



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:40 PM EDT

PDB ID : 4YXK / pdb_00004yxk
Title : Crystal structure of Elk prion protein complexed with POM1 FAB
Authors : Baral, P.K.; Swayampakula, M.; James, M.N.G.
Deposited on : 2015-03-23
Resolution : 2.81 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

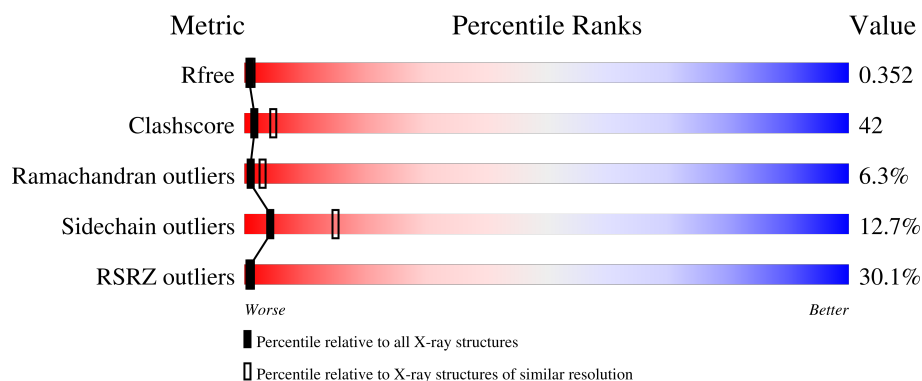
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	135	16% 30% 36% 8% 25%
2	H	218	30% 54% 34% 10%
3	L	213	34% 47% 33% 15% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NA	L	301	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4208 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 Major prion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	S	0	0	0
			840	521	146	165	8			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	MET	-	expression tag	UNP P67986
A	94	GLY	-	expression tag	UNP P67986
A	95	SER	-	expression tag	UNP P67986
A	96	SER	-	expression tag	UNP P67986
A	97	HIS	-	expression tag	UNP P67986
A	98	HIS	-	expression tag	UNP P67986
A	99	HIS	-	expression tag	UNP P67986
A	100	HIS	-	expression tag	UNP P67986
A	101	HIS	-	expression tag	UNP P67986
A	102	HIS	-	expression tag	UNP P67986
A	103	SER	-	expression tag	UNP P67986
A	104	SER	-	expression tag	UNP P67986
A	105	GLY	-	expression tag	UNP P67986
A	106	LEU	-	expression tag	UNP P67986
A	107	VAL	-	expression tag	UNP P67986
A	108	PRO	-	expression tag	UNP P67986
A	109	ARG	-	expression tag	UNP P67986
A	110	GLY	-	expression tag	UNP P67986
A	111	SER	-	expression tag	UNP P67986
A	112	HIS	-	expression tag	UNP P67986
A	113	MET	-	expression tag	UNP P67986
A	114	LEU	-	expression tag	UNP P67986
A	115	GLU	-	expression tag	UNP P67986
A	116	ASP	-	expression tag	UNP P67986
A	117	PRO	-	expression tag	UNP P67986
A	118	HIS	-	expression tag	UNP P67986
A	119	MET	-	expression tag	UNP P67986

- Molecule 2 is a protein called POM1 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1642	1037	265	330	10			

- Molecule 3 is a protein called POM1 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1652	1022	280	345	5			

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Na	0	0
			1	1		

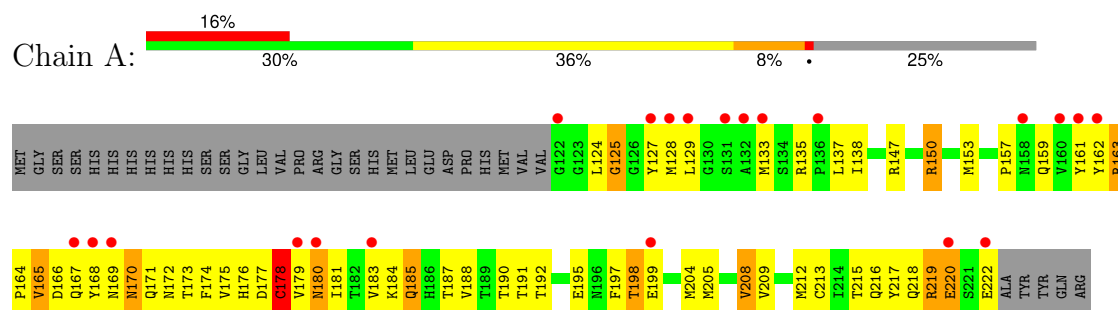
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		
5	H	28	Total	O	0	0
			28	28		
5	L	22	Total	O	0	0
			22	22		

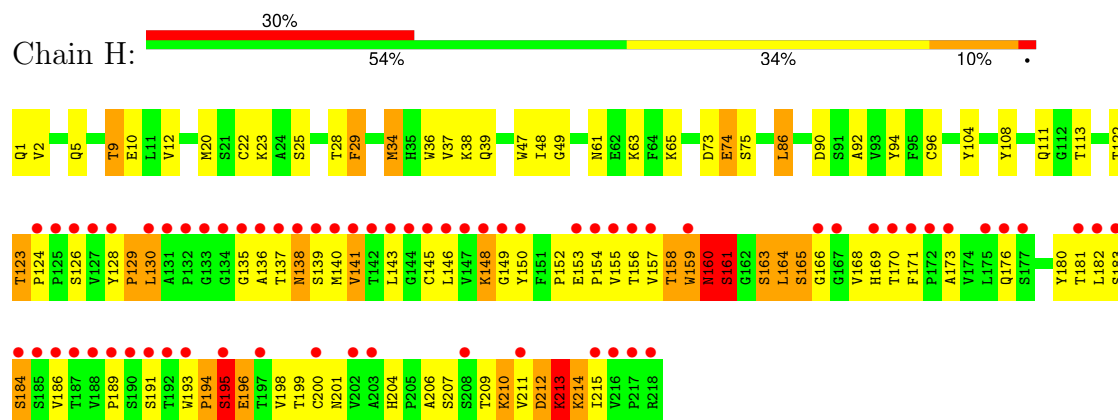
3 Residue-property plots

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.

