



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:44 PM UTC

PDB ID : 6W5O / pdb_00006w5o
Title : Class D beta-lactamase BAT-2 delta mutant
Authors : Smith, C.A.; Vakulenko, S.B.; Stewart, N.K.; Toth, M.
Deposited on : 2020-03-13
Resolution : 2.55 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

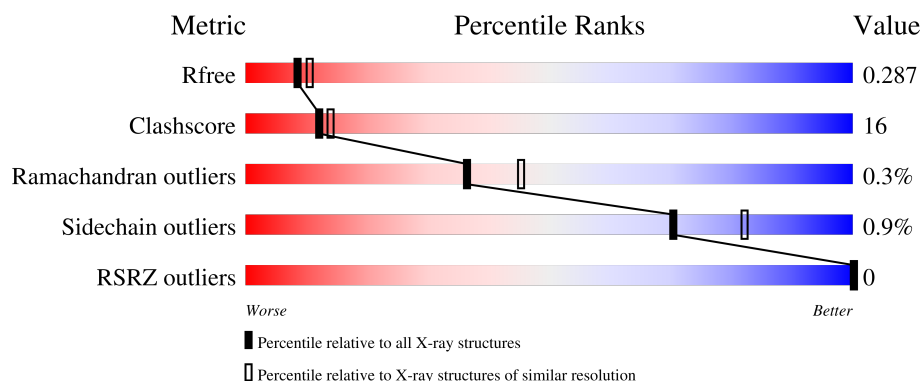
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	264	 56% 32% 11%
1	B	264	 60% 27% 11%
1	C	264	 59% 27% 11%
1	D	264	 61% 27% 11%
1	E	264	 62% 25% 11%

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Mol	Chain	Length	Quality of chain
1	F	264	 56%32%•11%
1	G	264	 53%33%•11%
1	H	264	 62%26%•11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15710 atoms, of which 6 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 BAT-2 Beta-lactamase delta mutant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	2	0
			1948	1237	330	375	6			
1	B	234	Total	C	N	O	S	0	1	0
			1940	1232	327	375	6			
1	C	234	Total	C	N	O	S	0	1	0
			1940	1232	327	375	6			
1	D	234	Total	C	N	O	S	0	1	0
			1932	1226	330	370	6			
1	E	234	Total	C	N	O	S	0	0	0
			1934	1228	327	373	6			
1	F	234	Total	C	N	O	S	0	1	0
			1939	1232	330	371	6			
1	G	234	Total	C	N	O	S	0	0	0
			1934	1228	327	373	6			
1	H	234	Total	C	N	O	S	0	1	0
			1940	1232	327	375	6			

There are 24 discrepancies between the modelled and reference sequences:

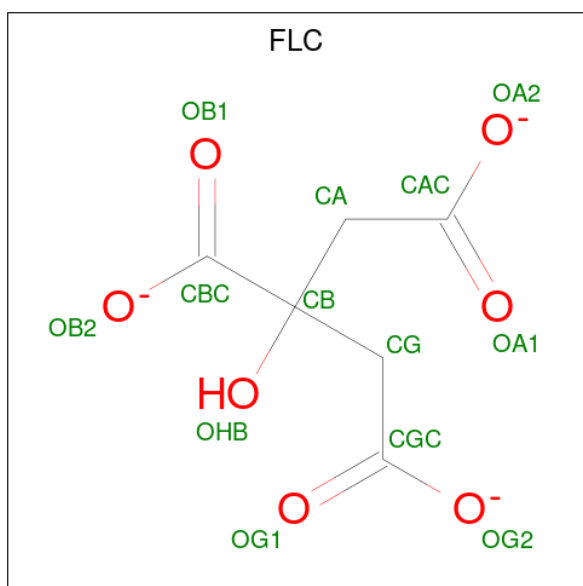
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP A0A0H3EA14
A	?	-	LEU	deletion	UNP A0A0H3EA14
A	?	-	THR	deletion	UNP A0A0H3EA14
B	?	-	ARG	deletion	UNP A0A0H3EA14
B	?	-	LEU	deletion	UNP A0A0H3EA14
B	?	-	THR	deletion	UNP A0A0H3EA14
C	?	-	ARG	deletion	UNP A0A0H3EA14
C	?	-	LEU	deletion	UNP A0A0H3EA14
C	?	-	THR	deletion	UNP A0A0H3EA14
D	?	-	ARG	deletion	UNP A0A0H3EA14
D	?	-	LEU	deletion	UNP A0A0H3EA14
D	?	-	THR	deletion	UNP A0A0H3EA14
E	?	-	ARG	deletion	UNP A0A0H3EA14

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LEU	deletion	UNP A0A0H3EA14
E	?	-	THR	deletion	UNP A0A0H3EA14
F	?	-	ARG	deletion	UNP A0A0H3EA14
F	?	-	LEU	deletion	UNP A0A0H3EA14
F	?	-	THR	deletion	UNP A0A0H3EA14
G	?	-	ARG	deletion	UNP A0A0H3EA14
G	?	-	LEU	deletion	UNP A0A0H3EA14
G	?	-	THR	deletion	UNP A0A0H3EA14
H	?	-	ARG	deletion	UNP A0A0H3EA14
H	?	-	LEU	deletion	UNP A0A0H3EA14
H	?	-	THR	deletion	UNP A0A0H3EA14

- Molecule 2 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is water.

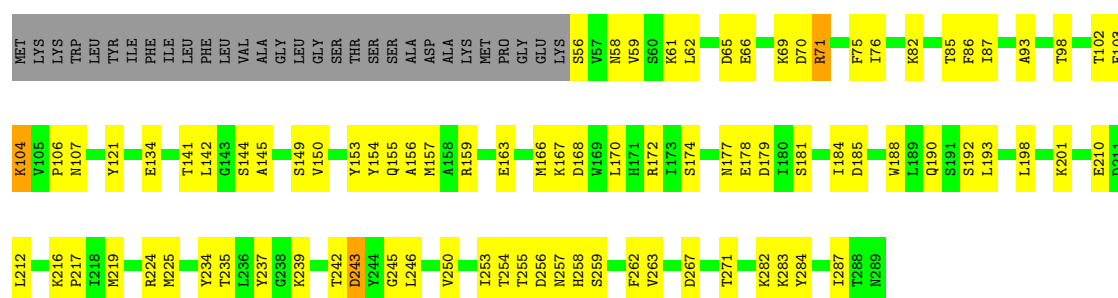
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	B	28	Total	O	0	0
			28	28		
4	C	29	Total	O	0	0
			29	29		
4	D	21	Total	O	0	0
			21	21		
4	E	21	Total	O	0	0
			21	21		
4	F	19	Total	O	0	0
			19	19		
4	G	15	Total	O	0	0
			15	15		
4	H	18	Total	O	0	0
			18	18		

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.

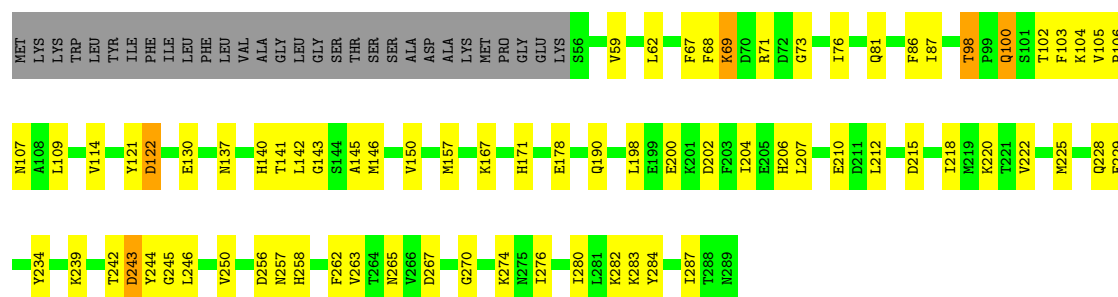
• Molecule 1: BAT-2 Beta-lactamase delta mutant

Chain A: 



