ARG:HB3	1.97	0.47
1:B:403:LEU:C	1:B:403:LEU:HD12	2.40	0.47
1:B:275:LYS:O	1:B:278:VAL:HG22	2.14	0.46
1:A:242:ASN:ND2	1:A:265:HIS:H	2.13	0.46
3:E:189:LYS:O	3:E:190:GLU:O	2.33	0.46
1:B:425:ILE:HG22	1:B:426:LYS:HG2	1.98	0.46
1:A:122:GLN:HG3	1:A:144:ARG:HB3	1.98	0.46
1:A:146:ASP:CB	1:A:170:ASP:HB3	2.44	0.46
1:B:96:ARG:HA	1:B:120:MET:HB2	1.98	0.46
1:B:298:ARG:HE	1:B:320:GLU:HG2	1.81	0.46
3:E:49:ARG:NH1	3:E:61:LEU:HB3	2.29	0.46
3:E:70:ALA:CB	3:E:161:VAL:HG22	2.45	0.46
3:F:48:ILE:HB	3:F:65:LEU:HD22	1.96	0.46
1:A:403:LEU:C	1:A:403:LEU:HD12	2.41	0.46
1:B:143:LEU:O	1:B:168:TRP:HD1	1.97	0.46
1:B:269:ILE:H	1:B:291:ASN:HD22	1.64	0.46
1:B:299:SER:O	1:B:300:ALA:C	2.57	0.46
3:E:90:LEU:HA	3:E:128:MET:CE	2.46	0.46
1:A:336:THR:HG22	1:A:360:SER:HB2	1.98	0.46
1:A:457:GLN:O	1:A:459:LEU:N	2.44	0.46
2:P:48:SER:OG	3:F:110:GLU:OE2	2.23	0.46
3:E:177:TYR:O	3:E:178:LYS:C	2.58	0.46
1:A:459:LEU:HD23	1:A:475:TYR:HD1	1.81	0.46
2:P:69:ILE:N	2:P:69:ILE:HD13	2.31	0.46
3:E:135:SER:O	3:E:160:PRO:HD2	2.16	0.46
1:A:410:ILE:HG23	1:A:433:LEU:H	1.81	0.46
1:A:416:ASN:ND2	1:A:441:GLY:HA3	2.31	0.46
1:B:457:GLN:C	1:B:459:LEU:N	2.73	0.46
1:B:168:TRP:CD1	1:B:168:TRP:N	2.84	0.46
2:P:99:ILE:HG23	2:P:102:CYS:CB	2.46	0.46
1:B:154:PRO:HA	1:B:155:PRO:HD3	1.83	0.45
1:A:200:HIS:HB3	6:A:712:HOH:O	2.15	0.45
2:M:70:ARG:CG	3:E:181:LYS:HB3	2.45	0.45
2:P:68:ASP:OD2	3:F:178:LYS:HB3	2.16	0.45
1:A:51:ASP:OD1	1:A:53:SER:HB3	2.17	0.45
3:E:93:ALA:O	3:E:94:SER:O	2.34	0.45
1:A:275:LYS:O	1:A:278:VAL:HG22	2.15	0.45
1:A:425:ILE:HG22	1:A:426:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ILE:HG21	1:A:418:PHE:HE2	1.82	0.45
1:B:478:GLN:HA	1:B:481:ALA:HB3	1.98	0.45
1:B:335:LEU:C	1:B:335:LEU:CD2	2.90	0.45
3:E:72:VAL:HG12	3:E:157:LEU:HD12	1.98	0.45
3:F:184:VAL:CG1	3:F:185:ARG:H	2.30	0.45
1:A:411:ALA:HA	1:A:433:LEU:O	2.17	0.45
3:F:117:ARG:CZ	3:F:117:ARG:HB3	2.47	0.45
1:A:413:ILE:HG21	1:A:418:PHE:CE2	2.52	0.45
1:A:448:LEU:HB3	1:A:471:ILE:CD1	2.46	0.45
1:B:461:SER:O	1:B:461:SER:OG	2.20	0.45
1:B:82:LEU:N	1:B:83:PRO:CD	2.80	0.45
3:F:128:MET:HE3	3:F:132:ARG:CZ	2.46	0.45
1:A:199:HIS:HB2	1:A:223:HIS:HE1	1.78	0.45