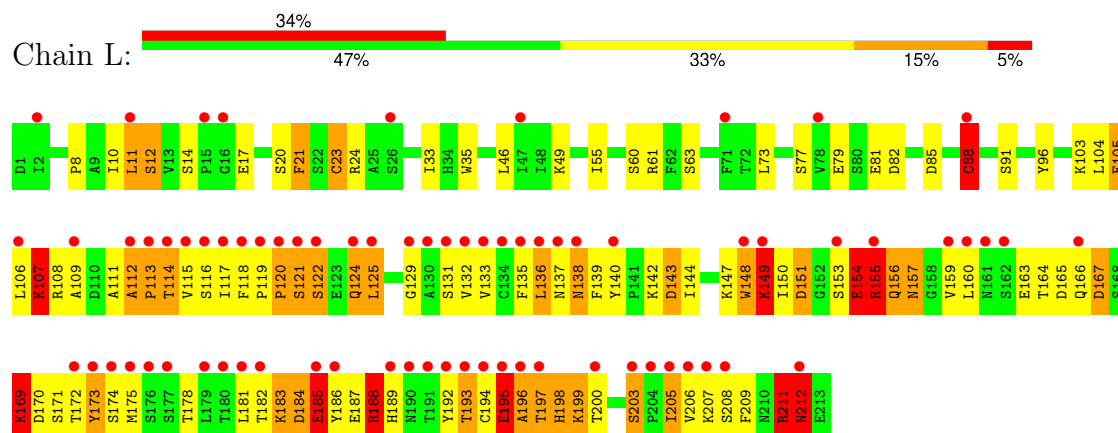
• Molecule 1: Major prion protein



• Molecule 2: POM1 FAB HEAVY CHAIN



• Molecule 3: POM1 FAB LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	84.67Å 105.51Å 76.11Å 90.00° 95.22° 90.00°	Depositor
Resolution (Å)	42.16 – 2.81 42.16 – 2.81	Depositor EDS
% Data completeness (in resolution range)	97.4 (42.16-2.81) 97.6 (42.16-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.300 , 0.353 0.314 , 0.352	Depositor DCC
R_{free} test set	809 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.808	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4208	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.06	0/858	1.30	6/1159 (0.5%)
2	H	1.07	1/1688 (0.1%)	1.53	23/2306 (1.0%)
3	L	0.85	0/1687	1.43	24/2291 (1.0%)
All	All	0.99	1/4233 (0.0%)	1.45	53/5756 (0.9%)

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
3	L	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	37	VAL	CA-C	-6.85	1.44	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	123	THR	CA-C-N	17.82	132.49	119.66
2	H	123	THR	C-N-CA	17.82	132.49	119.66
3	L	196	ALA	N-CA-C	-9.88	96.26	110.59
2	H	156	THR	CA-C-N	-9.58	110.59	123.14
2	H	156	THR	C-N-CA	-9.58	110.59	123.14
2	H	86	LEU	N-CA-C	8.36	122.66	110.28
3	L	105	GLU	N-CA-C	8.27	121.73	109.24
2	H	210	LYS	N-CA-C	8.03	127.89	110.80
3	L	119	PRO	CA-C-N	7.71	129.48	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	119	PRO	C-N-CA	7.71	129.48	119.84
2	H	212	ASP	N-CA-C	7.27	121.29	109.59
3	L	203	SER	CA-C-N	7.24	127.22	119.76
3	L	203	SER	C-N-CA	7.24	127.22	119.76
3	L	113	PRO	N-CA-C	7.17	122.44	111.19
2	H	213	LYS	N-CA-C	-7.10	93.74	107.44
2	H	214	LYS	N-CA-C	7.03	121.14	108.69
2	H	61	ASN	N-CA-C	-6.99	98.22	109.96
3	L	155	ARG	N-CA-C	6.59	119.19	108.26
2	H	214	LYS	CA-C-N	6.53	133.73	121.97
2	H	214	LYS	C-N-CA	6.53	133.73	121.97
3	L	178	THR	N-CA-C	6.23	118.21	107.93
2	H	138	ASN	N-CA-C	-6.20	104.32	113.61
2	H	160	ASN	N-CA-C	-5.93	98.17	110.80
3	L	96	TYR	N-CA-C	-5.93	102.14	110.50
3	L	107	LYS	N-CA-C	5.87	119.10	109.76
3	L	206	VAL	N-CA-C	5.74	116.12	107.80
2	H	130	LEU	N-CA-C	5.72	118.43	108.76
2	H	145	CYS	N-CA-C	-5.71	99.12	108.76
3	L	142	LYS	N-CA-C	5.68	118.41	111.82
3	L	115	VAL	N-CA-C	5.66	116.09	108.17
1	A	178	CYS	CA-C-N	-5.64	113.34	120.56
1	A	178	CYS	C-N-CA	-5.64	113.34	120.56
3	L	192	TYR	N-CA-C	5.61	118.05	108.90
2	H	157	VAL	N-CA-C	-5.60	100.27	108.11
1	A	185	GLN	N-CA-C	-5.54	105.24	111.28
3	L	195	GLU	N-CA-C	5.52	117.85	108.02
3	L	112	ALA	CA-C-N	5.52	125.28	119.76
3	L	112	ALA	C-N-CA	5.52	125.28	119.76
3	L	211	ARG	N-CA-C	5.42	122.34	110.80
2	H	211	VAL	N-CA-C	5.34	116.42	108.46
3	L	205	ILE	N-CA-C	-5.34	100.64	108.54
3	L	143	ASP	N-CA-C	5.33	118.04	110.10
2	H	124	PRO	CA-C-N	5.28	126.44	119.84
2	H	124	PRO	C-N-CA	5.28	126.44	119.84
2	H	158	THR	N-CA-C	-5.18	101.82	109.18
1	A	178	CYS	N-CA-C	-5.13	99.86	110.80
1	A	198	THR	N-CA-C	-5.13	103.27	110.35
1	A	162	TYR	N-CA-C	5.10	116.60	108.79
3	L	188	ARG	N-CA-C	5.08	121.63	110.80
2	H	29	PHE	N-CA-C	5.07	117.46	111.33
3	L	131	SER	N-CA-C	5.06	116.77	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	88	CYS	CA-CB-SG	5.05	126.03	114.40
2	H	74	GLU	N-CA-C	-5.03	105.92	111.71

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	148	TRP	Peptide
3	L	149	LYS	Peptide
3	L	154	GLU	Peptide
3	L	188	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	840	0	784	70	0
2	H	1642	0	1580	117	0
3	L	1652	0	1577	156	0
4	L	1	0	0	0	0
5	A	23	0	0	5	0
5	H	28	0	0	3	1
5	L	22	0	0	0	0
All	All	4208	0	3941	334	1

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 42.