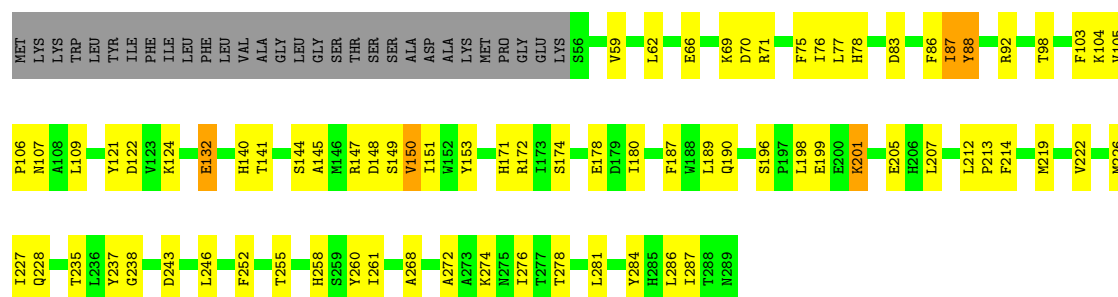
• Molecule 1: BAT-2 Beta-lactamase delta mutant

Chain B: 



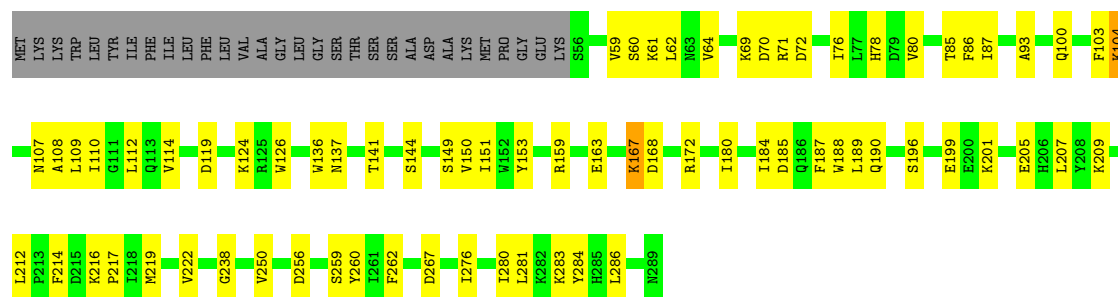
• Molecule 1: BAT-2 Beta-lactamase delta mutant

Chain C: 



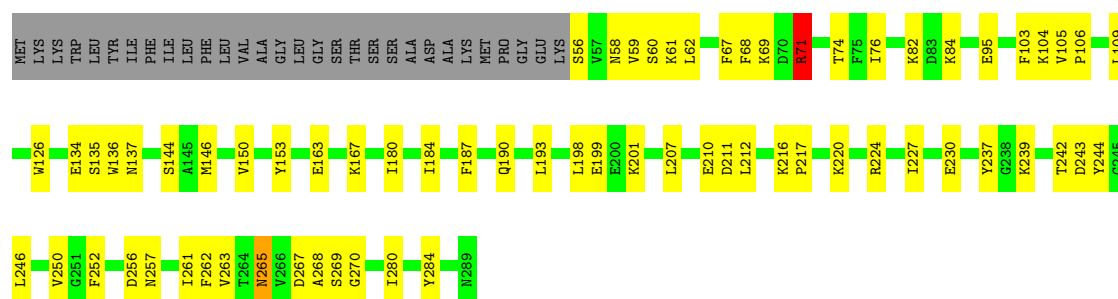
- Molecule 1: BAT-2 Beta-lactamase delta mutant

Chain D: 



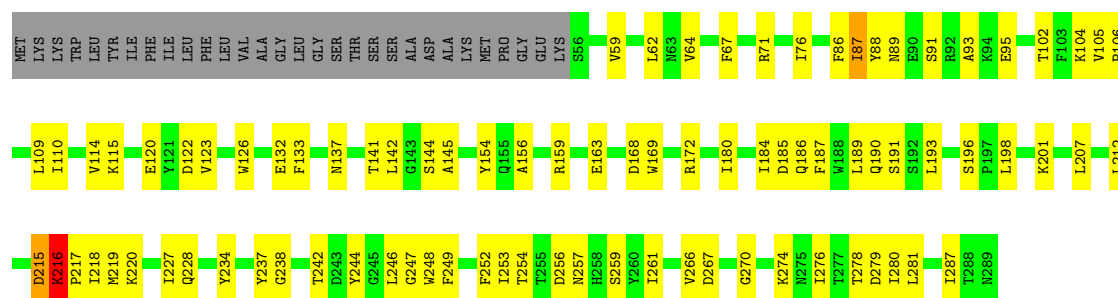
- Molecule 1: BAT-2 Beta-lactamase delta mutant

Chain E: 



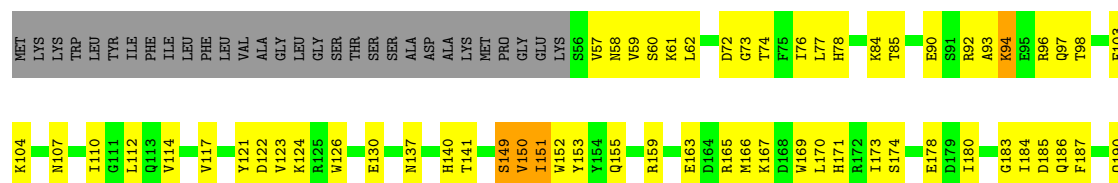
- Molecule 1: BAT-2 Beta-lactamase delta mutant

Chain F: 



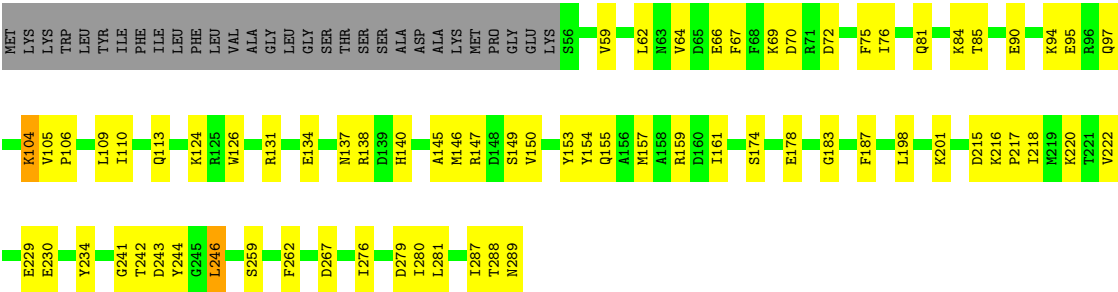
- Molecule 1: BAT-2 Beta-lactamase delta mutant

Chain G: 





