



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:13 AM UTC

PDB ID : 6XLQ / pdb_00006xlq
Title : Crystal Structure of the Human BTN3A1 Ectodomain in Complex with the CTX-2026 Fab
Authors : Payne, K.K.; Mine, J.A.; Biswas, S.; Chaurio, R.A.; Perales-Puchalt, A.; Anadon, C.M.; Costich, T.L.; Harro, C.M.; Walrath, J.; Ming, Q.; Tcyganov, E.; Buras, A.L.; Rigolizzo, K.E.; Mandal, G.; Lajoie, J.; Ophir, M.; Tchou, J.; Marchion, D.; Luca, V.C.; Bobrowicz, P.; McLaughlin, B.; Eskiocak, U.; Schmidt, M.; Cubillos-Ruiz, J.R.; Rodriguez, P.C.; Gabrilovich, D.I.; Conejo-Garcia, J.R.
Deposited on : 2020-06-29
Resolution : 3.00 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

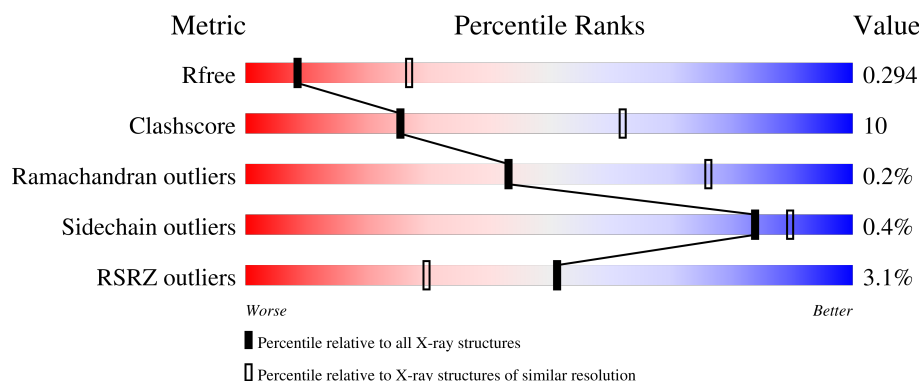
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	226	4% 74% 18% 7%
1	D	226	5% 76% 17% 7%
1	G	226	% 72% 20% 7%

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	J	226	4% 74% 18% 7%
2	B	223	2% 72% 23%
2	E	223	6% 71% 25%
2	H	223	3% 74% 22%
2	K	223	% 75% 22%
3	C	212	83% 17%
3	F	212	6% 82% 17%
3	I	212	2% 83% 17%
3	L	212	82% 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19387 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 Butyrophilin subfamily 3 member A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1588	1003	270	307	8			
1	D	210	Total	C	N	O	S	0	0	0
			1588	1003	270	307	8			
1	G	210	Total	C	N	O	S	0	0	0
			1588	1003	270	307	8			
1	J	210	Total	C	N	O	S	0	0	0
			1588	1003	270	307	8			

- Molecule 2 is a protein called CTX-2026 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1641	1038	277	316	10			
2	E	216	Total	C	N	O	S	0	0	0
			1641	1038	277	316	10			
2	H	216	Total	C	N	O	S	0	0	0
			1641	1038	277	316	10			
2	K	216	Total	C	N	O	S	0	0	0
			1641	1038	277	316	10			

- Molecule 3 is a protein called CTX-2026 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	212	Total	C	N	O	S	0	0	0
			1611	1009	270	327	5			
3	F	212	Total	C	N	O	S	0	0	0
			1611	1009	270	327	5			
3	I	212	Total	C	N	O	S	0	0	0
			1611	1009	270	327	5			
3	L	212	Total	C	N	O	S	0	0	0
			1611	1009	270	327	5			

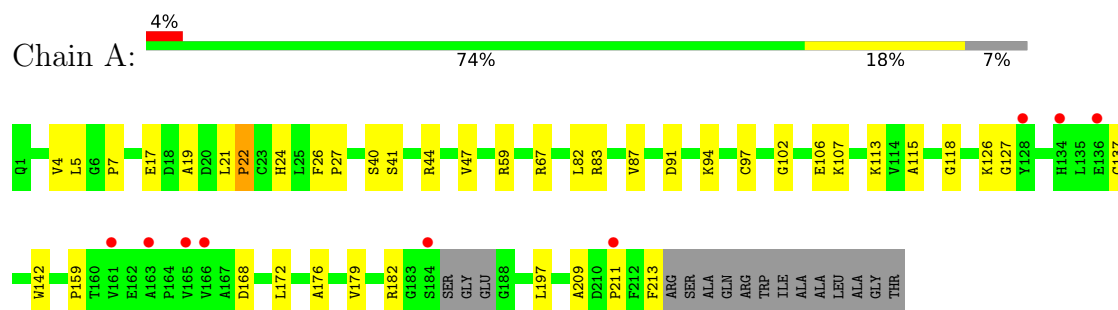
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	1	Total O 1 1	0	0
4	C	2	Total O 2 2	0	0
4	D	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0
4	G	5	Total O 5 5	0	0
4	H	1	Total O 1 1	0	0
4	J	6	Total O 6 6	0	0
4	K	3	Total O 3 3	0	0
4	L	5	Total O 5 5	0	0

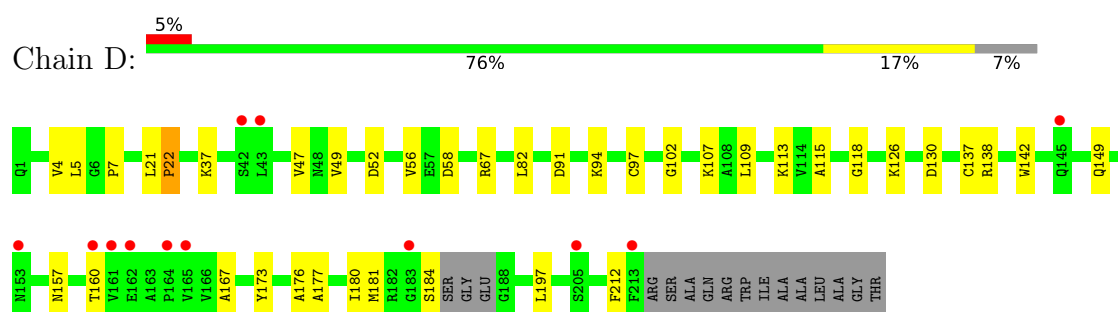
3 Residue-property plots [i](#)

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

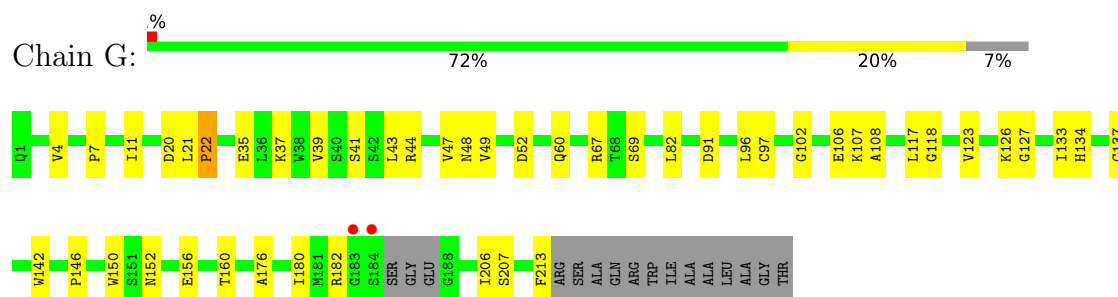
- Molecule 1: Butyrophilin subfamily 3 member A1