All (334) 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:L:198:HIS:CE1	3:L:199:LYS:HD2	1.48	1.47
3:L:198:HIS:ND1	3:L:199:LYS:CD	1.95	1.30
1:A:180:ASN:ND2	1:A:181:ILE:HD12	1.42	1.29
3:L:198:HIS:ND1	3:L:199:LYS:HD2	0.98	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:198:HIS:CE1	3:L:199:LYS:CD	2.16	1.26
3:L:198:HIS:HE1	3:L:199:LYS:CE	1.51	1.22
2:H:164:LEU:HD23	2:H:165:SER:N	1.57	1.19
2:H:160:ASN:HA	2:H:198:VAL:HG23	1.26	1.18
1:A:178:CYS:SG	1:A:213:CYS:SG	1.28	1.18
3:L:136:LEU:HD22	3:L:175:MET:HB2	1.21	1.17
3:L:33:ILE:HD11	3:L:88:CYS:SG	1.86	1.15
2:H:138:ASN:OD1	2:H:140:MET:HB2	1.45	1.14
3:L:198:HIS:HE1	3:L:199:LYS:NZ	1.45	1.14
3:L:198:HIS:CE1	3:L:199:LYS:NZ	2.16	1.12
3:L:198:HIS:CE1	3:L:199:LYS:CE	2.30	1.11
2:H:164:LEU:HD23	2:H:165:SER:H	0.94	1.08
2:H:164:LEU:CD2	2:H:165:SER:N	2.16	1.07
3:L:185:GLU:N	3:L:185:GLU:OE1	1.89	1.05
1:A:133:MET:HE2	5:A:316:HOH:O	1.59	1.03
2:H:160:ASN:HB3	2:H:163:SER:CB	1.89	1.03
2:H:160:ASN:HA	2:H:198:VAL:CG2	1.91	1.01
1:A:180:ASN:HD21	1:A:181:ILE:HD12	1.21	1.00
2:H:20:MET:HE1	2:H:94:TYR:HB2	1.41	1.00
2:H:129:PRO:HG2	3:L:124:GLN:OE1	1.62	0.98
1:A:180:ASN:HD22	1:A:181:ILE:H	1.11	0.98
1:A:180:ASN:ND2	1:A:181:ILE:CD1	2.28	0.96
1:A:180:ASN:HD22	1:A:181:ILE:HD12	1.27	0.95
1:A:178:CYS:SG	1:A:213:CYS:CB	2.56	0.94
2:H:193:TRP:CD1	2:H:194:PRO:HA	2.03	0.94
3:L:198:HIS:ND1	3:L:199:LYS:N	2.16	0.93
3:L:181:LEU:HD23	3:L:186:TYR:CE2	2.05	0.91
1:A:180:ASN:HD21	1:A:181:ILE:CD1	1.81	0.91
1:A:180:ASN:HD22	1:A:181:ILE:N	1.68	0.90
3:L:196:ALA:O	3:L:197:THR:OG1	1.91	0.89
2:H:138:ASN:OD1	2:H:140:MET:CB	2.20	0.89
2:H:20:MET:HE1	2:H:94:TYR:CB	2.02	0.88
2:H:164:LEU:CD2	2:H:166:GLY:H	1.86	0.88
3:L:133:VAL:HG13	3:L:135:PHE:CE2	2.09	0.87
1:A:170:ASN:OD1	1:A:173:THR:HG23	1.73	0.87
3:L:198:HIS:CE1	3:L:199:LYS:HZ1	1.90	0.86
2:H:199:THR:HG23	2:H:214:LYS:HB2	1.58	0.85
1:A:174:PHE:HD2	1:A:217:TYR:HD2	1.23	0.85
3:L:149:LYS:NZ	3:L:150:ILE:O	2.11	0.83
2:H:158:THR:CG2	2:H:201:ASN:O	2.27	0.83
3:L:182:THR:O	3:L:183:LYS:O	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:194:CYS:SG	3:L:195:GLU:N	2.54	0.81
3:L:23:CYS:SG	3:L:88:CYS:HB3	2.20	0.81
3:L:46:LEU:HG	3:L:55:ILE:HG12	1.64	0.80
3:L:33:ILE:CD1	3:L:88:CYS:SG	2.68	0.80
1:A:133:MET:CE	5:A:316:HOH:O	2.23	0.79
2:H:160:ASN:HB3	2:H:163:SER:OG	1.84	0.78
2:H:129:PRO:HG2	3:L:124:GLN:CD	2.07	0.78
3:L:136:LEU:CD2	3:L:175:MET:HB2	2.11	0.78
2:H:163:SER:OG	2:H:164:LEU:N	2.17	0.77
2:H:160:ASN:HB3	2:H:163:SER:HB3	1.65	0.76
3:L:113:PRO:HA	3:L:138:ASN:HB3	1.66	0.76
3:L:198:HIS:CE1	3:L:199:LYS:HA	2.19	0.76
3:L:23:CYS:SG	3:L:88:CYS:CB	2.73	0.76
3:L:133:VAL:CG1	3:L:135:PHE:CE2	2.70	0.75
3:L:198:HIS:CG	3:L:199:LYS:N	2.54	0.75
3:L:198:HIS:HE1	3:L:199:LYS:HZ1	1.26	0.75
3:L:184:ASP:HB3	3:L:185:GLU:OE1	1.87	0.75
1:A:197:PHE:HB2	5:A:308:HOH:O	1.87	0.74
2:H:63:LYS:HD2	2:H:63:LYS:O	1.87	0.74
3:L:183:LYS:HG3	3:L:184:ASP:N	2.02	0.74
2:H:138:ASN:O	2:H:140:MET:HG3	1.88	0.73
2:H:213:LYS:HD3	2:H:213:LYS:C	2.12	0.73
3:L:85:ASP:OD1	3:L:103:LYS:HG2	1.88	0.72
2:H:213:LYS:O	2:H:214:LYS:HD3	1.89	0.72
3:L:139:PHE:CE2	3:L:199:LYS:HG3	2.25	0.72
1:A:208:VAL:HG23	1:A:212:MET:HE3	1.72	0.72
2:H:22:CYS:CB	2:H:96:CYS:HG	2.01	0.72
3:L:137:ASN:OD1	3:L:174:SER:HA	1.90	0.71
3:L:124:GLN:OE1	3:L:124:GLN:N	2.24	0.71
1:A:183:VAL:O	1:A:187:THR:HG23	1.90	0.71
2:H:164:LEU:HD23	2:H:166:GLY:H	1.55	0.71
2:H:193:TRP:HA	2:H:194:PRO:O	1.92	0.70
3:L:108:ARG:NH1	3:L:171:SER:HB2	2.07	0.70
2:H:20:MET:CE	2:H:94:TYR:HB2	2.20	0.70
3:L:136:LEU:HD23	3:L:137:ASN:N	2.07	0.69
3:L:114:THR:N	3:L:137:ASN:O	2.25	0.69
1:A:174:PHE:CD2	1:A:217:TYR:HD2	2.08	0.69
1:A:218:GLN:O	1:A:220:GLU:N	2.26	0.69