3:E:190:GLU:HB2	3:E:191:PRO:HD3	1.98	0.45
1:A:403:LEU:HD11	1:A:405:LEU:HG	1.98	0.44
1:A:471:ILE:CG2	1:A:472:GLU:N	2.80	0.44
1:A:459:LEU:HD22	1:A:474:PRO:HG2	2.00	0.44
1:B:106:PRO:HD2	1:B:109:ALA:HB2	1.99	0.44
1:A:341:SER:HA	1:A:363:LEU:O	2.17	0.44
1:A:342:SER:C	6:A:735:HOH:O	2.61	0.44
2:M:50:VAL:HG11	3:E:108:LYS:HB2	1.99	0.44
1:B:242:ASN:HD22	1:B:265:HIS:N	2.16	0.44
1:B:457:GLN:C	1:B:459:LEU:H	2.24	0.44
1:B:61:PRO:HB3	1:B:62:SER:CA	2.48	0.43
1:B:84:ASN:ND2	1:B:85:PRO:O	2.50	0.43
1:B:456:LEU:HD23	1:B:474:PRO:HG2	1.99	0.43
3:F:56:ASP:N	3:F:56:ASP:OD1	2.50	0.43
3:F:90:LEU:HA	3:F:128:MET:HE2	1.99	0.43
1:B:118:VAL:HG22	1:B:142:SER:HB2	2.00	0.43
3:E:175:PHE:CE2	3:E:182:ALA:HB3	2.53	0.43
1:B:351:LEU:N	1:B:352:PRO:HD2	2.34	0.43
2:P:88:ASN:HB3	2:P:91:MET:O	2.18	0.43
3:E:90:LEU:HA	3:E:128:MET:HE2	2.01	0.43
3:F:54:LYS:CA	3:F:55:MET:CB	2.94	0.43
2:M:50:VAL:HG11	3:E:108:LYS:CB	2.49	0.43
1:A:388:GLU:HB3	6:A:738:HOH:O	2.17	0.43
1:A:442:LEU:CD2	1:A:445:LEU:HD13	2.48	0.43
1:B:171:ASP:HA	1:B:195:LEU:O	2.19	0.43
1:B:414:HIS:CG	1:B:415:PRO:HD2	2.54	0.43
1:B:459:LEU:HD12	1:B:474:PRO:HG2	1.99	0.43
1:A:59:GLU:C	1:A:60:LEU:O	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ILE:CG2	1:A:439:ILE:HD12	2.48	0.43
1:B:52:CYS:HB2	1:B:73:LEU:HD12	2.00	0.43
3:E:74:GLU:C	3:E:75:ILE:HG13	2.43	0.43
1:B:335:LEU:HD23	1:B:335:LEU:O	2.19	0.43
1:B:418:PHE:HD1	1:B:418:PHE:N	2.17	0.43
1:B:438:PRO:C	1:B:439:ILE:CG2	2.92	0.43
2:P:99:ILE:HG23	2:P:102:CYS:HB2	2.01	0.42
1:B:146:ASP:CB	1:B:170:ASP:HB3	2.48	0.42
1:B:442:LEU:HD11	1:B:445:LEU:CD2	2.49	0.42
1:A:51:ASP:OD1	1:A:51:ASP:C	2.62	0.42
1:B:84:ASN:ND2	1:B:86:LEU:HD11	2.34	0.42
1:B:435:SER:CB	1:B:455:ALA:HB3	2.50	0.42
3:E:93:ALA:C	3:E:94:SER:O	2.63	0.42
1:B:371:SER:N	6:B:745:HOH:O	2.53	0.42
1:B:442:LEU:HD11	1:B:445:LEU:HD22	2.01	0.42
1:A:52:CYS:HB2	1:A:73:LEU:HD12	2.01	0.42
1:A:333:LEU:C	1:A:333:LEU:CD2	2.92	0.42
1:B:75:MET:CE	1:B:75:MET:HA	2.49	0.42
2:P:69:ILE:HG22	3:F:83:MET:HA	2.01	0.42
1:A:351:LEU:N	1:A:352:PRO:HD2	2.35	0.42
1:A:265:HIS:HB2	1:A:289:TYR:O	2.20	0.42
1:A:266:SER:HA	1:A:290:ASP:O	2.20	0.42
1:B:265:HIS:HB2	1:B:289:TYR:O	2.20	0.42
