



Full wwPDB X-ray Structure Validation Report

Nov 20, 2014 – 10:25 PM EST

PDB ID : 4KPF
Title : Novel fluoroquinolones in complex with topoisomerase IV from *S. pneumoniae* and E-site G-gate
Authors : Laponogov, I.; Pan, X.-S.; Vesekov, D.A.; Cirz, R.T.; Wagman, A.S.; Moser, H.E.; Fisher, L.M.; Sanderson, M.R.
Deposited on : 2013-05-13
Resolution : 3.24 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

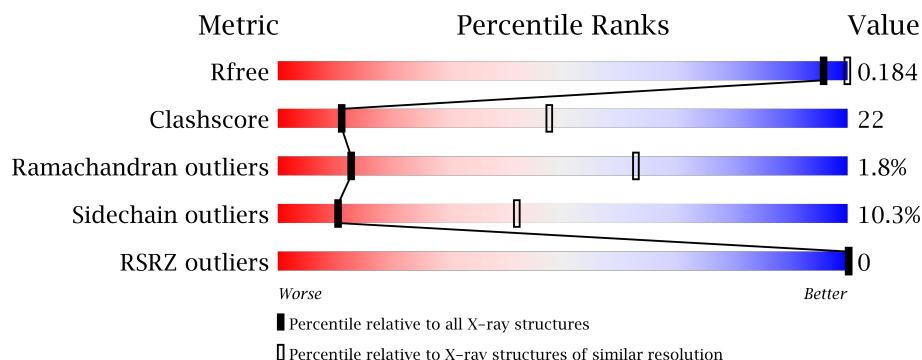
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24195
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24195

1 Overall quality at a glance

The reported resolution of this entry is 3.24 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}	66092	1080 (3.30-3.18)
Clashscore	79885	1369 (3.30-3.18)
Ramachandran outliers	78287	1342 (3.30-3.18)
Sidechain outliers	78261	1340 (3.30-3.18)
RSRZ outliers	66119	1081 (3.30-3.18)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	496	
1	B	496	
2	C	268	
2	D	268	
3	E	7	
4	F	11	
5	G	7	
6	H	11	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
7	MG	A	502	-	X
7	MG	C	701	-	X
7	MG	D	701	-	X
7	MG	G	100	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11197 atoms, of which 38 are hydrogens and 0 are deuterium.

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 ParC55.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	1	0
			3730	2365	643	709	13			
1	B	482	Total	C	N	O	S	0	1	0
			3713	2357	637	706	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	THR	ILE	CONFLICT	UNP P72525
A	489	LEU	-	EXPRESSION TAG	UNP P72525
A	490	GLU	-	EXPRESSION TAG	UNP P72525
A	491	HIS	-	EXPRESSION TAG	UNP P72525
A	492	HIS	-	EXPRESSION TAG	UNP P72525
A	493	HIS	-	EXPRESSION TAG	UNP P72525
A	494	HIS	-	EXPRESSION TAG	UNP P72525
A	495	HIS	-	EXPRESSION TAG	UNP P72525
A	496	HIS	-	EXPRESSION TAG	UNP P72525
B	257	THR	ILE	CONFLICT	UNP P72525
B	489	LEU	-	EXPRESSION TAG	UNP P72525
B	490	GLU	-	EXPRESSION TAG	UNP P72525
B	491	HIS	-	EXPRESSION TAG	UNP P72525
B	492	HIS	-	EXPRESSION TAG	UNP P72525
B	493	HIS	-	EXPRESSION TAG	UNP P72525
B	494	HIS	-	EXPRESSION TAG	UNP P72525
B	495	HIS	-	EXPRESSION TAG	UNP P72525
B	496	HIS	-	EXPRESSION TAG	UNP P72525