3:L:181:LEU:HD23	3:L:186:TYR:HE2	1.56	0.69
3:L:61:ARG:HD2	3:L:77:SER:O	1.92	0.68
3:L:133:VAL:HG13	3:L:135:PHE:HE2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:198:HIS:CE1	3:L:199:LYS:HZ2	2.12	0.68
3:L:212:ASN:N	3:L:212:ASN:OD1	2.27	0.67
3:L:139:PHE:N	3:L:173:TYR:HD2	1.92	0.67
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.75	0.67
2:H:160:ASN:CB	2:H:163:SER:H	2.07	0.67
2:H:164:LEU:HD22	2:H:165:SER:N	2.07	0.67
3:L:23:CYS:HG	3:L:88:CYS:CB	2.06	0.67
2:H:22:CYS:CB	2:H:96:CYS:SG	2.82	0.67
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.75	0.67
2:H:22:CYS:HB2	2:H:96:CYS:SG	2.34	0.67
3:L:136:LEU:HD23	3:L:136:LEU:C	2.19	0.67
3:L:153:SER:OG	3:L:154:GLU:N	2.28	0.67
2:H:128:TYR:CZ	2:H:130:LEU:HD13	2.30	0.67
3:L:108:ARG:NH1	3:L:171:SER:O	2.28	0.67
3:L:149:LYS:HG3	3:L:154:GLU:HA	1.77	0.67
2:H:20:MET:HE3	2:H:113:THR:HB	1.77	0.66
1:A:170:ASN:CG	1:A:173:THR:HG23	2.21	0.66
3:L:185:GLU:H	3:L:185:GLU:CD	2.00	0.66
2:H:158:THR:HG22	2:H:201:ASN:O	1.96	0.66
2:H:12:VAL:HG11	2:H:86:LEU:HD12	1.78	0.65
2:H:160:ASN:O	2:H:161:SER:HB3	1.95	0.65
2:H:160:ASN:HB2	2:H:163:SER:H	1.62	0.65
1:A:135:ARG:NH1	1:A:153:MET:O	2.31	0.64
1:A:171:GLN:HB2	1:A:217:TYR:CZ	2.32	0.64
3:L:23:CYS:HB2	3:L:35:TRP:CH2	2.33	0.64
2:H:29:PHE:HE1	2:H:34:MET:HE1	1.62	0.64
2:H:160:ASN:ND2	2:H:164:LEU:O	2.32	0.63
3:L:108:ARG:HH12	3:L:171:SER:C	2.06	0.63
1:A:166:ASP:OD1	1:A:166:ASP:C	2.42	0.62
3:L:113:PRO:HA	3:L:137:ASN:O	1.98	0.62
2:H:140:MET:HG2	2:H:189:PRO:HA	1.81	0.62
2:H:2:VAL:HA	2:H:25:SER:O	2.00	0.62
2:H:138:ASN:O	2:H:139:SER:C	2.40	0.61
2:H:171:PHE:CZ	3:L:174:SER:HB3	2.35	0.61
3:L:198:HIS:ND1	3:L:199:LYS:CA	2.63	0.61
2:H:164:LEU:HD23	2:H:166:GLY:N	2.15	0.61
1:A:170:ASN:OD1	1:A:172:ASN:HB2	2.00	0.61
2:H:212:ASP:HB2	2:H:214:LYS:HG2	1.83	0.60
3:L:184:ASP:O	3:L:186:TYR:N	2.34	0.60
1:A:181:ILE:HD12	1:A:181:ILE:H	1.65	0.60
3:L:61:ARG:NH1	3:L:79:GLU:OE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:129:PRO:O	3:L:124:GLN:NE2	2.35	0.60
2:H:138:ASN:OD1	2:H:140:MET:N	2.35	0.60
2:H:164:LEU:HD21	2:H:166:GLY:H	1.67	0.60
3:L:111:ALA:O	3:L:139:PHE:HD1	1.84	0.60
1:A:171:GLN:O	1:A:175:VAL:HG23	2.02	0.60
2:H:148:LYS:HA	2:H:181:THR:HG22	1.84	0.59
3:L:137:ASN:O	3:L:138:ASN:HB3	2.01	0.59
3:L:143:ASP:O	3:L:199:LYS:HD3	2.02	0.59
3:L:198:HIS:CG	3:L:199:LYS:H	2.20	0.59
3:L:113:PRO:CA	3:L:137:ASN:O	2.50	0.59
3:L:114:THR:O	3:L:137:ASN:HB2	2.03	0.59
3:L:181:LEU:CD2	3:L:186:TYR:HE2	2.15	0.59
3:L:139:PHE:CD2	3:L:199:LYS:HG3	2.38	0.58
1:A:165:VAL:HG13	1:A:166:ASP:H	1.67	0.58
3:L:167:ASP:OD1	3:L:171:SER:N	2.37	0.58
1:A:174:PHE:HE2	1:A:217:TYR:HA	1.67	0.58
3:L:198:HIS:HE1	3:L:199:LYS:HE3	1.60	0.58
3:L:155:ARG:CD	3:L:156:GLN:HB3	2.34	0.57
3:L:197:THR:O	3:L:197:THR:HG22	2.03	0.57
1:A:177:ASP:HA	1:A:181:ILE:CD1	2.34	0.57
1:A:127:TYR:CE1	1:A:181:ILE:HG21	2.40	0.57
1:A:168:TYR:OH	1:A:177:ASP:OD2	2.21	0.57
2:H:135:GLY:O	2:H:136:ALA:HB2	2.05	0.57
1:A:165:VAL:HG13	1:A:166:ASP:N	2.20	0.57
1:A:161:TYR:CE2	1:A:185:GLN:HG2	2.41	0.56
2:H:164:LEU:CD2	2:H:166:GLY:N	2.64	0.56
3:L:183:LYS:HG3	3:L:184:ASP:H	1.70	0.56
2:H:159:TRP:HZ2	2:H:168:VAL:HG11	1.70	0.56
1:A:188:VAL:O	1:A:192:THR:HG23	2.06	0.56
1:A:178:CYS:N	1:A:181:ILE:HD13	2.20	0.55
3:L:182:THR:O	3:L:183:LYS:C	2.48	0.55
1:A:215:THR:HB	5:A:316:HOH:O	2.07	0.55
3:L:23:CYS:CB	3:L:88:CYS:SG	2.94	0.55
3:L:155:ARG:HD2	3:L:156:GLN:HB3	1.88	0.55
1:A:188:VAL:O	1:A:191:THR:HG22	2.07	0.54
3:L:150:ILE:HG22	3:L:151:ASP:CG	2.33	0.54
3:L:196:ALA:C	3:L:197:THR:HG1	2.05	0.54
2:H:12:VAL:HG11	2:H:86:LEU:CD1	2.38	0.54
2:H:160:ASN:CA	2:H:198:VAL:CG2	2.78	0.54
3:L:136:LEU:HG	3:L:137:ASN:H	1.72	0.54