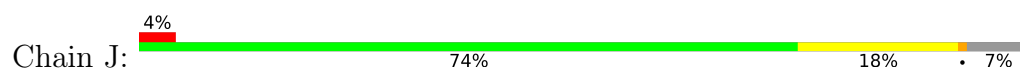
- Molecule 1: Butyrophilin subfamily 3 member A1

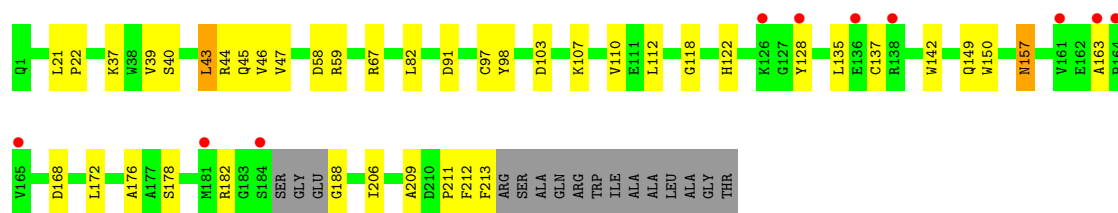


- Molecule 1: Butyrophilin subfamily 3 member A1

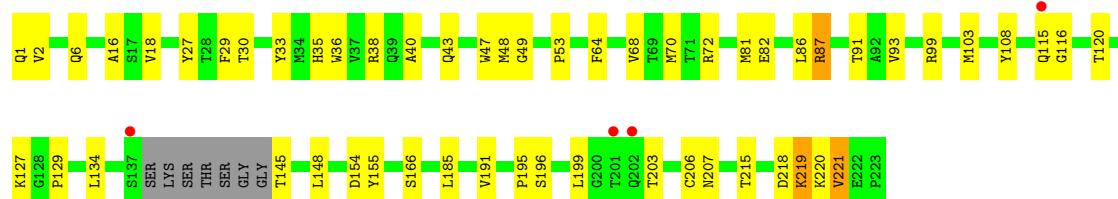
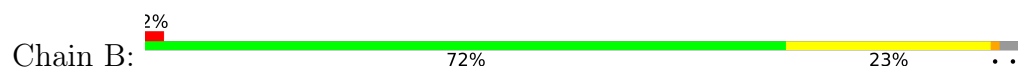


- Molecule 1: Butyrophilin subfamily 3 member A1

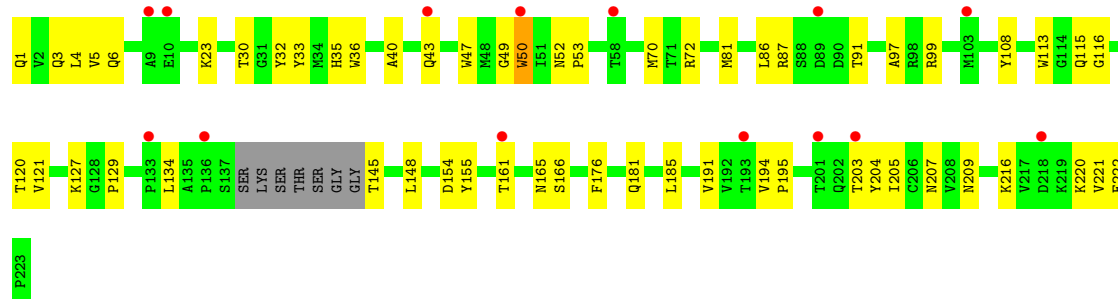




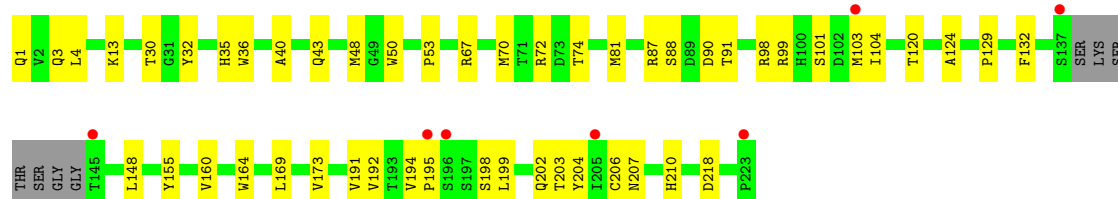
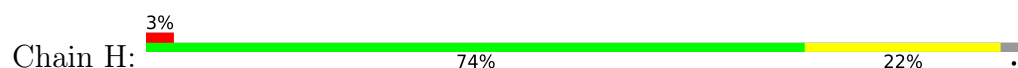
• Molecule 2: CTX-2026 Heavy Chain



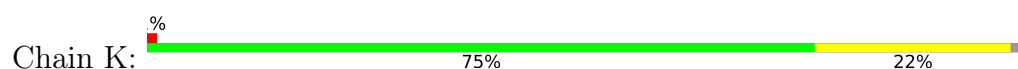
• Molecule 2: CTX-2026 Heavy Chain



• Molecule 2: CTX-2026 Heavy Chain

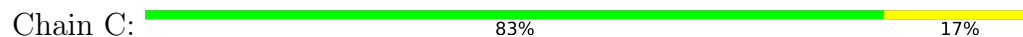


• Molecule 2: CTX-2026 Heavy Chain

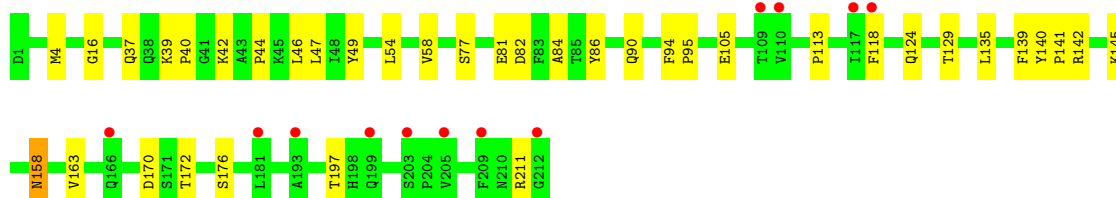
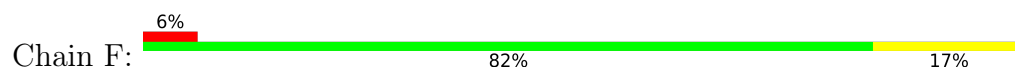




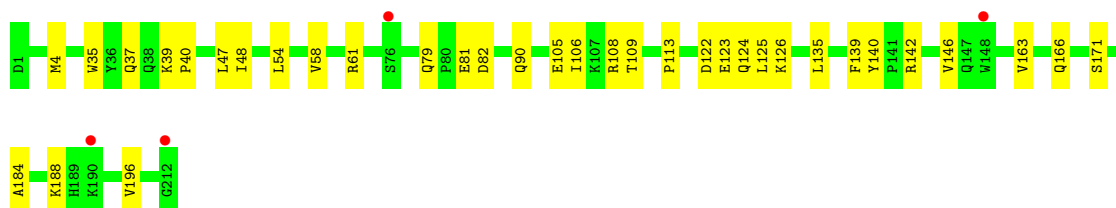
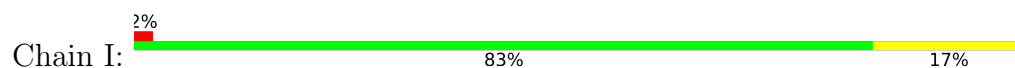
• Molecule 3: CTX-2026 Light Chain