2:P:124:ARG:HG3	2:P:126:TYR:CZ	2.55	0.42
1:A:459:LEU:HD11	1:A:473:MET:CE	2.50	0.42
1:B:438:PRO:CB	1:B:439:ILE:HG22	2.36	0.42
3:F:175:PHE:HA	3:F:179:ASN:HD21	1.84	0.42
1:A:82:LEU:HD13	1:A:84:ASN:HB2	2.02	0.41
2:M:42:LYS:HB3	2:M:42:LYS:HE2	1.74	0.41
3:E:185:ARG:C	3:E:186:ILE:HD12	2.45	0.41
1:A:123:ASN:HA	1:A:147:ALA:O	2.20	0.41
1:A:394:PHE:O	1:A:421:LEU:HD11	2.19	0.41
1:B:418:PHE:N	1:B:418:PHE:CD1	2.87	0.41
1:B:479:CYS:SG	1:B:542:SER:N	2.93	0.41
1:A:373:CYS:O	1:A:376:LEU:HB2	2.20	0.41
1:A:390:LYS:HA	1:A:414:HIS:CG	2.54	0.41
1:A:408:ASN:C	1:A:410:ILE:HG22	2.44	0.41
1:A:409:LYS:HA	6:F:301:HOH:O	2.20	0.41
1:A:459:LEU:HD23	1:A:475:TYR:CD1	2.55	0.41
2:P:60:LEU:HD22	2:P:77:PRO:HA	2.02	0.41
2:P:116:GLU:HA	2:P:117:GLY:HA2	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PRO:HA	1:A:155:PRO:HD3	1.83	0.41
1:B:61:PRO:CB	1:B:62:SER:CA	2.98	0.41
1:B:341:SER:HA	1:B:363:LEU:O	2.20	0.41
3:F:185:ARG:C	3:F:186:ILE:HD12	2.46	0.41
1:A:410:ILE:HG23	1:A:410:ILE:O	2.21	0.41
3:F:178:LYS:O	3:F:182:ALA:HB2	2.21	0.41
1:A:144:ARG:HG2	1:A:168:TRP:CE3	2.55	0.41
1:A:415:PRO:O	1:A:439:ILE:CD1	2.69	0.41
1:A:457:GLN:C	1:A:459:LEU:N	2.79	0.41
1:B:61:PRO:CG	1:B:64:LEU:HD13	2.49	0.41
1:B:333:LEU:C	1:B:333:LEU:CD2	2.88	0.41
1:A:414:HIS:HB3	1:A:415:PRO:CD	2.35	0.41
1:A:468:LEU:HD21	1:A:471:ILE:CD1	2.48	0.41
1:B:60:LEU:C	1:B:60:LEU:CD2	2.92	0.41
1:B:358:ASP:OD1	1:B:358:ASP:C	2.63	0.41
1:B:373:CYS:O	1:B:376:LEU:HB2	2.21	0.41
1:B:378:LYS:HG3	1:B:402:SER:HB3	2.02	0.41
2:M:116:GLU:HA	2:M:117:GLY:HA2	1.78	0.41
1:A:63:ASN:ND2	1:A:63:ASN:N	2.69	0.40
1:B:228:LYS:O	1:B:229:CYS:C	2.62	0.40
1:B:266:SER:HA	1:B:290:ASP:O	2.21	0.40
1:B:459:LEU:HD22	1:B:477:TYR:CE1	2.56	0.40
3:F:183:HIS:C	3:F:184:VAL:HG23	2.46	0.40
1:A:145:LEU:HB2	1:A:169:LEU:HD13	2.04	0.40
1:A:461:SER:O	1:A:478:GLN:NE2	2.54	0.40
1:B:192:THR:CG2	1:B:216:HIS:HB2	2.44	0.40
1:A:82:LEU:HD13	1:A:84:ASN:CB	2.52	0.40
1:A:134:LEU:O	1:A:161:LEU:HD21	2.21	0.40
1:A:299:SER:O	1:A:300:ALA:C	2.63	0.40
2:P:50:VAL:O	2:P:70:ARG:NH1	2.52	0.40
3:E:69:PHE:CZ	3:E:188:LEU:HD21	2.56	0.40
1:B:340:ILE:H	1:B:362:ASN:HD22	1.70	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	458/531 (86%)	389 (85%)	58 (13%)	11 (2%)	4	8