3:L:198:HIS:ND1	3:L:199:LYS:HA	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2:VAL:HG21	2:H:108:TYR:CE2	2.43	0.53
2:H:158:THR:HG23	2:H:201:ASN:O	2.05	0.53
2:H:168:VAL:HG12	2:H:186:VAL:HG13	1.90	0.53
3:L:33:ILE:CG1	3:L:88:CYS:SG	2.96	0.53
2:H:128:TYR:CZ	2:H:146:LEU:HB2	2.44	0.53
1:A:195:GLU:HA	1:A:195:GLU:OE1	2.08	0.52
3:L:137:ASN:O	3:L:138:ASN:CB	2.57	0.52
3:L:139:PHE:N	3:L:173:TYR:CD2	2.75	0.52
3:L:173:TYR:O	3:L:174:SER:OG	2.14	0.52
2:H:164:LEU:CD2	2:H:165:SER:H	1.81	0.52
3:L:108:ARG:HB3	3:L:140:TYR:CD2	2.45	0.52
1:A:173:THR:OG1	1:A:174:PHE:N	2.39	0.52
1:A:179:VAL:O	1:A:183:VAL:HG23	2.08	0.52
2:H:204:HIS:HD1	2:H:207:SER:CB	2.23	0.52
3:L:136:LEU:CD2	3:L:137:ASN:N	2.73	0.52
2:H:152:PRO:HD2	2:H:204:HIS:NE2	2.25	0.52
3:L:149:LYS:CG	3:L:154:GLU:HA	2.39	0.52
1:A:204:MET:O	1:A:208:VAL:HG13	2.10	0.52
3:L:12:SER:HB2	3:L:107:LYS:HG2	1.93	0.52
1:A:147:ARG:HD2	5:A:317:HOH:O	2.11	0.51
2:H:29:PHE:CE1	2:H:34:MET:HE1	2.44	0.51
1:A:174:PHE:HD2	1:A:217:TYR:CD2	2.15	0.51
2:H:1:GLN:CD	2:H:1:GLN:N	2.69	0.51
2:H:160:ASN:CA	2:H:198:VAL:HG23	2.18	0.51
2:H:5:GLN:HB2	2:H:23:LYS:HB3	1.91	0.51
3:L:149:LYS:CG	3:L:150:ILE:H	2.22	0.51
2:H:160:ASN:CB	2:H:163:SER:N	2.72	0.50
3:L:166:GLN:NE2	3:L:171:SER:C	2.69	0.50
3:L:163:GLU:HG2	3:L:164:THR:H	1.76	0.50
1:A:177:ASP:HA	1:A:181:ILE:HD11	1.94	0.50
2:H:138:ASN:CG	2:H:140:MET:HB2	2.31	0.50
2:H:153:GLU:HB3	2:H:154:PRO:HA	1.94	0.50
2:H:195:SER:O	2:H:196:GLU:HB2	2.11	0.50
1:A:157:PRO:O	1:A:212:MET:HE1	2.12	0.49
1:A:171:GLN:HB2	1:A:217:TYR:CE2	2.45	0.49
1:A:177:ASP:C	1:A:181:ILE:HD13	2.37	0.49
2:H:159:TRP:CE3	2:H:160:ASN:OD1	2.65	0.49
3:L:20:SER:HA	3:L:73:LEU:O	2.13	0.49
2:H:160:ASN:HB3	2:H:163:SER:CA	2.42	0.49
3:L:166:GLN:NE2	3:L:172:THR:O	2.45	0.49
1:A:208:VAL:HG23	1:A:212:MET:CE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:130:LEU:HD23	3:L:118:PHE:HB3	1.95	0.49
3:L:11:LEU:HD11	3:L:21:PHE:HD1	1.77	0.49
2:H:164:LEU:O	2:H:165:SER:HB2	2.13	0.49
2:H:161:SER:O	2:H:161:SER:OG	2.28	0.49
3:L:136:LEU:HG	3:L:137:ASN:N	2.28	0.49
2:H:155:VAL:HG11	2:H:182:LEU:HD21	1.95	0.49
3:L:136:LEU:CG	3:L:137:ASN:N	2.76	0.49
3:L:148:TRP:CD1	3:L:154:GLU:HG2	2.47	0.49
3:L:8:PRO:HG2	3:L:11:LEU:CD2	2.43	0.48
2:H:158:THR:O	2:H:159:TRP:HB3	2.13	0.48
2:H:164:LEU:CD2	2:H:164:LEU:C	2.84	0.48
3:L:166:GLN:HE21	3:L:171:SER:C	2.22	0.48
3:L:181:LEU:CD2	3:L:186:TYR:CE2	2.85	0.48
3:L:125:LEU:HD22	3:L:129:GLY:O	2.14	0.48
3:L:133:VAL:CG1	3:L:135:PHE:HE2	2.19	0.48
3:L:188:ARG:HG3	3:L:189:HIS:N	2.29	0.48
3:L:198:HIS:ND1	3:L:198:HIS:C	2.71	0.48
2:H:169:HIS:O	2:H:184:SER:HA	2.14	0.48
3:L:187:GLU:O	3:L:188:ARG:HB3	2.13	0.48
1:A:124:LEU:CG	1:A:125:GLY:H	2.27	0.47
2:H:159:TRP:C	2:H:161:SER:N	2.72	0.47
2:H:209:THR:O	2:H:210:LYS:HG2	2.13	0.47
3:L:108:ARG:HB3	3:L:140:TYR:HD2	1.79	0.47
3:L:133:VAL:HG11	3:L:135:PHE:CE2	2.47	0.47
3:L:184:ASP:O	3:L:187:GLU:HB3	2.14	0.47
1:A:179:VAL:HG22	1:A:209:VAL:HG23	1.95	0.47
3:L:173:TYR:N	3:L:173:TYR:CD1	2.79	0.47
2:H:86:LEU:HA	2:H:90:ASP:OD2	2.15	0.47
2:H:104:TYR:HB2	3:L:91:SER:OG	2.14	0.47
3:L:82:ASP:O	3:L:104:LEU:HD23	2.15	0.47
3:L:105:GLU:HG2	3:L:106:LEU:N	2.29	0.47
1:A:174:PHE:CD1	1:A:174:PHE:C	2.85	0.47
1:A:124:LEU:HG	1:A:125:GLY:H	1.80	0.47
1:A:216:GLN:O	1:A:219:ARG:CG	2.62	0.47
2:H:138:ASN:OD1	2:H:140:MET:CA	2.63	0.47
3:L:150:ILE:HG23	3:L:193:THR:OG1	2.15	0.47
2:H:2:VAL:HG21	2:H:108:TYR:CZ	2.50	0.46
2:H:159:TRP:HB3	2:H:200:CYS:CB	2.45	0.46
2:H:149:GLY:N	2:H:180:TYR:O	2.48	0.46
3:L:193:THR:HG23	3:L:208:SER:HB2	1.98	0.46
1:A:197:PHE:CE2	1:A:205:MET:HE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:204:HIS:HB3	2:H:209:THR:OG1	2.15	0.46