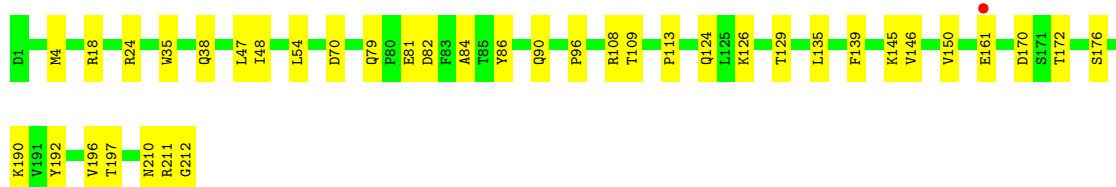
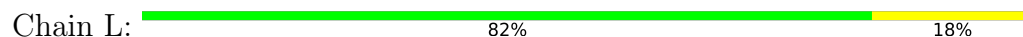
• Molecule 3: CTX-2026 Light Chain



• Molecule 3: CTX-2026 Light Chain



• Molecule 3: CTX-2026 Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.31Å 159.85Å 188.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.17 – 3.00 38.17 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (38.17-3.00) 98.6 (38.17-3.00)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.246 , 0.296 0.248 , 0.294	Depositor DCC
R_{free} test set	3332 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	19387	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5208e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.19	0/1620	0.50	0/2197
1	D	0.20	0/1620	0.49	0/2197
1	G	0.20	0/1620	0.53	0/2197
1	J	0.20	0/1620	0.53	0/2197
2	B	0.54	0/1676	0.65	0/2283
2	E	0.20	0/1676	0.57	1/2283 (0.0%)
2	H	0.22	0/1676	0.60	1/2283 (0.0%)
2	K	0.22	0/1676	0.57	0/2283
3	C	0.35	0/1647	0.54	0/2238
3	F	0.18	0/1647	0.50	0/2238
3	I	0.18	0/1647	0.49	0/2238
3	L	0.18	0/1647	0.48	0/2238
All	All	0.26	0/19772	0.54	2/26872 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	203	THR	CA-CB-CG2	7.12	122.61	110.50
2	E	50	TRP	CA-CB-CG	6.49	125.93	113.60

There are no chirality outliers.

There are no planarity outliers.

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	1588	0	1566	29	0
1	D	1588	0	1566	24	0
1	G	1588	0	1566	39	1
1	J	1588	0	1566	32	0
2	B	1641	0	1600	46	0
2	E	1641	0	1600	48	0
2	H	1641	0	1600	37	0
2	K	1641	0	1600	34	0
3	C	1611	0	1567	42	0
3	F	1611	0	1567	27	0
3	I	1611	0	1567	23	0
3	L	1611	0	1567	23	1
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	G	5	0	0	0	0
4	H	1	0	0	0	0
4	J	6	0	0	0	0
4	K	3	0	0	0	0
4	L	5	0	0	0	0
All	All	19387	0	18932	368	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 10.