1	B	459/531 (86%)	392 (85%)	56 (12%)	11 (2%)	4	8
2	M	94/115 (82%)	82 (87%)	10 (11%)	2 (2%)	5	9
2	P	91/115 (79%)	80 (88%)	8 (9%)	3 (3%)	3	4
3	E	147/160 (92%)	120 (82%)	19 (13%)	8 (5%)	1	1
3	F	146/160 (91%)	119 (82%)	19 (13%)	8 (6%)	1	1
All	All	1395/1612 (86%)	1182 (85%)	170 (12%)	43 (3%)	3	5

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	ILE
1	A	430	SER
1	B	84	ASN
1	B	430	SER
1	B	438	PRO
2	M	142	CYS
3	E	94	SER
3	E	166	GLY
3	E	190	GLU
3	F	55	MET
3	F	166	GLY
1	A	53	SER
1	A	170	ASP
1	B	458	SER
3	E	59	GLY
3	E	75	ILE
3	F	181	LYS
1	A	31	PRO
1	A	417	ALA
1	A	458	SER
1	B	170	ASP
1	B	435	SER
1	B	463	GLU
2	P	100	GLU
3	E	191	PRO
1	A	83	PRO

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Mol	Chain	Res	Type
1	A	437	PHE
1	A	451	THR
1	B	543	PRO
2	M	100	GLU
2	P	68	ASP
3	E	178	LYS
3	F	133	GLY
1	A	415	PRO
1	B	37	HIS
2	P	42	LYS
3	F	53	LEU
3	F	60	LYS
3	F	178	LYS
1	B	85	PRO
1	B	439	ILE
3	F	156	GLY
3	E	156	GLY

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	418/476 (88%)	354 (85%)	64 (15%)	3	5
1	B	419/476 (88%)	351 (84%)	68 (16%)	2	4
2	M	87/95 (92%)	76 (87%)	11 (13%)	4	9
2	P	83/95 (87%)	72 (87%)	11 (13%)	4	8
3	E	124/130 (95%)	104 (84%)	20 (16%)	2	4
3	F	123/130 (95%)	98 (80%)	25 (20%)	1	2
All	All	1254/1402 (89%)	1055 (84%)	199 (16%)	2	5

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	HIS

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Mol	Chain	Res	Type
1	A	53	SER
1	A	55	LEU
1	A	58	SER
1	A	63	ASN
1	A	73	LEU
1	A	81	LEU
1	A	82	LEU
1	A	96	ARG
1	A	113	LEU
1	A	122	GLN
1	A	127	ARG
1	A	146	ASP
1	A	169	LEU
1	A	176	GLU
1	A	192	THR
1	A	221	ARG
1	A	235	SER
1	A	246	LEU
1	A	247	ASP
1	A	251	THR
1	A	255	THR
1	A	256	LEU
1	A	266	SER
1	A	275	LYS
1	A	278	VAL
1	A	285	THR
1	A	299	SER
1	A	304	LEU
1	A	307	LEU
1	A	310	LEU
1	A	311	THR
1	A	313	ASN
1	A	316	SER
1	A	319	THR
1	A	330	LEU
1	A	335	LEU
1	A	365	GLU
1	A	367	LEU
1	A	389	ILE
1	A	390	LYS
1	A	392	ASP
1	A	398	LEU

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Mol	Chain	Res	Type
1	A	403	LEU
1	A	425	ILE
1	A	427	LEU
1	A	429	LEU
1	A	435	SER