- Molecule 2 is a protein called ParE30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	208	Total	C	N	O	S	0	0	0
			1466	932	256	272	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	210	Total	C	N	O	S	0	0	0
			1446	920	251	269	6			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	380	MET	-	EXPRESSION TAG	UNP Q59961
C	381	GLY	-	EXPRESSION TAG	UNP Q59961
C	382	HIS	-	EXPRESSION TAG	UNP Q59961
C	383	HIS	-	EXPRESSION TAG	UNP Q59961
C	384	HIS	-	EXPRESSION TAG	UNP Q59961
C	385	HIS	-	EXPRESSION TAG	UNP Q59961
C	386	HIS	-	EXPRESSION TAG	UNP Q59961
C	387	HIS	-	EXPRESSION TAG	UNP Q59961
C	388	HIS	-	EXPRESSION TAG	UNP Q59961
C	389	HIS	-	EXPRESSION TAG	UNP Q59961
C	390	HIS	-	EXPRESSION TAG	UNP Q59961
C	391	HIS	-	EXPRESSION TAG	UNP Q59961
C	392	SER	-	EXPRESSION TAG	UNP Q59961
C	393	SER	-	EXPRESSION TAG	UNP Q59961
C	394	GLY	-	EXPRESSION TAG	UNP Q59961
C	395	HIS	-	EXPRESSION TAG	UNP Q59961
C	396	ILE	-	EXPRESSION TAG	UNP Q59961
C	397	ASP	-	EXPRESSION TAG	UNP Q59961
C	398	ASP	-	EXPRESSION TAG	UNP Q59961
C	399	ASP	-	EXPRESSION TAG	UNP Q59961
C	400	ASP	-	EXPRESSION TAG	UNP Q59961
C	401	LYS	-	EXPRESSION TAG	UNP Q59961
C	402	HIS	-	EXPRESSION TAG	UNP Q59961
C	403	MET	-	EXPRESSION TAG	UNP Q59961
C	460	ILE	VAL	CONFLICT	UNP Q59961
C	644	ALA	THR	CONFLICT	UNP Q59961
D	380	MET	-	EXPRESSION TAG	UNP Q59961
D	381	GLY	-	EXPRESSION TAG	UNP Q59961
D	382	HIS	-	EXPRESSION TAG	UNP Q59961
D	383	HIS	-	EXPRESSION TAG	UNP Q59961
D	384	HIS	-	EXPRESSION TAG	UNP Q59961
D	385	HIS	-	EXPRESSION TAG	UNP Q59961
D	386	HIS	-	EXPRESSION TAG	UNP Q59961
D	387	HIS	-	EXPRESSION TAG	UNP Q59961
D	388	HIS	-	EXPRESSION TAG	UNP Q59961
D	389	HIS	-	EXPRESSION TAG	UNP Q59961

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Chain	Residue	Modelled	Actual	Comment	Reference
D	390	HIS	-	EXPRESSION TAG	UNP Q59961
D	391	HIS	-	EXPRESSION TAG	UNP Q59961
D	392	SER	-	EXPRESSION TAG	UNP Q59961
D	393	SER	-	EXPRESSION TAG	UNP Q59961
D	394	GLY	-	EXPRESSION TAG	UNP Q59961
D	395	HIS	-	EXPRESSION TAG	UNP Q59961
D	396	ILE	-	EXPRESSION TAG	UNP Q59961
D	397	ASP	-	EXPRESSION TAG	UNP Q59961
D	398	ASP	-	EXPRESSION TAG	UNP Q59961
D	399	ASP	-	EXPRESSION TAG	UNP Q59961
D	400	ASP	-	EXPRESSION TAG	UNP Q59961
D	401	LYS	-	EXPRESSION TAG	UNP Q59961
D	402	HIS	-	EXPRESSION TAG	UNP Q59961
D	403	MET	-	EXPRESSION TAG	UNP Q59961
D	460	ILE	VAL	CONFLICT	UNP Q59961
D	644	ALA	THR	CONFLICT	UNP Q59961

- Molecule 3 is a DNA chain called E-site1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	7	Total	C	N	O	P	0	0	0
			140	69	27	38	6			

- Molecule 4 is a DNA chain called E-site2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	11	Total	C	N	O	P	0	0	0
			225	108	39	67	11			

- Molecule 5 is a DNA chain called E-site3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	7	Total	C	N	O	P	0	0	0
			139	68	25	40	6			

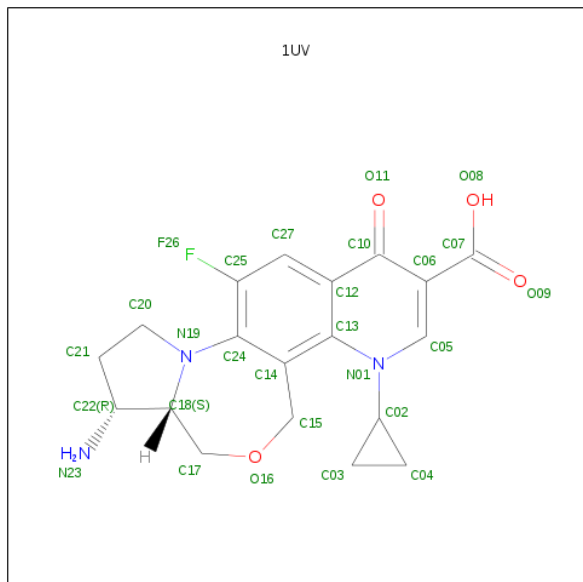
- Molecule 6 is a DNA chain called E-site4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	11	Total	C	N	O	P	0	0	0
			226	107	43	65	11			

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total Mg 1 1	0	0
7	B	1	Total Mg 1 1	0	0
7	A	2	Total Mg 2 2	0	0
7	D	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0

- Molecule 8 is (3AS,4R)-4-AMINO-13-CYCLOPROPYL-8-FLUORO-10-OXO-3A,4,5,6,10,13-HEXAHYDRO-1H,3H-PYRROLO[2',1':3,4][1,4]OXAZEPINO[5,6-H]QUINOLINE-11-CARBOXYLICACID (three-letter code: 1UV) (formula: C₁₉H₂₀FN₃O₄).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	H	1	Total 46	C 19	F 1	H 19	N 3	O 4	0	0
8	H	1	Total 46	C 19	F 1	H 19	N 3	O 4	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	8	Total O 8 8	0	0
9	B	3	Total O 3 3	0	0