All (368) 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:G:37:LYS:HE2	2:H:103:MET:SD	1.88	1.14
2:H:198:SER:OG	2:H:202:GLN:HG3	1.56	1.06
3:C:151:ASP:CG	3:C:189:HIS:HB3	1.89	0.98
2:B:219:LYS:NZ	3:C:123:GLU:OE2	2.01	0.94
2:E:35:HIS:CE1	2:E:50:TRP:CD1	2.56	0.94
2:E:35:HIS:CE1	2:E:50:TRP:HD1	1.88	0.92
2:E:40:ALA:CB	2:E:43:GLN:OE1	2.19	0.89
2:E:40:ALA:HB3	2:E:43:GLN:OE1	1.73	0.88
1:G:37:LYS:CE	2:H:103:MET:SD	2.62	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:35:HIS:CE1	2:K:50:TRP:HE3	1.94	0.85
2:H:198:SER:OG	2:H:202:GLN:CG	2.30	0.80
2:B:203:THR:HA	2:B:220:LYS:HE3	1.62	0.79
3:C:150:VAL:HG23	3:C:192:TYR:CE2	2.18	0.77
2:K:35:HIS:CE1	2:K:50:TRP:CE3	2.72	0.77
3:F:4:MET:HE3	3:F:90:GLN:HG2	1.67	0.77
1:A:67:ARG:NH2	1:A:91:ASP:OD2	2.20	0.74
2:B:219:LYS:NZ	3:C:123:GLU:CD	2.46	0.74
2:E:35:HIS:ND1	2:E:50:TRP:HD1	1.87	0.72
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.20	0.72
2:K:129:PRO:HB3	2:K:155:TYR:HB3	1.72	0.71
2:B:145:THR:HG22	2:B:195:PRO:HA	1.73	0.71
2:B:219:LYS:HZ1	3:C:123:GLU:CD	1.97	0.71
3:I:113:PRO:HB3	3:I:139:PHE:HB3	1.73	0.70
2:B:129:PRO:HB3	2:B:155:TYR:HB3	1.73	0.69
3:C:151:ASP:OD2	3:C:189:HIS:HB3	1.92	0.69
2:E:6:GLN:H	2:E:115:GLN:HE22	1.41	0.68
2:E:40:ALA:HB1	2:E:43:GLN:OE1	1.91	0.68
3:C:211:ARG:HH11	3:C:211:ARG:HB2	1.59	0.67
2:K:211:LYS:HG2	2:K:212:PRO:HD3	1.76	0.67
2:B:6:GLN:OE1	2:B:6:GLN:N	2.28	0.66
3:C:122:ASP:HA	3:C:125:LEU:HD12	1.75	0.66
2:K:35:HIS:HE1	2:K:50:TRP:CE3	2.12	0.66
2:H:91:THR:HG23	2:H:120:THR:HA	1.77	0.66
3:L:113:PRO:HB3	3:L:139:PHE:HB3	1.77	0.66
2:E:129:PRO:HB3	2:E:155:TYR:HB3	1.76	0.66
2:B:191:VAL:HG21	3:C:135:LEU:HD22	1.78	0.66
2:E:50:TRP:HE1	2:E:108:TYR:HD1	1.44	0.66
2:K:108:TYR:CG	3:L:96:PRO:HG3	2.31	0.66
1:A:21:LEU:HD12	1:A:82:LEU:HD23	1.76	0.65
1:J:67:ARG:NH2	1:J:91:ASP:OD2	2.18	0.65
2:K:67:ARG:NH2	2:K:90:ASP:OD2	2.30	0.64
2:B:6:GLN:NE2	2:B:115:GLN:HB3	2.12	0.64
1:G:21:LEU:HD12	1:G:82:LEU:HD23	1.79	0.64
1:J:128:TYR:OH	1:J:212:PHE:O	2.07	0.64
2:H:129:PRO:HB3	2:H:155:TYR:HB3	1.80	0.64
3:F:113:PRO:HB3	3:F:139:PHE:HB3	1.80	0.64
2:B:91:THR:HG23	2:B:120:THR:HA	1.80	0.64
2:E:191:VAL:HG11	3:F:135:LEU:HD22	1.78	0.64
1:J:103:ASP:HA	2:K:107:TYR:CD1	2.32	0.63
1:G:44:ARG:HH22	1:G:96:LEU:HD12	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:TYR:CG	3:C:96:PRO:HG3	2.33	0.63
2:B:219:LYS:NZ	3:C:123:GLU:OE1	2.32	0.63
1:D:149:GLN:HE21	1:D:157:ASN:HB3	1.62	0.63
2:B:206:CYS:O	2:B:218:ASP:HA	1.98	0.63
1:J:39:VAL:HG12	1:J:46:VAL:HA	1.81	0.62
2:K:91:THR:HG23	2:K:120:THR:HA	1.81	0.62
3:C:113:PRO:HB3	3:C:139:PHE:HB3	1.82	0.62
1:G:67:ARG:NH2	1:G:91:ASP:OD2	2.24	0.61
2:E:148:LEU:HD13	2:E:221:VAL:HG11	1.82	0.61
1:G:182:ARG:HA	1:G:213:PHE:HE2	1.65	0.61
1:D:181:MET:HE2	1:D:184:SER:HA	1.83	0.61
3:F:54:LEU:HD11	3:F:58:VAL:HB	1.84	0.60
1:J:149:GLN:NE2	1:J:157:ASN:OD1	2.35	0.60
2:K:203:THR:HA	2:K:220:LYS:HE3	1.84	0.59
1:J:163:ALA:HB3	1:J:176:ALA:HB3	1.84	0.59
2:B:203:THR:HG22	2:B:203:THR:O	2.01	0.59
1:D:118:GLY:HA3	1:D:142:TRP:CE2	2.38	0.59
3:I:4:MET:HE3	3:I:90:GLN:HG2	1.84	0.59
1:J:21:LEU:HD21	1:J:112:LEU:HB2	1.84	0.59
1:J:43:LEU:HB3	1:J:45:GLN:HG3	1.85	0.59
2:E:5:VAL:HG23	2:E:23:LYS:HB3	1.84	0.59
1:A:67:ARG:HH22	1:A:91:ASP:CG	2.11	0.58
3:C:151:ASP:OD2	3:C:189:HIS:CB	2.51	0.58
3:I:146:VAL:HG22	3:I:196:VAL:HG22	1.85	0.58
1:A:47:VAL:HG11	1:A:82:LEU:HD21	1.85	0.58
1:A:113:LYS:HD3	1:A:197:LEU:HD11	1.85	0.58
2:H:40:ALA:HB3	2:H:43:GLN:HB2	1.86	0.58
3:C:4:MET:HE3	3:C:90:GLN:HG2	1.86	0.58
2:K:191:VAL:HG21	3:L:135:LEU:HD22	1.86	0.58
3:F:81:GLU:OE1	3:F:81:GLU:N	2.25	0.58
2:K:206:CYS:O	2:K:218:ASP:HA	2.04	0.57
2:H:191:VAL:HG11	3:I:135:LEU:HD22	1.85	0.57
2:B:33:TYR:HB2	2:B:99:ARG:HD3	1.86	0.57
2:E:127:LYS:HD3	2:E:185:LEU:HD21	1.85	0.57
2:B:53:PRO:HA	2:B:72:ARG:HG2	1.87	0.56
2:E:134:LEU:HB3	3:F:118:PHE:CD2	2.40	0.56
1:A:126:LYS:O	1:A:126:LYS:HG3	2.06	0.56
3:C:189:HIS:N	3:C:189:HIS:CD2	2.72	0.56
2:E:40:ALA:HB3	2:E:43:GLN:HB2	1.88	0.56
3:L:4:MET:HE3	3:L:90:GLN:HG2	1.88	0.56
2:B:196:SER:O	2:B:199:LEU:HG	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:91:THR:HG23	2:E:120:THR:HA	1.87	0.56
2:K:53:PRO:HA	2:K:72:ARG:HG2	1.88	0.56
2:K:202:GLN:O	2:K:202:GLN:NE2	2.39	0.56
1:G:37:LYS:HG3	1:G:49:VAL:HG22	1.87	0.55
2:K:148:LEU:HD13	2:K:221:VAL:HG11	1.89	0.55
1:J:157:ASN:N	1:J:157:ASN:HD22	2.04	0.55
3:C:124:GLN:HG2	3:C:129:THR:O	2.07	0.55
2:K:36:TRP:CD1	2:K:70:MET:HE2	2.41	0.55
2:K:162:VAL:HG22	2:K:208:VAL:HG22	1.89	0.55
2:E:47:TRP:HZ2	2:E:50:TRP:CD1	2.23	0.55
3:C:209:PHE:C	3:C:209:PHE:CD1	2.85	0.54
3:F:158:ASN:HD22	3:F:158:ASN:H	1.55	0.54
1:G:48:ASN:OD1	1:G:60:GLN:NE2	2.40	0.54
2:B:40:ALA:HB3	2:B:43:GLN:HB2	1.90	0.54
2:B:30:THR:HA	2:B:53:PRO:HB2	1.90	0.54
2:E:72:ARG:HD2	2:E:72:ARG:C	2.33	0.53
2:H:36:TRP:CD1	2:H:70:MET:HE2	2.42	0.53
3:L:124:GLN:HG2	3:L:129:THR:O	2.07	0.53
1:J:118:GLY:HA3	1:J:142:TRP:CE2	2.42	0.53
3:C:142:ARG:NH2	3:C:163:VAL:HG21	2.23	0.53
1:A:40:SER:O	1:A:44:ARG:HA	2.09	0.53
2:E:36:TRP:HB2	2:E:70:MET:HE2	1.91	0.53
1:G:118:GLY:HA3	1:G:142:TRP:CE2	2.43	0.52
3:I:142:ARG:NH2	3:I:163:VAL:HG21	2.24	0.52
1:G:126:LYS:HD3	1:G:134:HIS:CE1	2.44	0.52
1:G:4:VAL:HG23	1:G:106:GLU:HB3	1.90	0.52
1:A:118:GLY:HA3	1:A:142:TRP:NE1	2.24	0.52
1:J:47:VAL:HG11	1:J:82:LEU:HD21	1.92	0.52
2:B:36:TRP:CD1	2:B:70:MET:HE2	2.45	0.52
2:B:129:PRO:HD2	2:B:215:THR:HG21	1.92	0.52