1	A	442	LEU
1	A	443	HIS
1	A	445	LEU
1	A	448	LEU
1	A	449	LYS
1	A	454	HIS
1	A	456	LEU
1	A	457	GLN
1	A	459	LEU
1	A	463	GLU
1	A	464	ASN
1	A	468	LEU
1	A	470	VAL
1	A	479	CYS
1	A	538	SER
1	A	541	CYS
1	B	55	LEU
1	B	59	GLU
1	B	62	SER
1	B	64	LEU
1	B	73	LEU
1	B	75	MET
1	B	77	ASN
1	B	81	LEU
1	B	82	LEU
1	B	92	LEU
1	B	96	ARG
1	B	113	LEU
1	B	122	GLN
1	B	146	ASP
1	B	156	SER
1	B	168	TRP
1	B	176	GLU
1	B	192	THR
1	B	195	LEU
1	B	221	ARG
1	B	227	LYS

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Mol	Chain	Res	Type
1	B	228	LYS
1	B	235	SER
1	B	246	LEU
1	B	251	THR
1	B	255	THR
1	B	256	LEU
1	B	266	SER
1	B	278	VAL
1	B	285	THR
1	B	304	LEU
1	B	307	LEU
1	B	310	LEU
1	B	311	THR
1	B	316	SER
1	B	319	THR
1	B	330	LEU
1	B	363	LEU
1	B	365	GLU
1	B	367	LEU
1	B	389	ILE
1	B	390	LYS
1	B	391	VAL
1	B	392	ASP
1	B	398	LEU
1	B	403	LEU
1	B	412	ILE
1	B	421	LEU
1	B	425	ILE
1	B	427	LEU
1	B	429	LEU
1	B	432	ASN
1	B	436	SER
1	B	440	THR
1	B	442	LEU
1	B	445	LEU
1	B	448	LEU
1	B	449	LYS
1	B	450	LEU
1	B	454	HIS
1	B	456	LEU
1	B	457	GLN
1	B	463	GLU

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Mol	Chain	Res	Type
1	B	464	ASN
1	B	468	LEU
1	B	469	LYS
1	B	479	CYS
1	B	482	PHE
2	M	40	CYS
2	M	42	LYS
2	M	72	VAL
2	M	76	LEU
2	M	81	PRO
2	M	85	ASP
2	M	100	GLU
2	M	112	THR
2	M	115	LYS
2	M	124	ARG
2	M	131	GLU
2	P	40	CYS
2	P	69	ILE
2	P	76	LEU
2	P	81	PRO
2	P	85	ASP
2	P	88	ASN
2	P	99	ILE
2	P	100	GLU
2	P	112	THR
2	P	115	LYS
2	P	131	GLU
3	E	56	ASP
3	E	63	LEU
3	E	65	LEU
3	E	66	GLU
3	E	75	ILE
3	E	76	THR
3	E	99	LEU
3	E	108	LYS
3	E	145	ARG
3	E	155	LEU
3	E	158	THR
3	E	161	VAL
3	E	164	ILE
3	E	165	TRP
3	E	167	ASN

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Mol	Chain	Res	Type
3	E	180	GLN
3	E	181	LYS
3	E	184	VAL
3	E	185	ARG
3	E	189	LYS
3	F	54	LYS
3	F	55	MET
3	F	56	ASP
3	F	61	LEU
3	F	63	LEU
3	F	65	LEU
3	F	66	GLU
3	F	72	VAL
3	F	84	GLN
3	F	92	ASN
3	F	99	LEU
3	F	108	LYS
3	F	114	ARG
3	F	117	ARG
3	F	155	LEU
3	F	158	THR
3	F	161	VAL
3	F	164	ILE
3	F	167	ASN
3	F	176	VAL
3	F	177	TYR
3	F	178	LYS
3	F	183	HIS
3	F	185	ARG
3	F	190	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	76	ASN
1	A	141	GLN
1	A	149	HIS
1	A	162	HIS