- Molecule 1: BAT-2 Beta-lactamase delta mutant



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	133.43Å 66.18Å 134.01Å 90.00° 91.66° 90.00°	Depositor
Resolution (Å)	60.56 – 2.55 60.56 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.6 (60.56-2.55) 89.6 (60.56-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.217 , 0.290 0.218 , 0.287	Depositor DCC
R_{free} test set	3574 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 25.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.140 for l,k,-h 0.053 for h,-k,-l 0.043 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15710	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 39.20 % 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 3.2864e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KCX, FLC, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	3/1987 (0.2%)	0.52	0/2680
1	B	0.57	4/1976 (0.2%)	0.51	2/2666 (0.1%)
1	C	0.77	11/1976 (0.6%)	0.57	0/2666
1	D	0.36	0/1967	0.48	2/2653 (0.1%)
1	E	0.70	6/1967 (0.3%)	0.56	0/2654
1	F	0.65	6/1975 (0.3%)	0.53	0/2664
1	G	0.83	8/1967 (0.4%)	0.66	3/2654 (0.1%)
1	H	0.49	2/1976 (0.1%)	0.47	0/2666
All	All	0.64	40/15791 (0.3%)	0.54	7/21303 (0.0%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	100	GLN	C-O	-7.50	1.17	1.24
1	G	150	VAL	C-O	-7.17	1.15	1.24
1	F	87	ILE	C-O	-6.96	1.16	1.24
1	E	68	PHE	C-O	-6.87	1.14	1.23
1	E	71	ARG	C-O	-6.83	1.15	1.23
1	E	265	ASN	C-O	-6.69	1.16	1.23
1	C	145	ALA	C-O	-6.64	1.15	1.24
1	E	268	ALA	C-O	-6.43	1.18	1.24
1	G	219	MET	C-O	-6.37	1.15	1.24
1	B	71	ARG	C-O	-6.28	1.16	1.23
1	C	147	ARG	C-O	-6.06	1.17	1.24
1	G	152	TRP	C-O	-6.06	1.17	1.24
1	G	193	LEU	C-O	-5.81	1.16	1.24
1	A	174	SER	C-O	-5.81	1.16	1.24
1	B	202	ASP	C-O	-5.71	1.17	1.24
1	F	89	ASN	C-O	-5.69	1.16	1.24
1	A	75	PHE	C-O	-5.60	1.17	1.23
1	C	148	ASP	C-O	-5.58	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	THR	C-O	-5.58	1.17	1.24
1	F	88	TYR	C-O	-5.57	1.17	1.24
1	C	149	SER	C-O	-5.55	1.17	1.23
1	C	87	ILE	C-O	-5.52	1.18	1.24
1	G	149	SER	C-O	-5.48	1.16	1.23
1	C	149	SER	C-N	-5.43	1.28	1.33
1	F	216	LYS	C-O	-5.29	1.19	1.24
1	E	95	GLU	C-O	-5.29	1.17	1.24
1	F	215	ASP	C-O	-5.28	1.17	1.24
1	C	148	ASP	N-CA	-5.21	1.40	1.46
1	C	151	ILE	C-O	-5.21	1.17	1.24
1	F	219	MET	C-O	-5.21	1.17	1.24
1	E	71	ARG	N-CA	-5.18	1.39	1.45
1	C	88	TYR	C-O	-5.15	1.17	1.24
1	G	151	ILE	C-O	-5.12	1.17	1.24
1	H	241	GLY	C-O	-5.12	1.17	1.23
1	C	150	VAL	C-O	-5.11	1.16	1.23
1	B	102	THR	C-O	-5.10	1.17	1.24
1	G	193	LEU	CA-C	-5.07	1.46	1.52
1	H	246	LEU	C-O	-5.06	1.18	1.24
1	C	92	ARG	C-O	-5.03	1.18	1.24
1	G	221	THR	C-O	-5.00	1.18	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	287	ILE	CB-CA-C	-6.20	105.62	112.68
1	G	282	LYS	N-CA-C	-5.62	104.63	112.45
1	B	69	LYS	N-CA-C	5.42	118.11	111.82
1	B	100	GLN	CB-CA-C	-5.37	110.40	116.63
1	D	167	LYS	CA-C-N	5.16	127.15	120.44
1	D	167	LYS	C-N-CA	5.16	127.15	120.44
1	G	285	HIS	N-CA-C	5.12	118.31	111.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1948	0	1878	76	0
1	B	1940	0	1865	60	0
1	C	1940	0	1865	62	0
1	D	1932	0	1863	54	0
1	E	1934	0	1859	59	0
1	F	1939	0	1870	55	0
1	G	1934	0	1859	82	0
1	H	1940	0	1865	48	0
2	B	13	0	5	0	0
3	F	4	6	6	0	0
4	A	29	0	0	2	0
4	B	28	0	0	2	0
4	C	29	0	0	1	0
4	D	21	0	0	0	0
4	E	21	0	0	1	0
4	F	19	0	0	0	0
4	G	15	0	0	1	0
4	H	18	0	0	2	0
All	All	15704	6	14935	474	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 16.