3:L:82:ASP:O	3:L:86:TYR:OH	2.22	0.52
3:C:211:ARG:HH11	3:C:211:ARG:CB	2.21	0.52
3:C:211:ARG:CB	3:C:211:ARG:NH1	2.72	0.52
1:G:137:CYS:O	1:G:176:ALA:HA	2.10	0.52
3:F:142:ARG:NH2	3:F:163:VAL:HG21	2.24	0.52
2:E:165:ASN:OD1	2:E:205:ILE:N	2.32	0.52
3:I:81:GLU:CD	3:I:81:GLU:H	2.18	0.51
1:G:118:GLY:HA3	1:G:142:TRP:NE1	2.26	0.51
1:D:97:CYS:O	1:D:107:LYS:HA	2.10	0.51
1:D:118:GLY:HA3	1:D:142:TRP:NE1	2.26	0.51
1:D:21:LEU:HD12	1:D:82:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:GLN:H	2:B:6:GLN:CD	2.19	0.51
3:I:122:ASP:HA	3:I:125:LEU:HD12	1.93	0.51
2:K:40:ALA:HB3	2:K:43:GLN:HB2	1.92	0.51
1:A:41:SER:N	1:A:94:LYS:O	2.43	0.51
2:E:194:VAL:HG11	2:E:204:TYR:CE1	2.46	0.51
2:H:72:ARG:HD3	2:H:74:THR:HG23	1.92	0.51
3:I:113:PRO:CB	3:I:139:PHE:HB3	2.41	0.50
1:D:47:VAL:HG11	1:D:82:LEU:HD21	1.94	0.50
3:I:108:ARG:HD2	3:I:171:SER:O	2.11	0.50
2:K:36:TRP:HB2	2:K:70:MET:HE2	1.93	0.50
2:B:6:GLN:CD	2:B:115:GLN:HB3	2.36	0.50
2:K:46:GLU:OE2	2:K:63:LYS:NZ	2.34	0.50
2:E:35:HIS:HA	2:E:50:TRP:HB3	1.93	0.50
2:E:113:TRP:CD2	3:F:44:PRO:HG2	2.47	0.50
2:K:13:LYS:NZ	2:K:124:ALA:O	2.44	0.50
1:D:52:ASP:OD1	2:E:32:TYR:OH	2.20	0.50
1:G:37:LYS:NZ	2:H:103:MET:SD	2.84	0.50
1:G:127:GLY:HA2	1:J:212:PHE:HE1	1.77	0.50
3:L:79:GLN:N	3:L:82:ASP:OD2	2.41	0.50
3:C:105:GLU:OE1	3:C:173:TYR:OH	2.25	0.50
3:C:150:VAL:CG2	3:C:192:TYR:CE2	2.92	0.50
2:B:18:VAL:O	2:B:82:GLU:HA	2.12	0.49
2:E:6:GLN:H	2:E:115:GLN:NE2	2.08	0.49
2:K:136:PRO:HG3	2:K:199:LEU:HD21	1.94	0.49
3:C:122:ASP:O	3:C:125:LEU:HB2	2.12	0.49
1:A:118:GLY:HA3	1:A:142:TRP:CD1	2.47	0.49
2:H:195:PRO:HG2	2:H:198:SER:HB2	1.95	0.49
3:L:113:PRO:CB	3:L:139:PHE:HB3	2.43	0.49
2:B:29:PHE:CE2	2:B:53:PRO:HB3	2.48	0.49
3:F:39:LYS:HE2	3:F:84:ALA:HB2	1.93	0.49
1:D:160:THR:CG2	1:D:177:ALA:HB1	2.43	0.49
2:E:6:GLN:OE1	2:E:116:GLY:N	2.45	0.49
2:K:36:TRP:CE2	2:K:81:MET:HB2	2.47	0.49
3:C:186:TYR:CD1	3:C:186:TYR:C	2.86	0.48
1:J:37:LYS:HD3	1:J:39:VAL:HG13	1.95	0.48
3:I:54:LEU:HD11	3:I:58:VAL:HB	1.95	0.48
1:A:59:ARG:HD3	2:B:103:MET:HE3	1.96	0.48
1:D:94:LYS:HB3	1:D:109:LEU:HD11	1.96	0.48
1:A:182:ARG:HA	1:A:213:PHE:HE2	1.78	0.48
2:H:87:ARG:NH2	2:H:88:SER:OG	2.46	0.48
3:L:18:ARG:HG2	3:L:18:ARG:HH11	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:VAL:HG21	2:H:103:MET:HE1	1.96	0.48
1:A:209:ALA:HB2	1:D:126:LYS:HA	1.96	0.47
1:J:182:ARG:HA	1:J:213:PHE:HE2	1.78	0.47
3:F:124:GLN:HG2	3:F:129:THR:O	2.13	0.47
3:F:16:GLY:HA2	3:F:77:SER:HA	1.96	0.47
1:A:168:ASP:OD1	1:A:172:LEU:N	2.45	0.47
3:C:113:PRO:CB	3:C:139:PHE:HB3	2.45	0.47
3:L:48:ILE:HD13	3:L:54:LEU:HA	1.97	0.47
1:D:130:ASP:HB3	1:D:180:ILE:HD13	1.96	0.47
2:H:207:ASN:ND2	2:H:218:ASP:OD2	2.48	0.47
1:D:7:PRO:HG3	1:D:22:PRO:HD2	1.97	0.47
2:E:36:TRP:CD1	2:E:70:MET:HE2	2.49	0.47
1:G:207:SER:HB2	1:J:122:HIS:NE2	2.30	0.47
3:L:108:ARG:NH1	3:L:109:THR:O	2.48	0.47
2:B:16:ALA:O	2:B:86:LEU:HG	2.14	0.47
3:C:151:ASP:OD1	3:C:189:HIS:HB3	2.13	0.47
1:G:39:VAL:HG22	1:G:96:LEU:HB2	1.97	0.47
3:L:81:GLU:H	3:L:81:GLU:CD	2.21	0.47
1:D:4:VAL:C	1:D:5:LEU:HD23	2.40	0.47
1:D:56:VAL:HG12	1:D:58:ASP:OD1	2.15	0.47
2:H:194:VAL:HG11	2:H:204:TYR:CZ	2.50	0.46
1:G:152:ASN:ND2	1:G:156:GLU:OE1	2.38	0.46
1:J:59:ARG:HD3	2:K:103:MET:CE	2.45	0.46
1:J:137:CYS:O	1:J:176:ALA:HA	2.16	0.46
2:H:164:TRP:CZ3	2:H:206:CYS:HB2	2.50	0.46
3:L:211:ARG:HH11	3:L:211:ARG:HB2	1.81	0.46
2:B:219:LYS:HZ3	3:C:123:GLU:CD	2.20	0.46
1:J:118:GLY:HA3	1:J:142:TRP:NE1	2.30	0.46
1:G:41:SER:HA	1:G:44:ARG:HH21	1.81	0.46
1:A:102:GLY:O	2:B:99:ARG:NH2	2.49	0.46
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.51	0.46
1:J:97:CYS:O	1:J:107:LYS:HA	2.16	0.46
3:L:24:ARG:NH2	3:L:70:ASP:OD1	2.49	0.46
3:L:145:LYS:HB3	3:L:197:THR:OG1	2.16	0.46
3:L:210:ASN:O	3:L:212:GLY:N	2.48	0.46
2:B:148:LEU:HD13	2:B:221:VAL:HG11	1.97	0.46
3:I:108:ARG:NH1	3:I:109:THR:O	2.49	0.46
1:D:137:CYS:O	1:D:176:ALA:HA	2.16	0.45
2:E:36:TRP:CE2	2:E:81:MET:HB2	2.50	0.45
2:E:203:THR:HA	2:E:220:LYS:HE3	1.98	0.45
2:H:36:TRP:HB2	2:H:70:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:168:ASP:OD1	1:J:172:LEU:N	2.49	0.45
2:B:93:VAL:CG1	2:B:116:GLY:HA3	2.46	0.45
3:F:105:GLU:OE2	3:F:140:TYR:OH	2.34	0.45
1:D:138:ARG:HE	1:D:138:ARG:HB3	1.58	0.45
2:B:166:SER:N	2:B:207:ASN:OD1	2.39	0.45
1:G:123:VAL:HG11	1:G:206:ILE:HD12	1.98	0.45
2:E:35:HIS:HE1	2:E:50:TRP:CD1	2.28	0.45
2:E:87:ARG:HD2	2:E:87:ARG:HA	1.55	0.45
2:B:36:TRP:CE2	2:B:81:MET:HB2	2.51	0.45
2:E:35:HIS:HB2	2:E:97:ALA:O	2.16	0.45
3:F:39:LYS:HB2	3:F:42:LYS:HG3	1.99	0.45
2:H:132:PHE:CE2	3:I:124:GLN:HG3	2.52	0.45
1:A:17:GLU:O	1:A:87:VAL:HG23	2.15	0.45
1:D:113:LYS:HD3	1:D:197:LEU:HD11	1.99	0.45
3:I:35:TRP:HB2	3:I:48:ILE:HB	1.99	0.44
2:B:47:TRP:CH2	2:B:49:GLY:HA2	2.53	0.44
1:G:127:GLY:HA2	1:J:212:PHE:CE1	2.52	0.44
3:C:113:PRO:HB3	3:C:139:PHE:CD2	2.52	0.44
2:E:30:THR:HA	2:E:53:PRO:HB2	1.99	0.44
2:E:47:TRP:CH2	2:E:49:GLY:HA2	2.53	0.44
2:E:166:SER:N	2:E:207:ASN:OD1	2.41	0.44
1:G:7:PRO:HD3	1:G:22:PRO:O	2.17	0.44
1:A:97:CYS:O	1:A:107:LYS:HA	2.17	0.44
3:F:158:ASN:H	3:F:158:ASN:ND2	2.15	0.44
2:H:3:GLN:O	2:H:4:LEU:HD23	2.17	0.44
3:I:123:GLU:H	3:I:123:GLU:CD	2.25	0.44
1:J:135:LEU:O	1:J:178:SER:HA	2.17	0.44
1:J:182:ARG:HA	1:J:213:PHE:CE2	2.53	0.44
2:B:127:LYS:HD3	2:B:185:LEU:HD21	2.00	0.44
3:C:123:GLU:HA	3:C:126:LYS:HD2	2.00	0.44
3:C:151:ASP:OD2	3:C:189:HIS:CG	2.71	0.44
1:A:159:PRO:O	1:A:179:VAL:HG12	2.18	0.44