1	A	166	HIS
1	A	200	HIS
1	A	216	HIS

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Mol	Chain	Res	Type
1	A	218	HIS
1	A	219	ASN
1	A	223	HIS
1	A	242	ASN
1	A	265	HIS
1	A	291	ASN
1	A	294	GLN
1	A	302	GLN
1	A	329	ASN
1	A	350	GLN
1	A	355	GLN
1	A	362	ASN
1	A	478	GLN
1	A	537	HIS
1	B	84	ASN
1	B	141	GLN
1	B	149	HIS
1	B	162	HIS
1	B	166	HIS
1	B	180	GLN
1	B	199	HIS
1	B	200	HIS
1	B	216	HIS
1	B	218	HIS
1	B	219	ASN
1	B	223	HIS
1	B	242	ASN
1	B	265	HIS
1	B	291	ASN
1	B	302	GLN
1	B	329	ASN
1	B	350	GLN
1	B	355	GLN
1	B	362	ASN
1	B	416	ASN
1	B	464	ASN
1	B	478	GLN
2	M	51	ASN
2	M	121	HIS
2	P	51	ASN
2	P	88	ASN
2	P	121	HIS

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Mol	Chain	Res	Type
3	E	183	HIS
3	F	180	GLN

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	602	1	14,14,15	0.88	0	17,19,21	1.93	5 (29%)
4	NAG	A	601	1	14,14,15	0.79	1 (7%)	17,19,21	2.12	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	602	1	-	0/6/23/26	0/1/1/1
4	NAG	A	601	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	C1-C2	2.41	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	C4-C3-C2	-5.33	103.20	111.02
4	B	602	NAG	C1-O5-C5	-4.71	105.87	112.19
4	A	601	NAG	C1-C2-N2	4.12	116.93	110.43
4	A	601	NAG	C1-O5-C5	3.67	117.10	112.19
4	B	602	NAG	O5-C5-C6	2.90	113.32	107.66
4	B	602	NAG	C6-C5-C4	2.89	120.11	113.02
4	B	602	NAG	O5-C1-C2	-2.47	107.47	111.29
4	B	602	NAG	O7-C7-N2	2.11	125.70	121.98
4	A	601	NAG	O3-C3-C2	2.09	113.74	109.40
4	A	601	NAG	O4-C4-C5	2.01	114.28	109.32

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	C1-C2-N2-C7
4	A	601	NAG	C4-C5-C6-O6
4	A	601	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	461/531 (86%)	0.66	66 (14%) 6 5	18, 66, 145, 192	1 (0%)
1	B	463/531 (87%)	0.37	39 (8%) 17 15	23, 52, 120, 159	0
2	M	98/115 (85%)	0.66	16 (16%) 4 3	32, 59, 110, 123	0
2	P	94/115 (81%)	1.22	24 (25%) 1 1	31, 83, 113, 125	0
3	E	149/160 (93%)	0.93	23 (15%) 5 4	40, 79, 132, 151	0
3	F	148/160 (92%)	1.99	69 (46%) 0 0	78, 133, 169, 200	0
All	All	1413/1612 (87%)	0.77	237 (16%) 4 3	18, 68, 148, 200	1 (0%)

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	LEU	9.5
1	B	81	LEU	9.2