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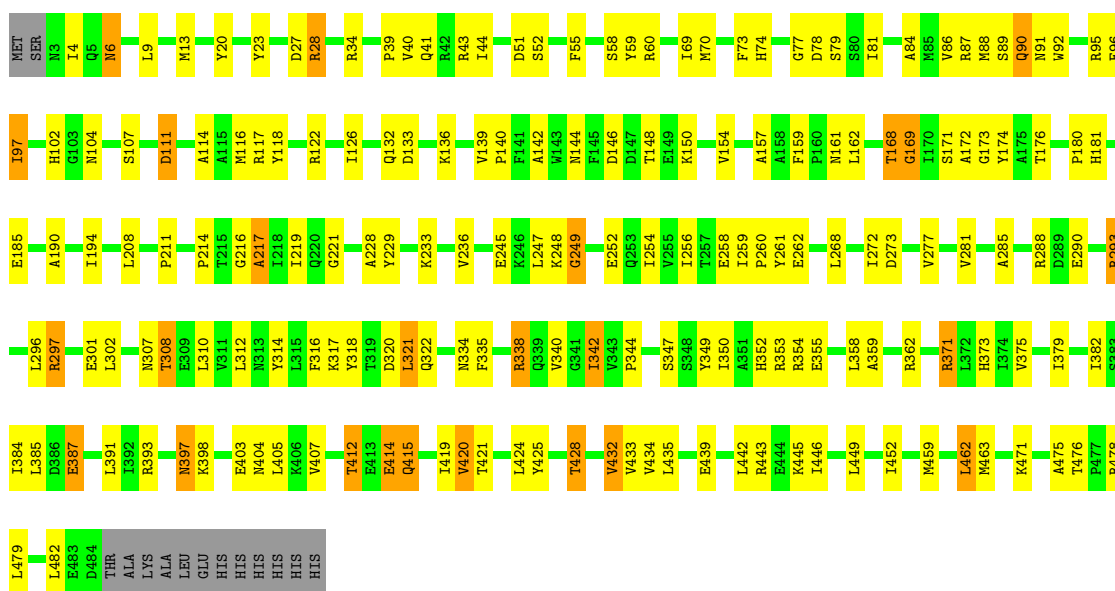
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	2	Total	O	0	0
			2	2		
9	D	1	Total	O	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

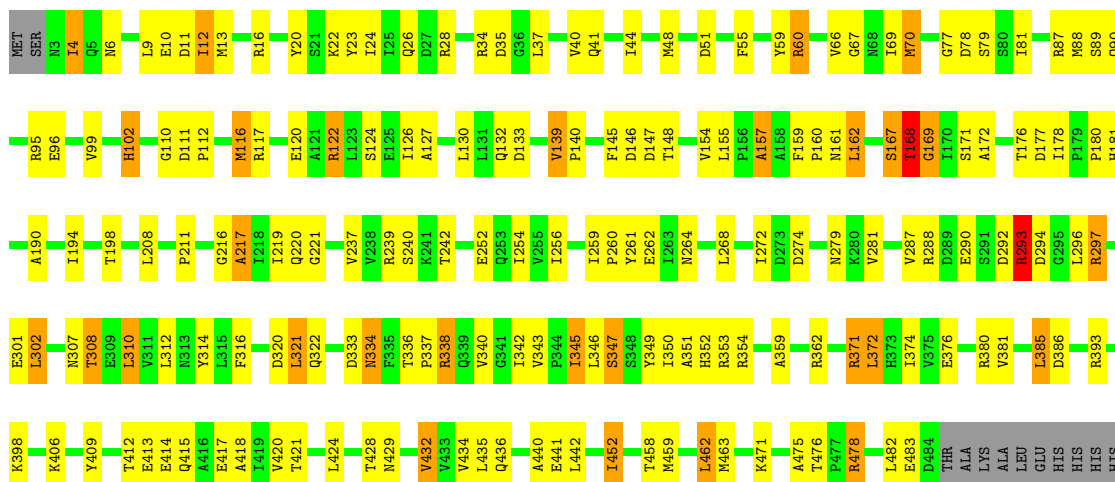
• Molecule 1: ParC55

Chain A:



• Molecule 1: ParC55

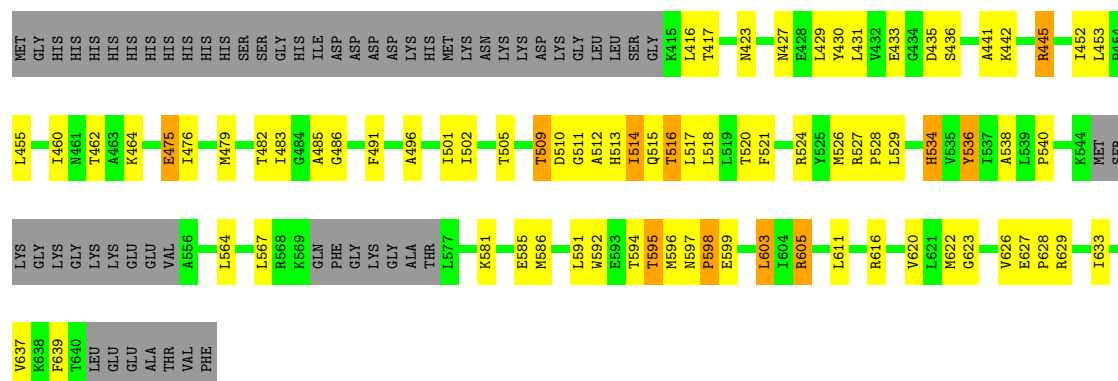
Chain B:



HIS
HIS

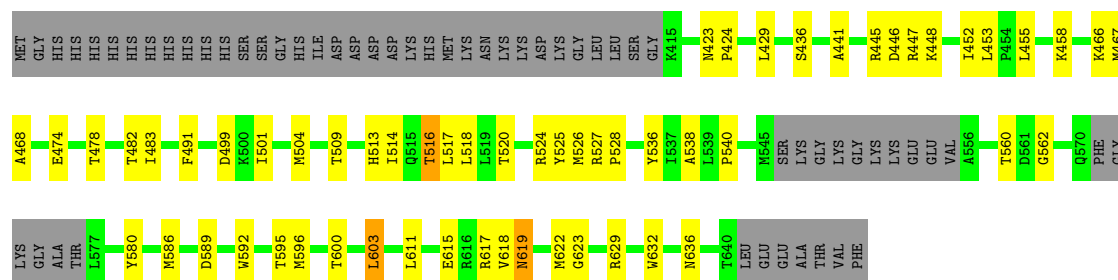
• Molecule 2: ParE30

Chain C:



• Molecule 2: ParE30

Chain D:



• Molecule 3: E-site1

Chain E:



• Molecule 4: E-site2

Chain F:



• Molecule 5: E-site3

Chain G:



• Molecule 6: E-site4

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.86Å 157.86Å 210.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.83 – 3.24 41.83 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.83-3.24) 99.9 (41.83-3.24)	Depositor EDS
R_{merge}	0.81	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.79 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.162 , 0.184 0.161 , 0.184	Depositor DCC
R_{free} test set	2446 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.9	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 48760 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11197	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 1UV