2:K:29:PHE:CE2	2:K:53:PRO:HB3	2.52	0.44
2:K:136:PRO:HG3	2:K:199:LEU:CD2	2.48	0.44
1:D:37:LYS:HG3	1:D:49:VAL:HG22	2.00	0.44
2:E:3:GLN:O	2:E:4:LEU:HD23	2.18	0.44
3:I:105:GLU:OE2	3:I:140:TYR:OH	2.34	0.44
1:J:137:CYS:HB2	1:J:150:TRP:CZ2	2.53	0.44
1:J:209:ALA:HB1	1:J:211:PRO:HD2	2.00	0.44
3:L:126:LYS:HB2	3:L:126:LYS:HE3	1.78	0.44
2:E:33:TYR:CE2	2:E:52:ASN:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:158:ASN:HD22	3:F:158:ASN:N	2.13	0.43
3:F:211:ARG:CZ	3:F:211:ARG:HB3	2.47	0.43
1:J:188:GLY:HA3	1:J:206:ILE:O	2.18	0.43
3:C:125:LEU:HD23	3:C:125:LEU:HA	1.74	0.43
3:F:170:ASP:CG	3:F:172:THR:HG22	2.43	0.43
1:G:52:ASP:OD1	2:H:32:TYR:OH	2.33	0.43
3:C:181:LEU:HA	3:C:181:LEU:HD23	1.76	0.43
2:B:129:PRO:CB	2:B:155:TYR:HB3	2.46	0.43
3:F:94:PHE:HA	3:F:95:PRO:HA	1.88	0.43
2:H:148:LEU:HD21	2:H:204:TYR:CD2	2.53	0.43
3:I:79:GLN:N	3:I:82:ASP:OD2	2.52	0.43
2:B:87:ARG:HH11	2:B:87:ARG:HD3	1.63	0.43
1:G:150:TRP:HD1	1:G:160:THR:HG23	1.84	0.43
2:B:36:TRP:HB2	2:B:70:MET:HE2	2.01	0.43
2:B:48:MET:HE2	2:B:48:MET:HB3	1.88	0.43
3:C:39:LYS:HB3	3:C:40:PRO:HD2	1.99	0.43
2:K:127:LYS:HG3	2:K:128:GLY:N	2.34	0.43
3:I:37:GLN:HB2	3:I:47:LEU:HD11	2.01	0.43
3:F:46:LEU:HD21	3:F:49:TYR:HB3	2.00	0.43
1:G:117:LEU:HD12	1:G:117:LEU:HA	1.91	0.43
3:I:106:ILE:HB	3:I:166:GLN:NE2	2.34	0.43
1:J:37:LYS:HB3	1:J:98:TYR:HB2	2.00	0.43
1:J:40:SER:O	1:J:44:ARG:HA	2.19	0.43
1:A:115:ALA:HB2	1:A:197:LEU:HD23	2.00	0.43
1:G:47:VAL:HG11	1:G:82:LEU:HD21	2.01	0.43
1:G:118:GLY:HA3	1:G:142:TRP:CD1	2.54	0.42
2:H:164:TRP:HB2	2:H:169:LEU:HB3	2.01	0.42
1:A:127:GLY:HA2	1:D:212:PHE:CZ	2.54	0.42
2:B:2:VAL:HG23	2:B:27:TYR:CD1	2.54	0.42
2:E:220:LYS:HE2	2:E:222:GLU:HG2	2.00	0.42
1:G:11:ILE:HD13	1:G:20:ASP:O	2.19	0.42
2:H:199:LEU:HD23	2:H:199:LEU:HA	1.66	0.42
2:B:203:THR:HG23	2:B:220:LYS:CD	2.50	0.42
1:J:37:LYS:HD3	1:J:39:VAL:CG1	2.50	0.42
1:A:118:GLY:HA3	1:A:142:TRP:CE2	2.55	0.42
3:F:145:LYS:HB3	3:F:197:THR:OG1	2.20	0.42
3:C:128:GLY:C	3:C:183:LYS:HB2	2.45	0.42
3:C:145:LYS:HB3	3:C:197:THR:OG1	2.19	0.42
1:G:11:ILE:HD11	1:G:22:PRO:CD	2.49	0.42
1:G:133:ILE:HG23	1:J:212:PHE:HZ	1.85	0.42
3:I:39:LYS:HB3	3:I:40:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:LEU:HB3	3:C:118:PHE:CD1	2.54	0.42
1:D:115:ALA:HB2	1:D:197:LEU:HD23	2.01	0.42
2:E:6:GLN:N	2:E:115:GLN:HE22	2.12	0.42
3:I:113:PRO:HB3	3:I:139:PHE:CD2	2.55	0.42
3:L:150:VAL:HG22	3:L:192:TYR:CD2	2.55	0.42
1:A:5:LEU:HB2	1:A:24:HIS:CD2	2.55	0.42
1:A:209:ALA:HB1	1:A:211:PRO:HD2	2.01	0.42
3:F:39:LYS:HB3	3:F:40:PRO:HD2	2.01	0.42
3:F:39:LYS:NZ	3:F:81:GLU:O	2.48	0.42
2:H:30:THR:HA	2:H:53:PRO:HB2	2.02	0.42
2:K:133:PRO:O	2:K:134:LEU:HD23	2.19	0.42
3:C:128:GLY:HA2	3:C:183:LYS:HB2	2.02	0.42
1:A:137:CYS:O	1:A:176:ALA:HA	2.19	0.41
2:H:103:MET:HG3	2:H:104:ILE:N	2.35	0.41
1:A:26:PHE:CD1	1:A:27:PRO:HA	2.54	0.41
2:E:154:ASP:OD1	2:E:181:GLN:NE2	2.50	0.41
1:J:21:LEU:HB3	1:J:110:VAL:HG11	2.02	0.41
2:K:50:TRP:CD1	2:K:59:LYS:HB3	2.55	0.41
1:A:7:PRO:HD3	1:A:22:PRO:O	2.20	0.41
1:D:102:GLY:O	2:E:99:ARG:NH2	2.52	0.41
3:F:37:GLN:HB2	3:F:47:LEU:HD11	2.03	0.41
1:G:97:CYS:SG	1:G:108:ALA:HB3	2.59	0.41
3:I:184:ALA:O	3:I:188:LYS:HG3	2.20	0.41
2:K:129:PRO:HD2	2:K:215:THR:HG21	2.01	0.41
2:B:127:LYS:HG2	2:B:154:ASP:O	2.20	0.41
1:G:97:CYS:O	1:G:107:LYS:HA	2.19	0.41
2:B:108:TYR:CB	3:C:96:PRO:HG3	2.50	0.41
2:E:161:THR:HB	2:E:209:ASN:HB3	2.02	0.41
3:L:170:ASP:OD1	3:L:172:THR:HG22	2.19	0.41
2:B:35:HIS:HE2	2:B:99:ARG:HG3	1.86	0.41
2:B:38:ARG:NH1	2:B:64:PHE:HE1	2.19	0.41
3:C:79:GLN:N	3:C:82:ASP:OD2	2.48	0.41
2:E:81:MET:HE3	2:E:81:MET:HB3	1.98	0.41
1:G:35:GLU:OE2	2:H:101:SER:OG	2.26	0.41
2:H:13:LYS:NZ	2:H:124:ALA:O	2.54	0.41
2:K:127:LYS:HD3	2:K:185:LEU:HD21	2.03	0.41
3:L:161:GLU:HA	3:L:176:SER:O	2.21	0.41
1:A:4:VAL:HG23	1:A:106:GLU:HB3	2.03	0.41
1:G:67:ARG:HH22	1:G:91:ASP:CG	2.24	0.41
1:G:133:ILE:O	1:G:180:ILE:HA	2.20	0.41
2:H:35:HIS:CE1	2:H:50:TRP:HE3	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ARG:HA	1:A:213:PHE:CE2	2.56	0.41
3:C:170:ASP:OD1	3:C:172:THR:HG22	2.20	0.41
1:D:67:ARG:NH2	1:D:91:ASP:OD2	2.36	0.41
2:E:176:PHE:CE2	3:F:176:SER:HB3	2.56	0.41
2:H:32:TYR:CG	2:H:98:ARG:HD2	2.56	0.41
2:H:160:VAL:CG2	2:H:210:HIS:HD2	2.34	0.41
3:I:61:ARG:NH1	3:I:82:ASP:OD1	2.48	0.41
1:J:58:ASP:OD1	1:J:58:ASP:N	2.53	0.41
2:E:145:THR:HG22	2:E:195:PRO:HA	2.03	0.41
3:F:140:TYR:CD1	3:F:141:PRO:HA	2.56	0.41
1:G:142:TRP:CG	1:G:146:PRO:HG3	2.56	0.41
2:H:173:VAL:HG22	2:H:192:VAL:HG23	2.03	0.41
2:E:154:ASP:HA	2:E:185:LEU:HB3	2.02	0.41
1:G:102:GLY:O	2:H:99:ARG:NH2	2.54	0.41
2:K:50:TRP:CD1	2:K:50:TRP:C	2.99	0.41
3:F:82:ASP:O	3:F:86:TYR:OH	2.26	0.40
2:H:160:VAL:HG22	2:H:210:HIS:HD2	1.86	0.40
2:K:60:TYR:HE1	2:K:70:MET:SD	2.44	0.40
3:L:38:GLN:O	3:L:84:ALA:HB1	2.21	0.40
3:C:170:ASP:CG	3:C:172:THR:HG22	2.47	0.40
1:D:167:ALA:HB2	1:D:173:TYR:CD1	2.57	0.40
2:E:207:ASN:HB3	2:E:216:LYS:NZ	2.37	0.40
1:G:43:LEU:HD12	1:G:43:LEU:HA	1.86	0.40
2:H:48:MET:HE2	2:H:48:MET:HB3	1.97	0.40
3:I:126:LYS:HE3	3:I:126:LYS:HB2	1.87	0.40
2:K:14:PRO:HB3	2:K:87:ARG:NH1	2.36	0.40
1:A:19:ALA:O	1:A:83:ARG:HA	2.21	0.40
3:C:185:ASP:N	3:C:185:ASP:OD1	2.55	0.40
2:E:86:LEU:HD13	2:E:121:VAL:HG22	2.04	0.40
3:L:35:TRP:O	3:L:47:LEU:HB2	2.21	0.40
3:L:146:VAL:HG22	3:L:196:VAL:HG22	2.03	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)
1:G:69:SER:OG	3:L:190:LYS:NZ[3_555]	2.19	0.01