All (474) 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:59:VAL:HA	1:G:62:LEU:HD13	1.36	1.07
1:A:98:THR:HG21	1:A:190:GLN:H	1.18	1.07
1:E:59:VAL:HA	1:E:62:LEU:HD13	1.42	1.02
1:A:212:LEU:HB2	1:A:219:MET:HE3	1.43	1.00
1:A:76:ILE:HD13	1:A:198:LEU:HD23	1.42	0.98
1:B:100:GLN:HE21	1:B:100:GLN:HA	1.32	0.95
1:G:278:THR:O	1:G:282:LYS:HG3	1.67	0.94
1:H:281:LEU:HB2	1:H:287:ILE:HD12	1.49	0.93
1:A:66:GLU:HA	1:A:69:LYS:HD3	1.51	0.90
1:A:70:ASP:HA	1:E:198:LEU:HD13	1.51	0.89
1:A:59:VAL:HA	1:A:62:LEU:HD13	1.52	0.89
1:D:59:VAL:HA	1:D:62:LEU:CD1	2.04	0.88
1:B:100:GLN:HA	1:B:100:GLN:NE2	1.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:GLN:HG2	1:E:244:TYR:CD2	2.10	0.86
1:B:76:ILE:HD13	1:B:198:LEU:HD23	1.57	0.85
1:G:163:GLU:HA	1:G:184:ILE:HD13	1.59	0.84
1:E:60:SER:OG	1:E:84:LYS:HE3	1.79	0.81
1:E:242:THR:HG23	1:E:270:GLY:H	1.44	0.81
1:G:187:PHE:CD1	1:G:193:LEU:HD22	2.16	0.80
1:D:59:VAL:O	1:D:62:LEU:HD12	1.82	0.80
1:A:98:THR:HG23	4:A:306:HOH:O	1.82	0.80
1:H:59:VAL:HA	1:H:62:LEU:CD1	2.12	0.80
1:A:163:GLU:HA	1:A:184:ILE:HD13	1.63	0.80
1:H:281:LEU:CB	1:H:287:ILE:HD12	2.12	0.79
1:G:74:THR:HG21	1:G:93:ALA:HB2	1.64	0.78
1:B:190:GLN:HG2	1:B:244:TYR:CD2	2.19	0.78
1:F:59:VAL:HA	1:F:62:LEU:HD13	1.66	0.78
1:A:242:THR:O	1:A:243:ASP:HB2	1.83	0.76
1:C:281:LEU:HB2	1:C:287:ILE:HD12	1.68	0.76
1:B:242:THR:HG23	1:B:270:GLY:H	1.51	0.75
1:E:242:THR:HG22	1:E:243:ASP:H	1.51	0.75
1:A:98:THR:HG21	1:A:190:GLN:N	2.00	0.75
1:A:70:ASP:HA	1:E:198:LEU:CD1	2.17	0.74
1:A:58:ASN:HD22	1:A:61:LYS:HD2	1.51	0.74
1:G:198:LEU:CD2	1:G:201:LYS:HE3	2.17	0.74
1:F:215:ASP:HB2	1:F:218:ILE:HD12	1.70	0.74
1:G:187:PHE:HD1	1:G:193:LEU:HD22	1.51	0.74
1:B:242:THR:O	1:B:243:ASP:HB2	1.87	0.74
1:A:212:LEU:HB2	1:A:219:MET:CE	2.17	0.74
1:F:109:LEU:HD11	1:F:207:LEU:HD13	1.69	0.74
1:D:59:VAL:HA	1:D:62:LEU:HD12	1.70	0.73
1:B:146:MET:HG3	1:B:239:LYS:HD3	1.71	0.72
1:D:59:VAL:HA	1:D:62:LEU:HD11	1.71	0.72
1:B:276:ILE:O	1:B:280:ILE:HG13	1.88	0.72
1:E:59:VAL:HA	1:E:62:LEU:CD1	2.20	0.72
1:C:71:ARG:HG2	1:C:71:ARG:HH11	1.54	0.72
1:G:74:THR:OG1	1:G:92:ARG:HB3	1.88	0.72
1:F:274:LYS:O	1:F:278:THR:HG23	1.90	0.72
1:G:76:ILE:HD13	1:G:198:LEU:HG	1.72	0.71
1:A:71:ARG:HH21	1:E:199:GLU:HG2	1.57	0.70
1:D:214:PHE:O	1:D:219:MET:HE2	1.92	0.70
1:H:72:ASP:HB3	1:H:267:ASP:OD2	1.92	0.70
1:G:110:ILE:HD13	1:G:166:MET:HE1	1.73	0.70
1:D:109:LEU:HD23	1:D:222:VAL:HG21	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114:VAL:HB	1:G:165:ARG:NH2	2.08	0.69
1:C:87:ILE:HD11	1:C:198:LEU:HD21	1.73	0.69
1:E:220:LYS:HE2	1:G:230:GLU:O	1.92	0.69
1:F:189:LEU:O	1:F:190:GLN:HG2	1.93	0.69
1:D:71:ARG:HG2	1:D:71:ARG:HH11	1.58	0.68
1:B:242:THR:HG22	1:B:243:ASP:H	1.58	0.68
1:G:163:GLU:CA	1:G:184:ILE:HD13	2.23	0.68
1:D:86:PHE:O	1:D:87:ILE:HG13	1.93	0.68
1:E:246:LEU:HD11	1:E:265:ASN:HD21	1.57	0.67
1:F:168:ASP:OD2	1:F:172[B]:ARG:NH2	2.23	0.67
1:A:76:ILE:HD13	1:A:198:LEU:CD2	2.22	0.67
1:B:234:TYR:CZ	1:B:287:ILE:HG23	2.30	0.66
1:G:73:GLY:CA	1:G:266:VAL:HG23	2.25	0.66
1:A:76:ILE:O	1:A:262:PHE:HA	1.96	0.66
1:A:134:GLU:OE2	1:A:134:GLU:HA	1.95	0.66
1:E:76:ILE:HD13	1:E:198:LEU:HD23	1.77	0.66
1:G:163:GLU:HA	1:G:184:ILE:CD1	2.26	0.65
1:A:155:GLN:HG2	1:A:185:ASP:HB2	1.79	0.65
1:G:110:ILE:HD13	1:G:166:MET:CE	2.27	0.65
1:H:215:ASP:HB2	1:H:218:ILE:HG13	1.79	0.64
1:A:59:VAL:O	1:A:86:PHE:HB2	1.97	0.64
1:E:210:GLU:OE1	1:E:216:LYS:HE3	1.98	0.64
1:E:239:LYS:HD2	4:E:320:HOH:O	1.97	0.64
1:A:93:ALA:HB1	1:A:198:LEU:HG	1.79	0.64
1:F:141:THR:H	1:F:144:SER:HB3	1.63	0.64
1:F:220:LYS:HE3	1:H:230:GLU:O	1.98	0.64
1:F:228:GLN:OE1	1:F:274:LYS:HE3	1.99	0.63
1:C:196:SER:OG	1:C:199:GLU:HG3	1.98	0.63
1:D:205:GLU:CG	1:D:209:LYS:HE3	2.29	0.62
1:G:60:SER:OG	1:G:84:LYS:HE3	1.99	0.62
1:C:214:PHE:O	1:C:219:MET:HE2	2.00	0.62
1:A:179:ASP:OD1	1:A:181:SER:HB3	2.00	0.62
1:A:58:ASN:ND2	1:A:61:LYS:HD2	2.14	0.62
1:F:145:ALA:HB3	1:F:154:TYR:HE1	1.65	0.62
1:G:98:THR:HG21	1:G:190:GLN:HA	1.82	0.61
1:B:215:ASP:HB2	1:B:218:ILE:HD12	1.80	0.61
1:B:109:LEU:HD23	1:B:222:VAL:HG21	1.82	0.61
1:E:211:ASP:O	1:E:212:LEU:HD23	2.00	0.61
1:B:143:GLY:HA2	1:B:225:MET:HG2	1.82	0.61
1:C:201:LYS:C	1:C:201:LYS:HD2	2.26	0.61
1:G:59:VAL:HA	1:G:62:LEU:CD1	2.22	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:ILE:HG22	1:D:187:PHE:CD2	2.35	0.61
1:G:96:ARG:C	1:G:97:GLN:HG3	2.26	0.61
1:E:242:THR:CG2	1:E:270:GLY:H	2.14	0.61
1:F:59:VAL:HA	1:F:62:LEU:CD1	2.31	0.60
1:B:145:ALA:HA	1:B:150:VAL:HG23	1.82	0.60
1:E:242:THR:HG23	1:E:270:GLY:N	2.14	0.60
1:B:67:PHE:CD2	1:B:280:ILE:HG12	2.36	0.60
1:E:109:LEU:HD11	1:E:207:LEU:HD13	1.82	0.60
1:C:207:LEU:HA	1:C:212:LEU:HD12	1.82	0.60
1:F:187:PHE:O	1:F:191:SER:HB3	2.01	0.60
1:A:210:GLU:HA	1:A:219:MET:CE	2.32	0.60
1:C:66:GLU:O	1:C:69:LYS:HE3	2.01	0.60
1:D:110:ILE:O	1:D:114:VAL:HG22	2.02	0.59
1:G:205:GLU:HA	1:G:261:ILE:HD12	1.84	0.59
1:E:227:ILE:HG12	1:E:237:TYR:CE2	2.37	0.59
1:G:214:PHE:O	1:G:219:MET:HE2	2.02	0.59
1:A:256:ASP:O	1:A:257:ASN:HB2	2.01	0.59
1:E:252:PHE:HB3	1:E:261:ILE:HD13	1.84	0.59
1:A:212:LEU:H	1:A:219:MET:HE1	1.68	0.59
1:C:71:ARG:HG2	1:C:71:ARG:NH1	2.14	0.59
1:C:243:ASP:HB3	1:C:246:LEU:HB3	1.84	0.59
1:A:144:SER:HB3	1:C:121:TYR:CG	2.37	0.58
1:F:281:LEU:HB2	1:F:287:ILE:HD12	1.85	0.58
1:G:74:THR:CG2	1:G:93:ALA:HB2	2.31	0.58
1:A:142:LEU:HG	1:A:225:MET:HE1	1.85	0.58
1:F:102:THR:HG21	1:F:248:TRP:HB3	1.83	0.58
1:E:58:ASN:ND2	1:E:61:LYS:HD2	2.19	0.58
1:H:155:GLN:O	1:H:159:ARG:HG3	2.03	0.58
1:F:156:ALA:HA	1:F:159:ARG:NH2	2.19	0.57
1:H:216:LYS:N	1:H:217:PRO:HD2	2.19	0.57
1:F:207:LEU:HA	1:F:212:LEU:HD12	1.85	0.57
1:A:156:ALA:HA	1:A:159:ARG:NH2	2.19	0.57
1:B:81:GLN:OE1	1:B:258:HIS:HA	2.04	0.57
1:A:71:ARG:NH2	1:E:199:GLU:HG2	2.18	0.57
1:A:103:PHE:O	1:A:106:PRO:HG2	2.04	0.57
1:A:104:KCX:HG3	1:A:154:TYR:CD2	2.38	0.57
1:A:142:LEU:HG	1:A:225:MET:CE	2.34	0.57
1:D:100:GLN:HE22	1:D:190:GLN:HE21	1.51	0.57
1:H:59:VAL:HA	1:H:62:LEU:HD12	1.87	0.57
1:H:243:ASP:HB3	1:H:246:LEU:HB3	1.87	0.57
1:E:58:ASN:HD22	1:E:61:LYS:HD2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:ILE:CD1	1:G:166:MET:HE1	2.35	0.57
1:G:174:SER:HA	1:G:178:GLU:OE2	2.04	0.57
1:C:87:ILE:CD1	1:C:198:LEU:HD21	2.35	0.56
1:E:103:PHE:C	1:E:106:PRO:HD2	2.30	0.56
1:F:64:VAL:HG11	1:F:280:ILE:HD13	1.88	0.56
1:G:74:THR:HG21	1:G:93:ALA:CB	2.35	0.56
1:H:157:MET:O	1:H:161:ILE:HG13	2.06	0.56
1:G:243:ASP:HB3	1:G:246:LEU:HB3	1.86	0.56
1:F:93:ALA:HB1	1:F:198:LEU:HG	1.88	0.56
1:F:252:PHE:HB3	1:F:261:ILE:HD13	1.88	0.56
1:A:144:SER:HB3	1:C:121:TYR:CB	2.35	0.56
1:D:59:VAL:C	1:D:62:LEU:HD12	2.31	0.55
1:F:126:TRP:CZ2	1:F:137:ASN:HB3	2.41	0.55
1:G:207:LEU:HA	1:G:212:LEU:HD12	1.88	0.55
1:D:59:VAL:CA	1:D:62:LEU:HD12	2.35	0.55
1:D:124:LYS:HD2	1:D:153:TYR:CD2	2.41	0.55
1:C:62:LEU:HD23	1:C:284:TYR:CE1	2.42	0.55
1:E:210:GLU:OE1	1:E:216:LYS:HG2	2.06	0.55
1:B:140:HIS:CE1	1:B:150:VAL:HG21	2.41	0.55
1:C:124:LYS:HB2	1:C:153:TYR:CE2	2.42	0.55
1:G:76:ILE:CD1	1:G:198:LEU:HG	2.37	0.55
1:C:66:GLU:O	1:C:69:LYS:HG2	2.07	0.55
1:G:72:ASP:O	1:G:266:VAL:HG23	2.07	0.55
1:G:249:PHE:CE1	1:G:274:LYS:HG3	2.42	0.55