3:L:184:ASP:C	3:L:186:TYR:N	2.72	0.46
2:H:28:THR:HA	5:H:310:HOH:O	2.16	0.46
2:H:128:TYR:CE2	2:H:130:LEU:HD13	2.50	0.46
2:H:163:SER:HG	2:H:164:LEU:H	1.58	0.46
3:L:147:LYS:HG3	3:L:197:THR:HG21	1.97	0.46
1:A:170:ASN:OD1	1:A:172:ASN:N	2.48	0.46
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.50	0.46
1:A:173:THR:O	1:A:176:HIS:N	2.45	0.46
1:A:198:THR:HG22	1:A:199:GLU:N	2.30	0.45
2:H:159:TRP:O	2:H:161:SER:N	2.42	0.45
1:A:169:ASN:O	1:A:170:ASN:HB2	2.16	0.45
2:H:146:LEU:HD11	3:L:133:VAL:HB	1.98	0.45
2:H:153:GLU:OE2	2:H:173:ALA:HB3	2.17	0.45
2:H:204:HIS:CE1	2:H:206:ALA:HB3	2.51	0.45
1:A:174:PHE:CD1	1:A:174:PHE:O	2.70	0.45
3:L:133:VAL:HG11	3:L:135:PHE:CZ	2.51	0.45
3:L:149:LYS:CD	3:L:150:ILE:H	2.30	0.45
2:H:39:GLN:O	2:H:92:ALA:HB1	2.17	0.45
3:L:108:ARG:HG3	3:L:109:ALA:H	1.81	0.45
3:L:166:GLN:NE2	3:L:171:SER:O	2.51	0.44
3:L:184:ASP:O	3:L:187:GLU:N	2.50	0.44
2:H:164:LEU:CD2	2:H:165:SER:CA	2.95	0.44
2:H:193:TRP:CG	2:H:194:PRO:HA	2.48	0.44
3:L:207:LYS:NZ	3:L:209:PHE:HD1	2.14	0.44
3:L:121:SER:OG	3:L:122:SER:N	2.36	0.44
3:L:149:LYS:HD2	3:L:150:ILE:H	1.83	0.44
2:H:36:TRP:NE1	5:H:308:HOH:O	2.42	0.44
3:L:169:LYS:HG3	3:L:170:ASP:OD1	2.18	0.44
2:H:160:ASN:HB2	2:H:163:SER:N	2.30	0.44
3:L:14:SER:O	3:L:17:GLU:HG2	2.18	0.44
2:H:73:ASP:OD1	2:H:75:SER:OG	2.23	0.44
3:L:46:LEU:HD11	3:L:49:LYS:HB3	2.00	0.44
1:A:198:THR:HG22	1:A:199:GLU:H	1.83	0.43
2:H:176:GLN:OE1	2:H:181:THR:HG21	2.17	0.43
3:L:149:LYS:HA	3:L:195:GLU:OE1	2.18	0.43
1:A:129:LEU:HA	1:A:129:LEU:HD12	1.70	0.43
2:H:129:PRO:O	2:H:130:LEU:HD12	2.18	0.43
2:H:146:LEU:HA	2:H:146:LEU:HD23	1.78	0.43
3:L:183:LYS:CG	3:L:184:ASP:H	2.30	0.43
2:H:159:TRP:C	2:H:161:SER:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:148:TRP:CD1	3:L:148:TRP:N	2.86	0.43
1:A:180:ASN:ND2	1:A:181:ILE:H	1.95	0.43
2:H:159:TRP:CZ2	2:H:168:VAL:HG11	2.53	0.43
3:L:11:LEU:CD1	3:L:21:PHE:HD1	2.31	0.43
1:A:150:ARG:NH2	1:A:150:ARG:HB3	2.34	0.43
3:L:138:ASN:HA	3:L:173:TYR:CD2	2.53	0.43
3:L:150:ILE:HG22	3:L:151:ASP:OD2	2.19	0.43
1:A:180:ASN:O	1:A:184:LYS:HG3	2.18	0.43
3:L:112:ALA:HA	3:L:113:PRO:HD3	1.82	0.43
2:H:122:THR:HG22	2:H:152:PRO:HD3	2.00	0.43
3:L:116:SER:O	3:L:135:PHE:HD2	2.02	0.42
3:L:167:ASP:O	3:L:171:SER:HA	2.19	0.42
1:A:137:LEU:HD12	1:A:138:ILE:N	2.34	0.42
2:H:28:THR:HB	5:H:301:HOH:O	2.19	0.42
3:L:139:PHE:HE1	3:L:200:THR:HG23	1.85	0.42
3:L:197:THR:O	3:L:198:HIS:CB	2.67	0.42
3:L:167:ASP:OD1	3:L:170:ASP:N	2.53	0.42
1:A:187:THR:HA	1:A:190:THR:HB	2.01	0.42
1:A:170:ASN:OD1	1:A:173:THR:N	2.53	0.42
1:A:205:MET:O	1:A:209:VAL:HG13	2.20	0.42
2:H:171:PHE:CE2	3:L:174:SER:HB3	2.54	0.42
3:L:138:ASN:HA	3:L:173:TYR:HD2	1.85	0.41
3:L:197:THR:O	3:L:198:HIS:HB3	2.20	0.41
2:H:150:TYR:OH	2:H:154:PRO:O	2.28	0.41
2:H:158:THR:OG1	2:H:159:TRP:N	2.53	0.41
3:L:23:CYS:HB2	3:L:35:TRP:CZ2	2.54	0.41
3:L:167:ASP:OD1	3:L:167:ASP:C	2.63	0.41
3:L:155:ARG:NH1	3:L:157:ASN:O	2.53	0.41
2:H:164:LEU:O	2:H:165:SER:CB	2.66	0.41
3:L:155:ARG:HD3	3:L:156:GLN:HB3	2.01	0.41
3:L:167:ASP:HB3	3:L:172:THR:N	2.36	0.41
3:L:160:LEU:HD12	3:L:160:LEU:HA	1.91	0.41
3:L:187:GLU:O	3:L:187:GLU:CG	2.69	0.41
1:A:217:TYR:CD1	1:A:217:TYR:C	2.98	0.41
1:A:168:TYR:HH	1:A:177:ASP:CG	2.29	0.41
3:L:63:SER:O	3:L:73:LEU:HD12	2.20	0.41
3:L:140:TYR:CE1	3:L:173:TYR:CE1	3.09	0.40
2:H:158:THR:O	2:H:159:TRP:CB	2.68	0.40
1:A:163:ARG:O	1:A:168:TYR:HE2	2.05	0.40
2:H:9:THR:C	2:H:10:GLU:HG2	2.45	0.40
2:H:129:PRO:HD2	3:L:124:GLN:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:141:VAL:O	2:H:143:LEU:HD12	2.21	0.40
3:L:91:SER:OG	3:L:91:SER:O	2.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:303:HOH:O	5:H:311:HOH:O[2_555]	2.04	0.16