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	206/226 (91%)	204 (99%)	1 (0%)	1 (0%)	24	60
1	D	206/226 (91%)	202 (98%)	3 (2%)	1 (0%)	24	60
1	G	206/226 (91%)	204 (99%)	1 (0%)	1 (0%)	24	60
1	J	206/226 (91%)	204 (99%)	1 (0%)	1 (0%)	24	60
2	B	212/223 (95%)	205 (97%)	7 (3%)	0	100	100
2	E	212/223 (95%)	207 (98%)	5 (2%)	0	100	100
2	H	212/223 (95%)	208 (98%)	4 (2%)	0	100	100
2	K	212/223 (95%)	207 (98%)	5 (2%)	0	100	100
3	C	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
3	F	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
3	I	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
3	L	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
All	All	2512/2644 (95%)	2452 (98%)	56 (2%)	4 (0%)	43	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	22	PRO
1	G	22	PRO
1	J	22	PRO
1	A	22	PRO

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	171/181 (94%)	171 (100%)	0	100	100
1	D	171/181 (94%)	171 (100%)	0	100	100
1	G	171/181 (94%)	171 (100%)	0	100	100
1	J	171/181 (94%)	169 (99%)	2 (1%)	63	82
2	B	181/186 (97%)	177 (98%)	4 (2%)	45	74
2	E	181/186 (97%)	181 (100%)	0	100	100
2	H	181/186 (97%)	181 (100%)	0	100	100
2	K	181/186 (97%)	181 (100%)	0	100	100
3	C	183/183 (100%)	181 (99%)	2 (1%)	65	83
3	F	183/183 (100%)	182 (100%)	1 (0%)	81	89
3	I	183/183 (100%)	183 (100%)	0	100	100
3	L	183/183 (100%)	183 (100%)	0	100	100
All	All	2140/2200 (97%)	2131 (100%)	9 (0%)	84	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	68	VAL
2	B	87	ARG
2	B	219	LYS
2	B	221	VAL
3	C	182	SER
3	C	189	HIS
3	F	158	ASN
1	J	43	LEU
1	J	157	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
2	B	54	ASN
3	C	37	GLN
3	C	79	GLN
2	E	181	GLN
3	F	166	GLN