1:H:288:THR:OG1	1:H:289:ASN:N	2.39	0.55
1:G:90:GLU:O	1:G:94:LYS:HE3	2.07	0.54
1:H:113:GLN:HE22	1:H:215:ASP:CG	2.15	0.54
1:F:59:VAL:O	1:F:86:PHE:HB2	2.07	0.54
1:A:87:ILE:CD1	1:A:198:LEU:HD21	2.37	0.54
1:A:163:GLU:HA	1:A:184:ILE:CD1	2.36	0.54
1:G:180:ILE:HG22	1:G:187:PHE:CD1	2.43	0.54
1:A:69:LYS:O	1:A:70:ASP:HB2	2.07	0.53
1:B:242:THR:HG23	1:B:270:GLY:N	2.23	0.53
1:C:274:LYS:O	1:C:278:THR:HG23	2.09	0.53
1:H:109:LEU:HD23	1:H:222:VAL:HG21	1.89	0.53
1:B:200:GLU:O	1:B:204:ILE:HG12	2.07	0.53
1:E:167:LYS:HD3	1:E:180:ILE:HD11	1.91	0.53
1:H:59:VAL:HA	1:H:62:LEU:HD13	1.91	0.53
1:H:106:PRO:O	1:H:110:ILE:HD12	2.08	0.53
1:H:174:SER:HA	1:H:178:GLU:OE2	2.08	0.52
1:B:142:LEU:HG	1:B:225:MET:CE	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:216:LYS:N	1:G:217:PRO:HD2	2.25	0.52
1:B:76:ILE:HD13	1:B:198:LEU:CD2	2.34	0.52
1:B:171:HIS:HA	1:B:178:GLU:OE1	2.10	0.52
1:C:109:LEU:HD11	1:C:207:LEU:HD13	1.92	0.52
1:D:104:KCX:HE3	1:D:149:SER:HA	1.91	0.52
1:D:276:ILE:O	1:D:280:ILE:HG13	2.09	0.52
1:D:196:SER:OG	1:D:199:GLU:HG3	2.09	0.52
1:D:109:LEU:CD2	1:D:222:VAL:HG21	2.38	0.52
1:C:174:SER:HA	1:C:178:GLU:OE2	2.10	0.52
1:A:62:LEU:HG	1:A:284:TYR:CZ	2.44	0.52
1:C:62:LEU:HD11	1:C:77:LEU:HD23	1.92	0.52
1:H:131:ARG:HD2	4:H:309:HOH:O	2.10	0.52
1:D:59:VAL:CA	1:D:62:LEU:CD1	2.85	0.51
1:D:72:ASP:HB3	1:D:267:ASP:OD2	2.10	0.51
1:F:110:ILE:HG12	1:F:169:TRP:HB3	1.90	0.51
1:A:121:TYR:CD2	1:C:144:SER:HB3	2.45	0.51
1:A:245:GLY:O	1:A:246:LEU:HD23	2.10	0.51
1:C:255:THR:OG1	1:C:258:HIS:HB2	2.10	0.51
1:C:272:ALA:O	1:C:276:ILE:HD12	2.10	0.51
1:D:103:PHE:O	1:D:107:ASN:HB2	2.11	0.51
1:G:238:GLY:HA2	1:G:250:VAL:O	2.11	0.51
1:G:72:ASP:C	1:G:266:VAL:HG23	2.36	0.51
1:E:74:THR:CG2	1:E:265:ASN:HB3	2.40	0.51
1:A:85:THR:HB	1:F:244:TYR:CD2	2.45	0.51
1:D:76:ILE:O	1:D:262:PHE:HA	2.10	0.51
1:E:136:TRP:NE1	1:E:150:VAL:HA	2.26	0.51
1:B:190:GLN:HG2	1:B:244:TYR:CE2	2.46	0.51
1:F:187:PHE:CE1	1:F:193:LEU:HD22	2.45	0.51
1:H:76:ILE:O	1:H:262:PHE:HA	2.11	0.51
1:D:205:GLU:HG2	1:D:209:LYS:HE3	1.93	0.50
1:E:103:PHE:O	1:E:106:PRO:HD2	2.11	0.50
1:H:137:ASN:O	1:H:138:ARG:HB3	2.11	0.50
1:H:67:PHE:CE1	1:H:279:ASP:HB3	2.46	0.50
1:F:234:TYR:CZ	1:F:287:ILE:HG23	2.47	0.50
1:B:100:GLN:HE21	1:B:100:GLN:CA	2.02	0.50
1:B:100:GLN:NE2	1:B:100:GLN:CA	2.59	0.50
1:B:105:VAL:HB	1:B:106:PRO:HD3	1.94	0.50
1:C:75:PHE:CE2	1:C:77:LEU:HB2	2.47	0.50
1:D:126:TRP:CZ2	1:D:137:ASN:HB3	2.47	0.50
1:A:167:LYS:NZ	1:A:178:GLU:O	2.42	0.50
1:A:250:VAL:HG12	1:A:263:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:THR:HG21	1:C:190:GLN:HA	1.92	0.50
1:H:64:VAL:HG11	1:H:280:ILE:HD13	1.94	0.50
1:A:87:ILE:HD13	1:A:198:LEU:HD21	1.93	0.50
1:B:109:LEU:CD2	1:B:222:VAL:HG21	2.42	0.50
1:H:134[A]:GLU:HA	1:H:134[A]:GLU:OE2	2.10	0.50
1:A:104:KCX:HE3	1:A:149:SER:HA	1.92	0.50
1:C:69:LYS:O	1:C:70:ASP:HB2	2.11	0.50
1:G:57:VAL:HG21	1:G:284:TYR:O	2.12	0.49
1:A:177:ASN:OD1	1:A:193:LEU:HD12	2.12	0.49
1:C:212:LEU:C	1:C:214:PHE:H	2.20	0.49
1:E:71:ARG:CG	1:E:267:ASP:O	2.60	0.49
1:F:105:VAL:HB	1:F:106:PRO:CD	2.42	0.49
1:H:183:GLY:O	1:H:187:PHE:HD2	1.95	0.49
1:C:59:VAL:HA	1:C:62:LEU:HG	1.93	0.49
1:B:145:ALA:HA	1:B:150:VAL:CG2	2.42	0.49
1:C:205:GLU:HA	1:C:261:ILE:HD12	1.94	0.49
1:D:71:ARG:HG2	1:D:71:ARG:NH1	2.23	0.49
1:G:155:GLN:O	1:G:159:ARG:HG3	2.11	0.49
1:B:103:PHE:C	1:B:106:PRO:HD2	2.38	0.49
1:D:283:LYS:HE2	1:D:284:TYR:CE2	2.48	0.49
1:B:76:ILE:O	1:B:262:PHE:HA	2.12	0.49
1:F:180:ILE:O	1:F:180:ILE:HG13	2.13	0.49
1:A:234:TYR:HA	1:A:254:THR:O	2.13	0.49
1:C:76:ILE:HD13	1:C:198:LEU:HD23	1.95	0.49
1:G:166:MET:HE2	1:G:170:LEU:HG	1.94	0.49
1:C:260:TYR:CD2	1:C:286:LEU:HD13	2.48	0.49
1:C:281:LEU:HB2	1:C:287:ILE:CD1	2.41	0.49
1:E:67:PHE:CD2	1:E:280:ILE:HG12	2.48	0.49
1:F:76:ILE:HD13	1:F:198:LEU:HD23	1.95	0.49
1:A:255:THR:OG1	1:A:258:HIS:HB2	2.12	0.49
1:B:142:LEU:HG	1:B:225:MET:HE1	1.95	0.49
1:F:163:GLU:HA	1:F:184:ILE:HD13	1.94	0.49
1:H:95:GLU:O	1:H:97:GLN:HG3	2.13	0.48
1:G:76:ILE:HD13	1:G:198:LEU:CG	2.41	0.48
1:A:56:SER:OG	1:A:82:LYS:NZ	2.46	0.48
1:A:201:LYS:HD2	1:A:201:LYS:C	2.37	0.48
1:B:246:LEU:HD11	1:B:265:ASN:HD21	1.77	0.48
1:G:183:GLY:O	1:G:187:PHE:HD2	1.96	0.48
1:G:78:HIS:HB3	1:G:261:ILE:HB	1.96	0.48
1:A:102:THR:HA	1:A:239:LYS:HG2	1.94	0.48
1:C:180:ILE:HG22	1:C:187:PHE:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:GLY:HA2	1:D:250:VAL:O	2.13	0.48
1:H:104:KCX:HE3	1:H:149:SER:HA	1.96	0.48
1:H:146:MET:HB2	1:H:154:TYR:OH	2.14	0.48
1:A:283:LYS:O	1:A:283:LYS:HG3	2.14	0.48
1:G:58:ASN:ND2	1:G:61:LYS:HD2	2.29	0.48
1:A:168:ASP:OD2	1:A:172[B]:ARG:NH2	2.42	0.48
1:B:103:PHE:O	1:B:106:PRO:HD2	2.13	0.48
1:G:124:LYS:HB2	1:G:153:TYR:CE2	2.48	0.48
1:G:140:HIS:CE1	1:G:150:VAL:HG21	2.49	0.48
1:C:109:LEU:HD23	1:C:222:VAL:HG21	1.96	0.47
1:E:201:LYS:C	1:E:201:LYS:HD2	2.38	0.47
1:F:87:ILE:CD1	1:F:198:LEU:HD21	2.44	0.47
1:F:122:ASP:O	1:F:141:THR:HA	2.14	0.47
1:F:216:LYS:N	1:F:217:PRO:HD2	2.29	0.47
1:G:73:GLY:HA3	1:G:266:VAL:HG23	1.94	0.47
1:C:124:LYS:HB2	1:C:153:TYR:CD2	2.49	0.47
1:G:130:GLU:HG2	1:G:137:ASN:ND2	2.30	0.47
1:E:163:GLU:N	1:E:184:ILE:HD13	2.29	0.47
1:F:142:LEU:O	1:F:154:TYR:OH	2.30	0.47
1:E:146:MET:HG3	1:E:239:LYS:HD3	1.95	0.47
1:E:184:ILE:O	1:E:184:ILE:HG13	2.13	0.47
1:E:220:LYS:HD2	1:G:230:GLU:HG2	1.97	0.47
1:H:81:GLN:HE22	1:H:259:SER:N	2.12	0.47
1:C:88:TYR:CD1	1:C:88:TYR:C	2.93	0.47
1:D:64:VAL:HG11	1:D:280:ILE:HD13	1.96	0.47
1:D:201:LYS:HD2	1:D:201:LYS:C	2.40	0.47
1:E:250:VAL:HG12	1:E:263:VAL:HG22	1.97	0.47
1:G:103:PHE:O	1:G:107:ASN:HB2	2.15	0.47
1:G:159:ARG:HD3	1:G:185:ASP:OD2	2.15	0.47
1:A:71:ARG:HG2	1:A:267:ASP:O	2.13	0.47
1:H:90:GLU:O	1:H:94:LYS:HG3	2.15	0.47
1:H:147:ARG:HG3	4:H:311:HOH:O	2.15	0.47
1:D:281:LEU:HD23	1:D:286:LEU:HD12	1.96	0.47
1:H:140:HIS:CE1	1:H:150:VAL:HG21	2.50	0.47
1:B:256:ASP:O	1:B:257:ASN:HB2	2.15	0.46
1:F:201:LYS:HD2	1:F:201:LYS:C	2.39	0.46
1:A:107:ASN:O	1:A:157:MET:HE3	2.16	0.46
1:A:254:THR:HG22	1:A:259:SER:HB3	1.97	0.46
1:B:210:GLU:CD	1:B:220:LYS:HZ2	2.22	0.46
1:B:242:THR:CG2	1:B:270:GLY:H	2.23	0.46
1:C:171:HIS:HA	1:C:178:GLU:CD	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:ILE:HD11	1:F:198:LEU:HD21	1.97	0.46
1:F:95:GLU:O	1:F:196:SER:HA	2.15	0.46
1:F:145:ALA:CB	1:F:154:TYR:HE1	2.26	0.46
1:F:256:ASP:O	1:F:257:ASN:HB2	2.15	0.46
1:B:167:LYS:HE2	1:E:244:TYR:OH	2.15	0.46
1:B:228:GLN:C	1:B:229:GLU:HG3	2.40	0.46
1:C:76:ILE:HG21	1:C:201:LYS:HG3	1.97	0.46
1:D:108:ALA:O	1:D:112:LEU:HD12	2.16	0.46
1:E:187:PHE:HE1	1:E:193:LEU:HD22	1.81	0.46
1:G:58:ASN:HD22	1:G:61:LYS:HD2	1.80	0.46
1:C:59:VAL:O	1:C:86:PHE:HB2	2.15	0.46
1:D:168:ASP:OD2	1:D:172[B]:ARG:NH2	2.49	0.46
1:E:62:LEU:HG	1:E:284:TYR:CZ	2.51	0.46
1:E:134:GLU:HG2	1:E:135:SER:N	2.30	0.46
1:F:185:ASP:OD1	1:F:186:GLN:HG2	2.15	0.46
1:A:144:SER:HB3	1:C:121:TYR:HB3	1.98	0.46
1:B:68:PHE:CE1	1:B:73:GLY:HA3	2.51	0.46
1:B:109:LEU:HD23	1:B:222:VAL:CG2	2.45	0.46
1:E:167:LYS:HD3	1:E:180:ILE:CD1	2.46	0.46
1:E:246:LEU:HD11	1:E:265:ASN:ND2	2.29	0.46
1:F:132:GLU:HB2	1:F:133:PHE:CD1	2.51	0.46
1:D:159:ARG:HD3	1:D:185:ASP:OD2	2.16	0.46
1:D:163:GLU:HA	1:D:184:ILE:HD13	1.98	0.46