1	B	437	PHE	6.4
3	F	176	VAL	5.7
3	F	61	LEU	5.4
3	F	53	LEU	5.4
1	A	60	LEU	5.4
3	F	175	PHE	5.3
3	E	191	PRO	5.2
1	B	84	ASN	5.0
3	E	192	PRO	4.9
2	P	132	GLY	4.9
2	P	50	VAL	4.8
2	M	117	GLY	4.6
1	A	477	TYR	4.6
3	F	63	LEU	4.3
2	P	119	TYR	4.3
1	A	453	ASN	4.2
3	F	129	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
3	E	61	LEU	4.0
2	M	143	SER	4.0
2	M	100	GLU	4.0
1	A	394	PHE	3.9
3	F	85	SER	3.9
3	F	51	ILE	3.8
3	F	178	LYS	3.8
3	F	47	ILE	3.8
1	A	415	PRO	3.8
3	F	161	VAL	3.7
3	F	164	ILE	3.7
1	B	439	ILE	3.7
1	A	86	LEU	3.7
2	P	130	PRO	3.6
3	E	178	LYS	3.6
3	F	55	MET	3.6
2	M	130	PRO	3.6
3	F	165	TRP	3.5
1	A	370	PHE	3.5
1	B	61	PRO	3.5
3	F	191	PRO	3.5
3	F	158	THR	3.5
1	A	411	ALA	3.5
1	B	539	VAL	3.5
1	B	440	THR	3.4
3	E	184	VAL	3.4
3	E	57	PRO	3.4
1	B	59	GLU	3.4
1	A	429	LEU	3.4
3	F	155	LEU	3.4
1	A	432	ASN	3.4
3	F	159	TRP	3.4
3	F	138	LEU	3.4
1	A	410	ILE	3.4
1	A	455	ALA	3.4
2	P	114	CYS	3.3
1	A	460	ILE	3.3
2	P	117	GLY	3.3
1	A	437	PHE	3.3
2	M	140	MET	3.3
3	F	136	ALA	3.3
1	B	436	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	539	VAL	3.3
3	F	188	LEU	3.2
1	B	441	GLY	3.2
3	E	181	LYS	3.2
1	B	482	PHE	3.2
3	F	139	PHE	3.2
1	B	465	PHE	3.2
2	P	43	GLY	3.2
1	B	459	LEU	3.1
3	F	169	ALA	3.1
1	B	476	ALA	3.1
1	A	456	LEU	3.1
3	F	46	ALA	3.1
3	F	173	MET	3.0
1	B	443	HIS	3.0
1	A	364	LEU	3.0
1	A	417	ALA	3.0
3	F	58	THR	3.0
1	A	442	LEU	3.0
1	B	433	LEU	3.0
3	F	93	ALA	3.0
1	B	480	CYS	3.0
3	F	183	HIS	2.9
1	B	543	PRO	2.9
2	P	142	CYS	2.9
1	A	412	ILE	2.9
3	E	47	ILE	2.9
1	A	393	THR	2.9
1	B	62	SER	2.9
1	B	546	GLY	2.9
3	F	74	GLU	2.9
1	A	480	CYS	2.9
1	A	438	PRO	2.9
3	F	163	LEU	2.9
3	F	141	ILE	2.9
2	M	139	THR	2.9
3	E	44	GLN	2.9
3	F	186	ILE	2.8
2	M	118	LEU	2.8
3	F	108	LYS	2.8
3	F	105	SER	2.8
1	A	391	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	M	142	CYS	2.8
2	M	141	GLU	2.8
1	A	443	HIS	2.8
1	B	475	TYR	2.8
3	E	59	GLY	2.8
1	A	45	ARG	2.8
2	M	132	GLY	2.8
3	F	62	ASN	2.8
3	F	171	LYS	2.8
3	F	166	GLY	2.7
3	F	189	LYS	2.7
3	E	190	GLU	2.7
2	M	127	PRO	2.7
3	E	179	ASN	2.7
1	B	458	SER	2.7
3	E	165	TRP	2.7
1	B	545	PRO	2.7
2	P	74	VAL	2.7
3	F	99	LEU	2.7
1	A	365	GLU	2.7
1	A	82	LEU	2.6
1	B	442	LEU	2.6
1	A	59	GLU	2.6