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	0.44	0/3794	0.64	0/5142
1	B	0.45	0/3777	0.64	0/5123
2	C	0.34	0/1492	0.53	0/2037
2	D	0.33	0/1472	0.51	0/2014
3	E	0.82	0/157	1.50	4/241 (1.7%)
4	F	0.84	0/251	1.78	6/385 (1.6%)
5	G	0.76	0/155	1.54	3/238 (1.3%)
6	H	0.83	0/253	1.60	5/388 (1.3%)
All	All	0.46	0/11351	0.75	18/15568 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3	DT	O4'-C4'-C3'	-11.44	99.14	106.00
4	F	10	DT	O4'-C4'-C3'	-10.03	99.98	106.00
6	H	10	DC	O4'-C4'-C3'	-9.13	100.52	106.00
5	G	14	DA	O4'-C4'-C3'	-7.20	101.62	104.50
5	G	11	DT	N3-C4-O4	6.78	123.97	119.90
4	F	6	DT	O4'-C1'-N1	6.70	112.69	108.00
4	F	8	DC	O4'-C1'-N1	6.35	112.44	108.00
3	E	11	DT	N3-C4-O4	6.33	123.70	119.90
4	F	6	DT	C1'-O4'-C4'	-6.26	103.84	110.10
6	H	5	DA	O4'-C1'-N9	-6.24	103.63	108.00
6	H	3	DC	O4'-C4'-C3'	-6.22	102.01	104.50
3	E	12	DG	C4'-C3'-C2'	-6.11	97.60	103.10
4	F	10	DT	C1'-O4'-C4'	-6.11	103.99	110.10
3	E	12	DG	O4'-C4'-C3'	-5.81	102.18	104.50
6	H	10	DC	C1'-O4'-C4'	-5.44	104.66	110.10
5	G	11	DT	C5-C4-O4	-5.18	121.28	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	11	DT	C5-C4-O4	-5.15	121.30	124.90
6	H	1	DG	O4'-C1'-N9	5.00	111.50	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3730	0	3642	169	1
1	B	3713	0	3621	188	1
2	C	1466	0	1284	80	0
2	D	1446	0	1231	47	0
3	E	140	0	78	2	0
4	F	225	0	126	11	0
5	G	139	0	78	4	0
6	H	226	0	124	10	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	G	1	0	0	0	0
8	H	54	38	0	4	0
9	A	8	0	0	3	0
9	B	3	0	0	0	0
9	C	2	0	0	2	0
9	D	1	0	0	0	0
All	All	11159	38	10184	474	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (474) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:146:ASP:HB3	1:A:148:THR:HG23	1.24	1.11
1:B:256:ILE:HD13	1:B:321:LEU:HD21	1.30	1.09
1:B:146:ASP:HB3	1:B:148:THR:HG23	1.31	1.09
1:A:70:MET:HE1	1:A:78:ASP:HB3	1.28	1.09
1:B:194:ILE:HG12	1:B:350:ILE:HD13	1.24	1.09
1:A:293:ARG:HB3	1:A:293:ARG:HH11	1.03	1.08
1:B:70:MET:HE1	1:B:78:ASP:HB3	1.36	1.07
1:B:307:ASN:HD22	1:B:310:LEU:HB2	0.92	1.06
1:A:256:ILE:HD13	1:A:321:LEU:HD21	1.36	1.04
1:A:293:ARG:CB	1:A:293:ARG:HH11	1.72	1.02
1:B:307:ASN:ND2	1:B:310:LEU:HB2	1.74	1.01
1:A:139:VAL:HG11	1:A:154:VAL:O	1.64	0.96
1:B:194:ILE:HG12	1:B:350:ILE:CD1	1.93	0.96
1:A:70:MET:HE1	1:A:78:ASP:CB	1.94	0.96
1:B:307:ASN:HD22	1:B:310:LEU:CB	1.79	0.95
1:B:20:TYR:CD1	2:D:513:HIS:HB2	2.05	0.91
1:A:293:ARG:NH1	1:A:293:ARG:HB3	1.87	0.90
1:B:41:GLN:HG2	1:B:88:MET:HE2	1.54	0.90
1:B:252:GLU:OE1	1:B:308:THR:HG21	1.70	0.89
2:C:526:MET:CE	2:C:529:LEU:HD12	2.03	0.88
1:B:60:ARG:HH11	1:B:60:ARG:CG	1.87	0.88
1:A:211:PRO:O	1:A:478:ARG:NH2	2.07	0.87
2:C:536:TYR:HD1	2:C:603:LEU:HD12	1.38	0.87
1:A:146:ASP:HB3	1:A:148:THR:CG2	2.03	0.86
1:A:288:ARG:NH1	1:A:290:GLU:OE2	2.08	0.86
2:C:431:LEU:HD13	2:C:479:MET:HE3	1.58	0.85
1:B:281:VAL:HG21	1:B:314:TYR:CG	2.12	0.84
2:C:536:TYR:CD1	2:C:603:LEU:HD12	2.13	0.84
1:B:41:GLN:HA	1:B:88:MET:HE1	1.60	0.84
1:B:350:ILE:HA	1:B:463:MET:HE1	1.60	0.83
1:A:194:ILE:HD11	1:A:463:MET:HE3	1.61	0.82