1:D:207:LEU:HD12	1:D:207:LEU:O	2.15	0.46
1:F:266:VAL:HG22	1:F:267:ASP:N	2.31	0.46
1:G:198:LEU:HD23	1:G:201:LYS:HE3	1.97	0.46
1:B:121:TYR:CB	1:D:144:SER:HB3	2.46	0.45
1:E:187:PHE:CE1	1:E:193:LEU:HD22	2.51	0.45
1:H:146:MET:HB2	1:H:154:TYR:HH	1.80	0.45
1:C:180:ILE:HG12	4:C:304:HOH:O	2.16	0.45
1:D:216:LYS:HB3	1:D:216:LYS:HE3	1.67	0.45
1:E:56:SER:HB2	1:E:82:LYS:NZ	2.31	0.45
1:G:77:LEU:HD11	1:G:260:TYR:HB3	1.98	0.45
1:E:198:LEU:HD23	1:E:198:LEU:HA	1.84	0.45
1:G:286:LEU:HD23	1:G:286:LEU:HA	1.67	0.45
1:H:276:ILE:O	1:H:280:ILE:HG13	2.17	0.45
1:D:151:ILE:HD13	1:D:189:LEU:CD1	2.46	0.45
1:G:112:LEU:HD23	1:G:117:VAL:HG23	1.98	0.45
1:C:103:PHE:O	1:C:107:ASN:HB2	2.17	0.45
1:C:140:HIS:CD2	1:C:150:VAL:HG11	2.52	0.45
1:E:76:ILE:O	1:E:262:PHE:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:TRP:CZ2	1:E:137:ASN:HB3	2.51	0.45
1:G:90:GLU:HG2	1:G:94:LYS:NZ	2.32	0.45
1:A:210:GLU:HA	1:A:219:MET:HE1	1.98	0.45
1:B:282:LYS:O	1:B:283:LYS:C	2.59	0.45
1:C:71:ARG:NH1	1:C:268:ALA:HB2	2.32	0.45
1:D:69:LYS:O	1:D:70:ASP:HB2	2.17	0.45
1:B:107:ASN:OD1	1:B:157:MET:HE3	2.17	0.45
1:F:120:GLU:HA	1:F:142:LEU:HB3	1.99	0.45
1:G:205:GLU:HA	1:G:261:ILE:CD1	2.47	0.45
1:B:62:LEU:HD12	1:B:284:TYR:CE1	2.53	0.44
1:D:80:VAL:HB	1:D:259:SER:O	2.17	0.44
1:D:205:GLU:HG3	1:D:209:LYS:HE3	1.99	0.44
1:H:109:LEU:CD2	1:H:222:VAL:HG21	2.47	0.44
1:B:228:GLN:OE1	1:B:274:LYS:HE3	2.17	0.44
1:D:78:HIS:HB2	1:D:85:THR:HG23	1.98	0.44
1:E:105:VAL:N	1:E:106:PRO:HD2	2.33	0.44
1:F:114:VAL:O	1:F:115:LYS:HB2	2.17	0.44
1:B:130:GLU:HG3	1:B:137:ASN:ND2	2.32	0.44
1:E:224:ARG:HD3	1:G:230:GLU:OE2	2.17	0.44
1:G:185:ASP:OD1	1:G:186:GLN:HG2	2.17	0.44
1:H:124:LYS:HD2	1:H:153:TYR:CD2	2.53	0.44
1:A:216:LYS:N	1:A:217:PRO:HD2	2.32	0.44
1:A:254:THR:HG22	1:A:259:SER:CB	2.47	0.44
1:D:141:THR:H	1:D:144:SER:HG	1.65	0.44
1:F:71:ARG:CD	1:F:276:ILE:HD11	2.47	0.44
1:G:187:PHE:CE1	1:G:193:LEU:HD22	2.52	0.44
1:A:98:THR:CG2	1:A:190:GLN:H	2.08	0.44
1:A:234:TYR:CE2	1:A:287:ILE:HG12	2.53	0.44
1:B:146:MET:O	1:B:239:LYS:HE2	2.18	0.44
1:A:141:THR:HG21	1:C:141:THR:HG21	2.00	0.44
1:E:216:LYS:N	1:E:217:PRO:HD2	2.33	0.44
1:F:227:ILE:HG12	1:F:237:TYR:CE2	2.53	0.43
1:A:235:THR:HG22	1:A:237:TYR:CE1	2.53	0.43
1:C:189:LEU:O	1:C:190:GLN:HG2	2.17	0.43
1:C:222:VAL:O	1:C:226:MET:HG3	2.17	0.43
1:G:94:LYS:HB3	1:G:94:LYS:HE2	1.65	0.43
1:C:132[A]:GLU:H	1:C:132[A]:GLU:HG2	1.34	0.43
1:D:260:TYR:CE1	1:D:286:LEU:HD22	2.53	0.43
1:H:216:LYS:O	1:H:220:LYS:HG3	2.18	0.43
1:H:229:GLU:OE1	1:H:234:TYR:OH	2.31	0.43
1:H:244:TYR:O	1:H:244:TYR:CD2	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:THR:HG22	1:A:188:TRP:O	2.18	0.43
1:F:59:VAL:CA	1:F:62:LEU:HD13	2.44	0.43
1:G:123:VAL:HG22	1:G:141:THR:HG22	2.00	0.43
1:G:252:PHE:HB3	1:G:261:ILE:HD13	2.00	0.43
1:H:75:PHE:CE2	1:H:280:ILE:HG21	2.53	0.43
1:B:59:VAL:O	1:B:86:PHE:HB2	2.18	0.43
1:E:144:SER:HB3	1:G:121:TYR:HB3	2.01	0.43
1:H:126:TRP:HB2	1:H:138:ARG:C	2.44	0.43
1:H:201:LYS:HD2	1:H:201:LYS:C	2.43	0.43
1:D:86:PHE:C	1:D:87:ILE:HG13	2.44	0.43
1:D:112:LEU:HD21	1:D:119:ASP:HA	2.01	0.43
1:G:171:HIS:HA	1:G:178:GLU:OE1	2.19	0.43
1:A:70:ASP:O	1:A:71:ARG:NH1	2.52	0.43
1:A:153:TYR:CD1	1:A:153:TYR:C	2.96	0.43
1:B:87:ILE:HD13	1:B:198:LEU:HD21	2.01	0.43
1:C:78:HIS:HE1	1:C:83:ASP:OD1	2.01	0.43
1:F:254:THR:HG22	1:F:259:SER:HB3	2.01	0.43
1:G:167:LYS:HD3	1:G:180:ILE:HG12	2.01	0.43
1:G:114:VAL:HB	1:G:165:ARG:HH21	1.80	0.42
1:G:169:TRP:O	1:G:173:ILE:HG12	2.19	0.42
1:B:121:TYR:CG	1:D:144:SER:HB3	2.54	0.42
1:B:157:MET:HA	4:B:405:HOH:O	2.19	0.42
1:E:136:TRP:CD1	1:E:150:VAL:HG22	2.53	0.42
1:A:69:LYS:HB2	1:A:69:LYS:HE3	1.75	0.42
1:B:206:HIS:O	1:B:210:GLU:N	2.52	0.42
1:B:239:LYS:HZ2	1:B:239:LYS:HG3	1.73	0.42
1:D:207:LEU:HA	1:D:212:LEU:HD12	2.00	0.42
1:H:105:VAL:HB	1:H:106:PRO:CD	2.50	0.42
1:A:282:LYS:HE3	4:A:324:HOH:O	2.18	0.42
1:B:98:THR:HB	4:B:404:HOH:O	2.20	0.42
1:C:228:GLN:NE2	1:C:238:GLY:O	2.52	0.42
1:C:252:PHE:HB3	1:C:261:ILE:HD13	2.01	0.42
1:E:242:THR:HG23	1:E:269:SER:HA	2.00	0.42
1:F:253:ILE:CD1	1:F:287:ILE:HG13	2.49	0.42
1:A:145:ALA:HA	1:A:150:VAL:HG23	2.00	0.42
1:A:224:ARG:HD2	1:C:227:ILE:HD12	2.01	0.42
1:F:67:PHE:CE1	1:F:279:ASP:HB3	2.55	0.42
1:G:62:LEU:HG	1:G:284:TYR:CZ	2.54	0.42
1:G:151:ILE:O	1:G:155:GLN:HG3	2.19	0.42
1:F:249:PHE:CD2	1:F:274:LYS:HA	2.55	0.42
1:G:126:TRP:HA	4:G:304:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:PHE:CE2	1:B:107:ASN:HB2	2.55	0.42
1:D:76:ILE:HD11	1:D:93:ALA:HB1	2.02	0.42
1:A:121:TYR:CG	1:C:144:SER:HB3	2.55	0.42
1:A:253:ILE:O	1:A:259:SER:HA	2.20	0.42
1:B:245:GLY:O	1:B:267:ASP:HA	2.19	0.42
1:C:105:VAL:HB	1:C:106:PRO:CD	2.50	0.42
1:C:109:LEU:HD13	1:C:214:PHE:CE2	2.55	0.42
1:C:235:THR:HG22	1:C:237:TYR:CE1	2.55	0.42
1:G:247:GLY:O	1:G:265:ASN:HA	2.19	0.42
1:H:84:LYS:HD2	1:H:85:THR:H	1.84	0.42
1:A:166:MET:O	1:A:170:LEU:HG	2.19	0.41
1:B:250:VAL:HG12	1:B:263:VAL:HG22	2.02	0.41
1:D:188:TRP:CD1	1:D:189:LEU:HG	2.54	0.41
1:E:230:GLU:O	1:G:220:LYS:HD2	2.20	0.41
1:E:256:ASP:O	1:E:257:ASN:HB2	2.18	0.41
1:F:238:GLY:HA3	1:F:249:PHE:CE1	2.55	0.41
1:C:201:LYS:C	1:C:201:LYS:CD	2.91	0.41
1:D:136:TRP:CD1	1:D:150:VAL:HG22	2.54	0.41
1:G:166:MET:HE2	1:G:170:LEU:CG	2.50	0.41
1:C:226:MET:O	1:C:237:TYR:HA	2.20	0.41
1:F:123:VAL:HG22	1:F:141:THR:HG22	2.02	0.41
1:F:246:LEU:HD12	1:F:247:GLY:H	1.85	0.41
1:D:60:SER:O	1:D:61:LYS:HD3	2.20	0.41
1:G:166:MET:CE	1:G:170:LEU:HG	2.50	0.41
1:H:84:LYS:HD2	1:H:84:LYS:HA	1.83	0.41
1:H:198:LEU:HA	1:H:198:LEU:HD23	1.85	0.41
1:C:122:ASP:O	1:C:141:THR:HA	2.20	0.41
1:G:97:GLN:O	1:G:194:LYS:HA	2.20	0.41
1:C:172:ARG:HH11	1:C:172:ARG:HD3	1.65	0.41
1:G:98:THR:HA	1:G:193:LEU:O	2.21	0.41
1:B:122:ASP:O	1:B:141:THR:HA	2.20	0.41
1:F:105:VAL:HB	1:F:106:PRO:HD3	2.02	0.41
1:G:85:THR:HG21	1:G:201:LYS:HE2	2.03	0.41
1:G:170:LEU:HD23	1:G:170:LEU:HA	1.67	0.41
1:E:153:TYR:CD1	1:E:153:TYR:C	2.99	0.41
1:E:242:THR:O	1:E:243:ASP:HB2	2.21	0.41
1:A:65:ASP:OD1	1:A:65:ASP:N	2.54	0.41
1:F:242:THR:HG23	1:F:270:GLY:H	1.86	0.41
1:G:76:ILE:HD13	1:G:198:LEU:CD2	2.51	0.41
1:H:281:LEU:HB3	1:H:287:ILE:HD12	1.99	0.41
1:D:216:LYS:N	1:D:217:PRO:HD2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:69:LYS:O	1:H:70:ASP:HB2	2.20	0.40
1:A:179:ASP:CG	1:A:192:SER:HB2	2.47	0.40
1:B:207:LEU:HA	1:B:212:LEU:HD12	2.03	0.40
1:H:145:ALA:CB	1:H:154:TYR:HE1	2.34	0.40
1:C:171:HIS:HA	1:C:178:GLU:OE1	2.22	0.40
1:B:114:VAL:O	1:B:114:VAL:HG23	2.20	0.40
1:E:144:SER:HB3	1:G:121:TYR:CB	2.52	0.40
1:G:122:ASP:O	1:G:153:TYR:OH	2.39	0.40
1:A:184:ILE:HD12	1:A:184:ILE:HA	1.84	0.40
1:C:66:GLU:C	1:C:69:LYS:HG2	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	233/264 (88%)	210 (90%)	22 (9%)	1 (0%)	30	39
1	B	232/264 (88%)	209 (90%)	21 (9%)	2 (1%)	14	20
1	C	232/264 (88%)	213 (92%)	18 (8%)	1 (0%)	30	39
1	D	232/264 (88%)	212 (91%)	19 (8%)	1 (0%)	30	39
1	E	231/264 (88%)	215 (93%)	16 (7%)	0	100	100
1	F	232/264 (88%)	217 (94%)	15 (6%)	0	100	100
1	G	231/264 (88%)	215 (93%)	15 (6%)	1 (0%)	30	39
1	H	232/264 (88%)	214 (92%)	18 (8%)	0	100	100
All	All	1855/2112 (88%)	1705 (92%)	144 (8%)	6 (0%)	36	45