3	F	190	GLU	2.6
2	P	71	GLN	2.6
3	F	75	ILE	2.6
1	A	450	LEU	2.6
2	P	59	LYS	2.6
3	F	110	GLU	2.6
3	E	60	LYS	2.6
1	A	31	PRO	2.5
1	A	30	GLY	2.5
1	B	450	LEU	2.5
1	B	419	SER	2.5
3	F	76	THR	2.5
1	A	418	PHE	2.5
3	E	175	PHE	2.5
1	A	457	GLN	2.5
1	B	462	SER	2.5
1	A	452	GLY	2.5
3	F	102	GLY	2.5
1	A	459	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	183	HIS	2.5
1	A	448	LEU	2.4
3	F	172	LEU	2.4
3	E	62	ASN	2.4
3	E	70	ALA	2.4
3	F	59	GLY	2.4
3	F	80	GLY	2.4
2	P	69	ILE	2.4
1	B	60	LEU	2.4
2	P	109	ASN	2.4
3	F	179	ASN	2.4
2	P	128	ALA	2.4
2	M	131	GLU	2.4
1	A	78	ILE	2.4
1	B	391	VAL	2.4
2	M	128	ALA	2.4
1	A	389	ILE	2.4
1	A	481	ALA	2.4
3	F	57	PRO	2.3
3	F	101	PRO	2.3
3	E	164	ILE	2.3
2	P	98	LYS	2.3
2	P	127	PRO	2.3
1	A	483	GLY	2.3
2	P	54	LEU	2.3
3	F	83	MET	2.3
3	F	81	LYS	2.3
3	F	177	TYR	2.3
3	F	79	GLU	2.3
1	A	476	ALA	2.3
3	F	160	PRO	2.3
1	A	444	GLY	2.3
1	A	414	HIS	2.3
1	A	405	LEU	2.3
3	E	53	LEU	2.3
3	E	69	PHE	2.3
1	A	368	PRO	2.3
3	E	64	THR	2.3
1	A	33	GLY	2.3
1	A	537	HIS	2.3
1	B	537	HIS	2.3
2	P	72	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	137	VAL	2.3
1	A	85	PRO	2.3
1	A	39	HIS	2.2
1	A	458	SER	2.2
1	B	456	LEU	2.2
2	M	115	LYS	2.2
3	F	135	SER	2.2
2	M	119	TYR	2.2
1	A	446	THR	2.2
1	A	367	LEU	2.2
1	B	79	SER	2.2
1	B	31	PRO	2.2
3	F	50	VAL	2.2
1	A	409	LYS	2.2
1	B	83	PRO	2.2
3	F	107	VAL	2.2
1	A	395	GLN	2.2
1	A	343	LEU	2.2
1	B	448	LEU	2.2
3	F	65	LEU	2.2
3	F	109	LEU	2.2
1	A	386	ILE	2.2
1	B	58	SER	2.2
1	B	418	PHE	2.2
1	A	447	HIS	2.1
3	F	126	ALA	2.1
2	P	70	ARG	2.1
2	P	115	LYS	2.1
2	P	118	LEU	2.1
3	F	111	SER	2.1
2	M	68	ASP	2.1
2	P	40	CYS	2.1
3	E	152	GLN	2.1
3	F	69	PHE	2.1
1	A	403	LEU	2.1
2	P	46	LEU	2.1
1	A	413	ILE	2.1
1	B	460	ILE	2.1
3	F	48	ILE	2.1
1	A	465	PHE	2.0
3	F	148	ALA	2.0
1	A	434	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	F	181	LYS	2.0
3	F	68	VAL	2.0
3	F	54	LYS	2.0
1	A	425	ILE	2.0
1	A	435	SER	2.0
1	A	475	TYR	2.0
1	A	538	SER	2.0
2	P	101	HIS	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
4	NAG	A	601	14/15	0.79	0.12	66,82,88,95	0
4	NAG	B	602	14/15	0.86	0.10	54,60,66,67	0
5	NI	B	601	1/1	0.99	0.02	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.