1:A:41:GLN:HA	1:A:88:MET:HE1	1.61	0.82
1:B:254:ILE:HD13	1:B:312:LEU:HD13	1.61	0.81
1:B:380:ARG:NH2	1:B:409:TYR:O	2.11	0.81
2:D:516:THR:O	2:D:520:THR:HG23	1.80	0.80
2:C:520:THR:HG21	2:C:622:MET:HG3	1.64	0.80
2:C:486:GLY:O	2:C:491:PHE:HD2	1.64	0.80
1:B:167:SER:C	1:B:168:THR:HG22	2.01	0.79
1:B:12:ILE:HG22	1:B:13:MET:N	1.97	0.79
1:A:117[B]:ARG:HD2	1:B:77:GLY:HA2	1.64	0.79
2:C:476:ILE:HD12	2:C:521:PHE:CE2	2.18	0.79
1:B:60:ARG:HH11	1:B:60:ARG:HG2	1.47	0.78
5:G:13:DC:H42	6:H:7:DG:H1	1.32	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:229:TYR:CD1	1:A:342:ILE:HG12	2.18	0.77
2:C:526:MET:HE2	2:C:529:LEU:HD12	1.65	0.77
2:D:520:THR:HG21	2:D:622:MET:HG3	1.67	0.77
1:B:44:ILE:HD12	1:B:88:MET:HE3	1.66	0.77
1:B:41:GLN:HA	1:B:88:MET:CE	2.15	0.76
1:B:350:ILE:HG23	1:B:463:MET:CE	2.15	0.76
1:A:169:GLY:HA2	1:A:176:THR:HG22	1.68	0.75
1:A:259:ILE:HB	1:A:260:PRO:CD	2.17	0.75
1:A:229:TYR:CG	1:A:342:ILE:HG12	2.20	0.75
1:A:296:LEU:HD23	1:A:297:ARG:N	2.01	0.74
1:A:445:LYS:O	1:A:449:LEU:HD12	1.87	0.74
2:C:526:MET:HE1	2:C:529:LEU:HD12	1.68	0.74
1:B:70:MET:HE1	1:B:78:ASP:CB	2.14	0.74
1:B:146:ASP:HB3	1:B:148:THR:CG2	2.14	0.73
1:B:44:ILE:HD12	1:B:88:MET:CE	2.17	0.73
2:C:479:MET:O	2:C:483:ILE:HG13	1.89	0.73
1:A:23:TYR:CB	2:C:509:THR:HG21	2.19	0.73
1:A:338:ARG:HD2	1:A:340:VAL:CG1	2.19	0.73
1:A:317:LYS:HD3	1:A:318:TYR:CE2	2.23	0.73
1:B:190:ALA:O	1:B:194:ILE:HG13	1.88	0.73
1:B:87:ARG:HA	1:B:90:GLN:HG3	1.71	0.72
1:A:96:GLU:HG2	1:A:126:ILE:HD13	1.72	0.72
1:B:219:ILE:HB	1:B:482:LEU:HD23	1.70	0.72
2:C:516:THR:O	2:C:520:THR:HG23	1.89	0.72
6:H:6:DT:H2"	6:H:7:DG:H5'	1.71	0.72
1:A:307:ASN:ND2	1:A:310:LEU:HB2	2.04	0.71
1:A:60:ARG:HH11	1:A:60:ARG:CG	2.04	0.71
1:B:281:VAL:HG21	1:B:314:TYR:CB	2.20	0.71
2:C:431:LEU:HD13	2:C:479:MET:CE	2.20	0.71
2:D:516:THR:HG23	2:D:622:MET:CE	2.20	0.71
1:B:307:ASN:ND2	1:B:310:LEU:H	1.89	0.70
1:A:259:ILE:HB	1:A:260:PRO:HD2	1.74	0.70
1:A:194:ILE:HD11	1:A:463:MET:CE	2.21	0.69
1:A:41:GLN:HA	1:A:88:MET:CE	2.22	0.69
1:B:261:TYR:CD2	1:B:262:GLU:HG3	2.28	0.68
1:A:452:ILE:HD13	1:A:462:LEU:HD12	1.75	0.68
1:B:211:PRO:O	1:B:478:ARG:NH2	2.25	0.68
2:D:536:TYR:HB3	2:D:603:LEU:CD1	2.23	0.68
1:B:124:SER:OG	1:B:126:ILE:HG22	1.93	0.68
1:B:281:VAL:CG2	1:B:314:TYR:CG	2.77	0.67
1:A:338:ARG:HD2	1:A:340:VAL:HG12	1.76	0.67
1:B:41:GLN:CG	1:B:88:MET:HE2	2.25	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:101:1UV:C15	8:H:101:1UV:C04	2.72	0.67
1:B:350:ILE:HG23	1:B:463:MET:HE2	1.77	0.67
2:C:536:TYR:HB3	2:C:603:LEU:CD1	2.25	0.66
1:A:316:PHE:CE2	1:A:321:LEU:HD13	2.30	0.66
2:D:455:LEU:CD1	2:D:518:LEU:HD11	2.26	0.66
1:A:70:MET:CE	1:A:78:ASP:HB3	2.17	0.66
1:A:55:PHE:HA	1:A:122:ARG:HD2	1.77	0.66
1:A:44:ILE:HD12	1:A:88:MET:CE	2.26	0.66
1:A:6:ASN:HB3	2:C:605:ARG:HB3	1.76	0.66
1:A:41:GLN:HG2	1:A:88:MET:HE2	1.77	0.66
1:A:169:GLY:HA3	1:A:176:THR:O	1.96	0.65
1:B:55:PHE:HA	1:B:122:ARG:HD2	1.77	0.65
2:C:460:ILE:HD12	4:F:6:DT:H5''	1.78	0.65
2:D:516:THR:HG23	2:D:622:MET:HE2	1.79	0.65
4:F:3:DT:H4'	4:F:4:DC:OP1	1.97	0.65