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	99/135 (73%)	90 (91%)	4 (4%)	5 (5%)	1	5
2	H	216/218 (99%)	193 (89%)	13 (6%)	10 (5%)	2	6
3	L	211/213 (99%)	174 (82%)	19 (9%)	18 (8%)	0	1
All	All	526/566 (93%)	457 (87%)	36 (7%)	33 (6%)	1	3

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	219	ARG
2	H	129	PRO
2	H	161	SER
2	H	165	SER
2	H	194	PRO
2	H	195	SER
2	H	196	GLU
2	H	215	ILE
3	L	120	PRO

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Mol	Chain	Res	Type
3	L	121	SER
3	L	149	LYS
3	L	156	GLN
3	L	183	LYS
3	L	185	GLU
3	L	198	HIS
3	L	199	LYS
3	L	211	ARG
3	L	212	ASN
1	A	178	CYS
2	H	159	TRP
2	H	191	SER
3	L	154	GLU
3	L	157	ASN
3	L	169	LYS
1	A	164	PRO
3	L	122	SER
3	L	138	ASN
3	L	188	ARG
3	L	197	THR
2	H	126	SER
3	L	151	ASP
1	A	125	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	93/123 (76%)	82 (88%)	11 (12%)	5	17
2	H	187/187 (100%)	169 (90%)	18 (10%)	8	26
3	L	191/191 (100%)	160 (84%)	31 (16%)	2	8
All	All	471/501 (94%)	411 (87%)	60 (13%)	4	15