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Mol	Chain	Res	Type
1	G	45	GLN
2	H	181	GLN
1	J	149	GLN
1	J	157	ASN
3	L	37	GLN
3	L	79	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
2	PCA	H	1	2	7,8,9	1.94	1 (14%)	9,10,12	2.23	5 (55%)
2	PCA	E	1	2	7,8,9	1.92	1 (14%)	9,10,12	2.24	5 (55%)
2	PCA	K	1	2	7,8,9	1.95	1 (14%)	9,10,12	2.25	5 (55%)
2	PCA	B	1	2	7,8,9	1.94	1 (14%)	9,10,12	2.26	5 (55%)

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
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1
2	PCA	E	1	2	-	0/0/11/13	0/1/1/1
2	PCA	K	1	2	-	0/0/11/13	0/1/1/1
2	PCA	B	1	2	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	PCA	CD-N	5.06	1.47	1.34
2	H	1	PCA	CD-N	5.01	1.47	1.34
2	B	1	PCA	CD-N	5.01	1.47	1.34
2	E	1	PCA	CD-N	4.95	1.46	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	PCA	CB-CA-C	-3.15	108.34	112.66
2	K	1	PCA	OE-CD-CG	-3.04	121.30	126.72
2	H	1	PCA	CB-CA-N	3.00	111.50	103.24
2	H	1	PCA	OE-CD-CG	-2.99	121.39	126.72
2	E	1	PCA	OE-CD-CG	-2.97	121.41	126.72
2	B	1	PCA	OE-CD-CG	-2.97	121.42	126.72
2	E	1	PCA	CB-CA-N	2.96	111.40	103.24
2	B	1	PCA	CB-CA-N	2.94	111.34	103.24
2	H	1	PCA	CA-N-CD	-2.92	103.58	113.58
2	E	1	PCA	CA-N-CD	-2.91	103.62	113.58
2	B	1	PCA	CA-N-CD	-2.90	103.66	113.58
2	K	1	PCA	CA-N-CD	-2.78	104.07	113.58
2	K	1	PCA	CB-CA-N	2.74	110.78	103.24
2	E	1	PCA	CB-CA-C	-2.71	108.94	112.66
2	E	1	PCA	CG-CD-N	2.67	114.93	108.39
2	B	1	PCA	CG-CD-N	2.67	114.93	108.39
2	B	1	PCA	CB-CA-C	-2.66	109.01	112.66
2	H	1	PCA	CG-CD-N	2.65	114.88	108.39
2	K	1	PCA	CG-CD-N	2.60	114.74	108.39
2	H	1	PCA	CB-CA-C	-2.47	109.26	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

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	210/226 (92%)	0.41	9 (4%)	40 21	49, 79, 113, 127	0
1	D	210/226 (92%)	0.48	12 (5%)	29 15	51, 75, 114, 133	0
1	G	210/226 (92%)	0.04	2 (0%)	79 59	35, 59, 106, 129	0
1	J	210/226 (92%)	0.36	10 (4%)	35 19	46, 64, 109, 135	0
2	B	215/223 (96%)	0.15	4 (1%)	66 43	40, 61, 123, 146	0
2	E	215/223 (96%)	0.76	14 (6%)	25 13	61, 98, 148, 173	0
2	H	215/223 (96%)	0.29	7 (3%)	49 28	38, 71, 134, 156	0
2	K	215/223 (96%)	0.06	3 (1%)	73 51	41, 59, 95, 132	0
3	C	212/212 (100%)	0.27	1 (0%)	87 72	43, 77, 137, 150	0
3	F	212/212 (100%)	0.60	12 (5%)	29 15	46, 105, 132, 149	0
3	I	212/212 (100%)	0.22	4 (1%)	66 43	33, 76, 108, 124	0
3	L	212/212 (100%)	0.01	1 (0%)	87 72	41, 63, 85, 96	0
All	All	2548/2644 (96%)	0.30	79 (3%)	51 30	33, 72, 127, 173	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	164	PRO	5.3
3	F	118	PHE	3.6
1	J	161	VAL	3.6
1	D	164	PRO	3.4
1	A	184	SER	3.4
1	J	128	TYR	3.4
2	H	205	ILE	3.4
1	A	211	PRO	3.2
1	G	184	SER	3.2
3	F	193	ALA	3.1
2	H	196	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	E	103	MET	3.1
1	J	136	GLU	3.0
3	I	212	GLY	3.0
2	H	103	MET	3.0
2	E	50	TRP	2.9
1	A	161	VAL	2.8
2	B	137	SER	2.8
2	H	137	SER	2.8
3	F	166	GLN	2.7
2	H	223	PRO	2.7
1	J	165	VAL	2.6
1	A	128	TYR	2.6
1	A	136	GLU	2.6
1	D	160	THR	2.6
2	H	145	THR	2.6
1	D	183	GLY	2.6
3	I	148	TRP	2.6
2	K	103	MET	2.6
3	L	161	GLU	2.6
1	J	184	SER	2.5
2	B	115	GLN	2.5
2	K	2	VAL	2.5
1	J	163	ALA	2.4
1	G	183	GLY	2.4
2	B	201	THR	2.4
1	A	134	HIS	2.4
1	D	205	SER	2.4
3	F	199	GLN	2.4
2	E	218	ASP	2.4
3	F	212	GLY	2.4
1	D	43	LEU	2.4
1	D	161	VAL	2.3
2	E	203	THR	2.3
1	D	153	ASN	2.3
1	D	145	GLN	2.3
2	H	195	PRO	2.3
2	B	202	GLN	2.3
1	A	166	VAL	2.2
2	E	43	GLN	2.2
2	E	133	PRO	2.2
2	K	201	THR	2.2
3	F	205	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	89	ASP	2.2
1	D	213	PHE	2.2
1	D	42	SER	2.2
2	E	58	THR	2.1
2	E	161	THR	2.1
1	A	163	ALA	2.1
1	D	165	VAL	2.1
1	J	126	LYS	2.1
2	E	201	THR	2.1
3	F	109	THR	2.1
3	F	117	ILE	2.1
2	E	136	PRO	2.1
3	F	110	VAL	2.1
3	C	70	ASP	2.1
2	E	193	THR	2.1
2	E	10	GLU	2.1
3	I	76	SER	2.1
1	D	162	GLU	2.1
3	F	209	PHE	2.1
3	F	203	SER	2.0
1	J	138	ARG	2.0
1	J	181	MET	2.0
2	E	9	ALA	2.0
3	I	190	LYS	2.0
1	A	165	VAL	2.0
3	F	181	LEU	2.0

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

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(Å ²)	Q<0.9
2	PCA	B	1	8/9	0.67	0.14	73,76,81,82	0
2	PCA	E	1	8/9	0.68	0.13	89,95,100,103	0
2	PCA	K	1	8/9	0.68	0.14	66,80,86,89	0
2	PCA	H	1	8/9	0.80	0.13	57,75,89,95	0

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.