1:B:288:ARG:NH1	1:B:290:GLU:OE2	2.29	0.65
2:C:564:LEU:O	2:C:567:LEU:N	2.28	0.64
1:A:20:TYR:CD1	2:C:513:HIS:HB2	2.31	0.64
1:B:350:ILE:HG23	1:B:463:MET:HE1	1.79	0.64
1:A:87:ARG:HA	1:A:90:GLN:HG3	1.80	0.64
1:A:60:ARG:HH11	1:A:60:ARG:HG2	1.63	0.64
1:A:439:GLU:O	1:A:443:ARG:HG3	1.98	0.64
2:C:462:THR:HG21	2:C:521:PHE:HD2	1.63	0.64
3:E:13:DA:H2''	3:E:14:DA:O5'	1.97	0.64
2:D:478:THR:O	2:D:482:THR:HG23	1.98	0.63
1:B:12:ILE:CG2	1:B:13:MET:N	2.61	0.63
2:D:611:LEU:C	2:D:611:LEU:HD13	2.19	0.63
1:A:43:ARG:HG2	1:A:73:PHE:HB3	1.79	0.63
1:A:23:TYR:HB3	2:C:509:THR:HG21	1.81	0.63
1:A:281:VAL:HG21	1:A:314:TYR:CG	2.34	0.63
2:C:629:ARG:NH1	4:F:9:DA:OP1	2.26	0.63
1:B:259:ILE:HB	1:B:260:PRO:CD	2.30	0.62
8:H:102:1UV:C04	8:H:102:1UV:C15	2.76	0.62
1:B:281:VAL:CG2	1:B:314:TYR:CD2	2.81	0.62
1:B:194:ILE:CG1	1:B:350:ILE:HD13	2.16	0.62
1:A:340:VAL:HB	1:A:344:PRO:HG2	1.80	0.62
2:C:441:ALA:HB1	2:C:452:ILE:HD12	1.80	0.62
1:B:256:ILE:CD1	1:B:321:LEU:HD21	2.19	0.62
1:B:237:VAL:HG11	1:B:322:GLN:NE2	2.14	0.62
1:B:350:ILE:CA	1:B:463:MET:HE1	2.28	0.61
2:C:611:LEU:HD13	2:C:611:LEU:C	2.21	0.61
5:G:13:DC:N3	6:H:7:DG:N2	2.42	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:616:ARG:O	2:C:620:VAL:HG23	1.99	0.61
1:B:23:TYR:CB	2:D:509:THR:HG21	2.31	0.61
1:B:307:ASN:ND2	1:B:310:LEU:N	2.48	0.61
2:D:623:GLY:O	2:D:629:ARG:NH2	2.33	0.61
1:A:216:GLY:O	1:A:217:ALA:HB3	2.01	0.61
1:B:70:MET:CE	1:B:78:ASP:HB3	2.23	0.60
1:B:167:SER:O	1:B:168:THR:HG22	2.02	0.60
2:C:626:VAL:HG11	4:F:9:DA:H3'	1.83	0.60
1:B:168:THR:HA	1:B:176:THR:O	2.02	0.60
1:A:146:ASP:CB	1:A:148:THR:HG23	2.16	0.59
1:B:338:ARG:HD2	1:B:340:VAL:HG12	1.84	0.59
2:D:611:LEU:O	2:D:611:LEU:HD13	2.01	0.59
1:B:237:VAL:CG1	1:B:322:GLN:HE21	2.16	0.59
1:B:471:LYS:O	1:B:475:ALA:HB2	2.03	0.59
1:A:118:TYR:HE2	4:F:1:DA:H5'	1.66	0.59
1:B:159:PHE:HB2	1:B:160:PRO:HD2	1.83	0.59
1:B:24:ILE:HG13	1:B:28:ARG:HD2	1.84	0.59
1:A:350:ILE:HA	1:A:463:MET:HE1	1.85	0.59
2:C:475:GLU:O	2:C:479:MET:HB2	2.03	0.58
2:C:513:HIS:O	2:C:516:THR:HG22	2.03	0.58
1:B:371:ARG:O	1:B:371:ARG:HG3	2.02	0.58
1:A:44:ILE:HD12	1:A:88:MET:HE3	1.84	0.58
1:B:167:SER:C	1:B:168:THR:CG2	2.72	0.58
2:C:514:ILE:HA	2:C:517:LEU:HD12	1.85	0.58
1:B:336:THR:CG2	1:B:337:PRO:HD2	2.33	0.58
2:C:637:VAL:HG12	2:C:639:PHE:CE2	2.39	0.58
2:D:504:MET:HG3	2:D:538:ALA:HB3	1.86	0.58
2:C:486:GLY:O	2:C:491:PHE:CD2	2.51	0.58
1:A:185:GLU:OE1	1:A:478:ARG:NH1	2.37	0.57
5:G:13:DC:N4	6:H:7:DG:H1	2.02	0.57
1:B:169:GLY:HA2	1:B:176:THR:HG22	1.85	0.57
1:B:169:GLY:HA3	1:B:176:THR:O	2.05	0.57
2:C:430:TYR:CZ	2:C:502:ILE:HD12	2.39	0.57
1:A:302:LEU:CD1	1:A:308:THR:HB	2.35	0.57
1:B:371:ARG:HG2	1:B:442:LEU:HD11	1.86	0.57
1:B:145:PHE:CD1	1:B:146:ASP:N	2.73	0.57
1:A:375:VAL:O	1:A:379:ILE:HG13	2.05	0.57
1:A:296:LEU:C	1:A:296:LEU:HD23	2.24	0.56
1:A:43:ARG:HG2	1:A:73:PHE:CB	2.35	0.56
1:A:144:ASN:HA	9:A:602:HOH:O	2.04	0.56
1:B:194:ILE:HD13	1:B:463:MET:HE2	1.87	0.56
2:D:474:GLU:O	2:D:478:THR:HG23	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:107:SER:OG	1:A:111:ASP:OD2	2.15	0.56