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	MET
1	A	150	ARG
1	A	159	GLN
1	A	163	ARG
1	A	165	VAL
1	A	167	GLN
1	A	178	CYS
1	A	180	ASN
1	A	208	VAL
1	A	220	GLU
1	A	222	GLU
2	H	9	THR
2	H	34	MET
2	H	65	LYS
2	H	74	GLU
2	H	111	GLN
2	H	123	THR
2	H	137	THR
2	H	141	VAL
2	H	148	LYS
2	H	160	ASN
2	H	161	SER
2	H	163	SER
2	H	164	LEU
2	H	170	THR
2	H	183	SER
2	H	184	SER
2	H	195	SER
2	H	213	LYS
3	L	10	ILE
3	L	11	LEU
3	L	12	SER
3	L	21	PHE
3	L	23	CYS
3	L	24	ARG
3	L	60	SER
3	L	81	GLU
3	L	88	CYS
3	L	107	LYS
3	L	114	THR
3	L	117	ILE
3	L	124	GLN
3	L	125	LEU

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Mol	Chain	Res	Type
3	L	136	LEU
3	L	144	ILE
3	L	149	LYS
3	L	155	ARG
3	L	159	VAL
3	L	165	ASP
3	L	167	ASP
3	L	169	LYS
3	L	173	TYR
3	L	184	ASP
3	L	185	GLU
3	L	193	THR
3	L	195	GLU
3	L	203	SER
3	L	205	ILE
3	L	211	ARG
3	L	212	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
2	H	160	ASN
3	L	37	GLN
3	L	198	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	101/135 (74%)	1.19	21 (20%)	2 2	29, 68, 108, 120	0
2	H	218/218 (100%)	1.24	66 (30%)	1 1	23, 49, 163, 187	0
3	L	213/213 (100%)	1.57	73 (34%)	1 1	31, 90, 159, 165	0
All	All	532/566 (93%)	1.36	160 (30%)	1 1	23, 73, 158, 187	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	206	VAL	11.0
2	H	141	VAL	8.4
3	L	135	PHE	7.6
2	H	135	GLY	6.8
2	H	142	THR	6.7
2	H	143	LEU	6.7
3	L	196	ALA	6.4
3	L	133	VAL	5.7
2	H	147	VAL	5.2
3	L	132	VAL	5.2
1	A	179	VAL	4.9
1	A	161	TYR	4.9
2	H	131	ALA	4.7
2	H	145	CYS	4.7
2	H	184	SER	4.7
3	L	204	PRO	4.7
3	L	189	HIS	4.6
3	L	130	ALA	4.6
3	L	116	SER	4.6
2	H	191	SER	4.6
2	H	186	VAL	4.2
3	L	113	PRO	4.2
3	L	115	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
2	H	195	SER	4.2
1	A	183	VAL	4.1
3	L	136	LEU	4.1
3	L	117	ILE	4.0
3	L	207	LYS	4.0
2	H	144	GLY	4.0
2	H	215	ILE	3.9
2	H	187	THR	3.9
2	H	182	LEU	3.9
3	L	122	SER	3.8
2	H	188	VAL	3.7
2	H	134	GLY	3.7
2	H	157	VAL	3.7
2	H	132	PRO	3.7
3	L	190	ASN	3.7
1	A	131	SER	3.6
3	L	118	PHE	3.6
3	L	131	SER	3.6
2	H	126	SER	3.5
3	L	121	SER	3.5
2	H	211	VAL	3.5
2	H	148	LYS	3.5
3	L	120	PRO	3.4
2	H	176	GLN	3.4
2	H	167	GLY	3.4
2	H	130	LEU	3.3
3	L	106	LEU	3.3
3	L	119	PRO	3.3
3	L	186	TYR	3.2
2	H	183	SER	3.2
3	L	205	ILE	3.2
3	L	129	GLY	3.2
3	L	191	THR	3.2
3	L	16	GLY	3.1
1	A	127	TYR	3.1
2	H	124	PRO	3.1
3	L	197	THR	3.1
2	H	146	LEU	3.1
3	L	181	LEU	3.0
1	A	158	ASN	3.0
2	H	155	VAL	3.0
1	A	168	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	170	THR	3.0
3	L	192	TYR	2.9
3	L	112	ALA	2.9
3	L	114	THR	2.8
2	H	149	GLY	2.8
2	H	150	TYR	2.8
2	H	139	SER	2.8
2	H	127	VAL	2.8
2	H	128	TYR	2.8
3	L	173	TYR	2.8
2	H	136	ALA	2.8
3	L	161	ASN	2.8
3	L	153	SER	2.8
2	H	156	THR	2.7
3	L	174	SER	2.7
2	H	216	VAL	2.7
3	L	78	VAL	2.7
2	H	185	SER	2.7
2	H	200	CYS	2.7
2	H	133	GLY	2.7
1	A	220	GLU	2.7
3	L	193	THR	2.6
3	L	155	ARG	2.6
2	H	193	TRP	2.6
1	A	133	MET	2.6
2	H	197	THR	2.6
2	H	202	VAL	2.6
1	A	136	PRO	2.5
3	L	125	LEU	2.5
3	L	175	MET	2.5
3	L	180	THR	2.5
3	L	182	THR	2.5
3	L	177	SER	2.5
1	A	199	GLU	2.5
1	A	160	VAL	2.5
3	L	148	TRP	2.5
3	L	200	THR	2.5
2	H	190	SER	2.5
3	L	140	TYR	2.5
2	H	189	PRO	2.4
2	H	173	ALA	2.4
3	L	208	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	222	GLU	2.4
3	L	109	ALA	2.4
2	H	181	THR	2.4
2	H	140	MET	2.4
3	L	162	SER	2.4
3	L	124	GLN	2.4
1	A	180	ASN	2.4
2	H	125	PRO	2.4
3	L	212	ASN	2.4
2	H	218	ARG	2.4
2	H	153	GLU	2.4
3	L	195	GLU	2.4
1	A	132	ALA	2.3
3	L	172	THR	2.3
2	H	166	GLY	2.3
3	L	71	PHE	2.3
3	L	88	CYS	2.3
3	L	203	SER	2.3
2	H	217	PRO	2.3
3	L	185	GLU	2.3
2	H	175	LEU	2.3
2	H	137	THR	2.2
1	A	162	TYR	2.2
1	A	169	ASN	2.2
3	L	179	LEU	2.2
3	L	166	GLN	2.2
2	H	154	PRO	2.2
2	H	172	PRO	2.2
2	H	177	SER	2.2
1	A	167	GLN	2.2
3	L	134	CYS	2.2
1	A	122	GLY	2.2
3	L	149	LYS	2.2
3	L	159	VAL	2.2
3	L	176	SER	2.2
3	L	47	ILE	2.1
2	H	169	HIS	2.1
1	A	128	MET	2.1
2	H	208	SER	2.1
3	L	194	CYS	2.1
3	L	15	PRO	2.1
2	H	171	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
3	L	160	LEU	2.1
2	H	159	TRP	2.1
3	L	26	SER	2.1
2	H	138	ASN	2.1
1	A	129	LEU	2.1
3	L	11	LEU	2.0
3	L	137	ASN	2.0
2	H	192	THR	2.0
2	H	203	ALA	2.0
3	L	138	ASN	2.0
3	L	2	ILE	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	NA	L	301	1/1	0.46	0.53	99,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.