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ASP
1	B	243	ASP
1	G	244	TYR
1	B	122	ASP
1	D	256	ASP
1	C	213	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	211/233 (91%)	210 (100%)	1 (0%)	81	88
1	B	210/233 (90%)	208 (99%)	2 (1%)	68	80
1	C	210/233 (90%)	207 (99%)	3 (1%)	59	75
1	D	208/233 (89%)	207 (100%)	1 (0%)	81	88
1	E	209/233 (90%)	207 (99%)	2 (1%)	68	80
1	F	209/233 (90%)	207 (99%)	2 (1%)	68	80
1	G	209/233 (90%)	206 (99%)	3 (1%)	59	75
1	H	210/233 (90%)	208 (99%)	2 (1%)	68	80
All	All	1676/1864 (90%)	1660 (99%)	16 (1%)	70	80

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ARG
1	B	69	LYS
1	B	98	THR
1	C	132[A]	GLU
1	C	132[B]	GLU
1	C	201	LYS
1	D	167	LYS
1	E	69	LYS
1	E	71	ARG
1	F	91	SER

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Mol	Chain	Res	Type
1	F	216	LYS
1	G	94	LYS
1	G	149	SER
1	G	289	ASN
1	H	66	GLU
1	H	242	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	ASN
1	B	100	GLN
1	D	58	ASN
1	D	63	ASN
1	D	190	GLN
1	E	58	ASN
1	F	233	HIS
1	G	289	ASN
1	H	107	ASN
1	H	155	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	$\# Z > 2$
1	KCX	H	104	1	10,11,12	0.97	0	6,12,14	1.48	1 (16%)
1	KCX	D	104	1	10,11,12	1.07	0	6,12,14	0.93	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	B	104	1	10,11,12	0.86	0	6,12,14	1.57	2 (33%)
1	KCX	C	104	1	10,11,12	0.97	0	6,12,14	1.36	1 (16%)
1	KCX	A	104	1	10,11,12	0.95	0	6,12,14	1.56	1 (16%)
1	KCX	G	104	1	10,11,12	1.00	0	6,12,14	1.42	1 (16%)
1	KCX	E	104	1	10,11,12	0.94	0	6,12,14	1.58	2 (33%)
1	KCX	F	104	1	10,11,12	1.02	1 (10%)	6,12,14	1.08	1 (16%)

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
1	KCX	H	104	1	-	1/9/10/12	-
1	KCX	D	104	1	-	0/9/10/12	-
1	KCX	B	104	1	-	0/9/10/12	-
1	KCX	C	104	1	-	0/9/10/12	-
1	KCX	A	104	1	-	1/9/10/12	-
1	KCX	G	104	1	-	1/9/10/12	-
1	KCX	E	104	1	-	0/9/10/12	-
1	KCX	F	104	1	-	0/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	104	KCX	OQ1-CX	2.00	1.25	1.21

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	KCX	OQ1-CX-NZ	-3.67	119.34	124.92
1	H	104	KCX	OQ1-CX-NZ	-3.55	119.53	124.92
1	G	104	KCX	OQ1-CX-NZ	-3.29	119.93	124.92
1	C	104	KCX	OQ1-CX-NZ	-3.20	120.06	124.92
1	B	104	KCX	OQ1-CX-NZ	-2.95	120.44	124.92
1	E	104	KCX	OQ1-CX-NZ	-2.74	120.75	124.92
1	E	104	KCX	CE-NZ-CX	-2.47	117.79	121.98
1	F	104	KCX	OQ1-CX-NZ	-2.44	121.21	124.92
1	B	104	KCX	CE-NZ-CX	-2.39	117.92	121.98
1	D	104	KCX	OQ1-CX-NZ	-2.15	121.66	124.92

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	104	KCX	C-CA-CB-CG
1	H	104	KCX	C-CA-CB-CG
1	G	104	KCX	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	104	KCX	1	0
1	D	104	KCX	1	0
1	A	104	KCX	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
3	EDO	F	301	-	3,3,3	0.48	0	2,2,2	0.29	0
2	FLC	B	301	-	12,12,12	1.03	0	17,17,17	1.32	1 (5%)

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
3	EDO	F	301	-	-	0/1/1/1	-
2	FLC	B	301	-	-	6/16/16/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	FLC	OB2-CBC-CB	3.52	119.89	113.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	FLC	CA-CB-CBC-OB1
2	B	301	FLC	CA-CB-CBC-OB2
2	B	301	FLC	OHB-CB-CBC-OB1
2	B	301	FLC	OHB-CB-CBC-OB2
2	B	301	FLC	CB-CA-CAC-OA1
2	B	301	FLC	CB-CA-CAC-OA2

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	233/264 (88%)	-1.34	0 100 100	18, 31, 44, 52	5 (2%)
1	B	233/264 (88%)	-1.37	0 100 100	15, 27, 41, 48	4 (1%)
1	C	233/264 (88%)	-1.34	0 100 100	16, 30, 54, 67	4 (1%)
1	D	233/264 (88%)	-1.31	0 100 100	16, 31, 54, 63	4 (1%)
1	E	233/264 (88%)	-1.36	0 100 100	15, 27, 38, 50	3 (1%)
1	F	233/264 (88%)	-1.36	0 100 100	18, 31, 43, 59	4 (1%)
1	G	233/264 (88%)	-1.24	0 100 100	15, 31, 58, 70	3 (1%)
1	H	233/264 (88%)	-1.33	0 100 100	17, 31, 56, 71	4 (1%)
All	All	1864/2112 (88%)	-1.33	0 100 100	15, 30, 51, 71	31 (1%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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
1	KCX	A	104	12/13	0.99	0.04	19,24,27,32	2
1	KCX	B	104	12/13	0.99	0.04	13,21,24,27	0
1	KCX	D	104	12/13	0.99	0.03	15,21,24,28	1
1	KCX	E	104	12/13	0.99	0.03	19,21,23,25	1
1	KCX	F	104	12/13	0.99	0.03	20,23,32,32	1
1	KCX	G	104	12/13	0.99	0.04	14,21,24,24	1
1	KCX	H	104	12/13	0.99	0.02	19,22,26,26	1
1	KCX	C	104	12/13	1.00	0.02	18,22,23,25	1

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
3	EDO	F	301	4/4	0.98	0.08	33,47,51,57	0
2	FLC	B	301	13/13	0.99	0.04	34,42,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.