1:A:471:LYS:O	1:A:475:ALA:HB2	2.06	0.56
2:C:483:ILE:HD13	2:C:501:ILE:HD11	1.88	0.56
2:C:527:ARG:N	2:C:528:PRO:CD	2.69	0.56
2:D:536:TYR:HB3	2:D:603:LEU:HD11	1.88	0.56
1:A:171:SER:OG	1:A:172:ALA:N	2.38	0.56
2:C:594:THR:OG1	2:C:595:THR:HG22	2.06	0.56
1:A:293:ARG:H	1:A:293:ARG:NH1	2.03	0.56
1:B:281:VAL:HG23	1:B:314:TYR:CD2	2.40	0.56
2:D:632:TRP:CE2	2:D:636:ASN:ND2	2.71	0.56
1:B:24:ILE:CG1	1:B:28:ARG:HD2	2.35	0.55
1:A:97:ILE:HG12	1:A:97:ILE:O	2.06	0.55
1:A:293:ARG:NH1	1:A:293:ARG:CB	2.56	0.55
2:D:538:ALA:O	2:D:540:PRO:HD3	2.07	0.55
1:A:96:GLU:CG	1:A:126:ILE:HD13	2.36	0.55
1:B:12:ILE:HG22	1:B:13:MET:H	1.70	0.55
1:B:343:VAL:O	1:B:347:SER:HB3	2.05	0.55
1:B:44:ILE:CD1	1:B:88:MET:HE3	2.35	0.55
1:B:59:TYR:CE1	1:B:102:HIS:ND1	2.74	0.54
2:D:516:THR:HG22	2:D:517:LEU:HG	1.89	0.54
1:A:104:ASN:HB3	1:A:114:ALA:HB2	1.88	0.54
1:A:256:ILE:CD1	1:A:321:LEU:HD21	2.25	0.54
1:B:35:ASP:O	1:B:161:ASN:HB3	2.07	0.54
1:B:169:GLY:CA	1:B:176:THR:HG22	2.38	0.54
2:C:483:ILE:HD13	2:C:501:ILE:CD1	2.38	0.54
1:A:27:ASP:O	1:A:39:PRO:HG2	2.08	0.54
1:B:293:ARG:HH11	1:B:293:ARG:HB3	1.73	0.54
1:B:171:SER:OG	1:B:172:ALA:N	2.40	0.54
1:B:338:ARG:O	1:B:340:VAL:HG13	2.08	0.54
1:A:334:ASN:O	1:A:335:PHE:HB2	2.08	0.54
2:D:466:LYS:O	2:D:468:ALA:N	2.41	0.54
1:B:124:SER:HG	1:B:126:ILE:HG22	1.71	0.53
5:G:13:DC:H2''	5:G:14:DA:O5'	2.08	0.53
1:A:214:PRO:HA	1:A:479:LEU:HD12	1.90	0.53
1:B:126:ILE:HG23	1:B:127:ALA:N	2.22	0.53
6:H:4:DT:H2''	6:H:5:DA:H5'	1.89	0.53
1:A:293:ARG:CG	1:A:293:ARG:HH11	2.20	0.53
1:A:40:VAL:HG13	1:A:41:GLN:N	2.24	0.53
1:A:425:TYR:O	1:A:428:THR:OG1	2.20	0.53
1:A:442:LEU:O	1:A:446:ILE:HG13	2.09	0.53
2:D:520:THR:CG2	2:D:622:MET:HG3	2.37	0.52
1:A:434:VAL:CG1	1:A:435:LEU:N	2.71	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:194:ILE:CD1	1:B:463:MET:HE2	2.39	0.52
1:B:412:THR:OG1	1:B:415:GLN:HG3	2.09	0.52
1:A:23:TYR:CG	2:C:509:THR:HG21	2.44	0.52
6:H:3:DC:H2'	6:H:4:DT:C6	2.44	0.52
1:A:403:GLU:O	1:A:407:VAL:HG23	2.10	0.52
1:B:22:LYS:HE2	1:B:26:GLN:OE1	2.09	0.52
1:B:351:ALA:O	1:B:354:ARG:HB3	2.10	0.52
1:A:118:TYR:CE2	4:F:1:DA:H5'	2.43	0.52
2:C:529:LEU:HD22	2:C:534:HIS:HB2	1.91	0.52
1:A:414:GLU:CD	1:A:414:GLU:H	2.12	0.52
1:B:374:ILE:HD12	1:B:418:ALA:HB2	1.91	0.52
2:C:536:TYR:CD1	2:C:603:LEU:CD1	2.90	0.52
2:C:581:LYS:HB2	2:C:585:GLU:OE2	2.09	0.52
1:B:252:GLU:O	1:B:302:LEU:HD12	2.10	0.52
2:D:491:PHE:HE1	2:D:528:PRO:HB2	1.73	0.52
1:A:412:THR:HG23	1:A:415:GLN:OE1	2.10	0.52
1:A:168:THR:HA	1:A:176:THR:O	2.10	0.51
1:A:252:GLU:OE1	1:A:308:THR:HG21	2.10	0.51
1:A:126:ILE:HG12	1:A:159:PHE:CE1	2.45	0.51
1:A:60:ARG:NH1	1:A:60:ARG:CG	2.66	0.51
2:C:431:LEU:CD1	2:C:479:MET:CE	2.87	0.51
1:A:354:ARG:HG3	1:A:459:MET:CE	2.41	0.51
1:B:111:ASP:HB2	1:B:112:PRO:HD2	1.92	0.51
2:D:618:VAL:HG12	2:D:619:ASN:N	2.25	0.51
6:H:6:DT:C2'	6:H:7:DG:H5'	2.38	0.51
1:A:194:ILE:CD1	1:A:463:MET:CE	2.89	0.51
2:C:416:LEU:HD23	2:C:417:THR:C	2.30	0.51
2:C:526:MET:C	2:C:528:PRO:HD2	2.31	0.51
1:A:86:VAL:O	1:A:90:GLN:HG2	2.11	0.51
2:D:455:LEU:HD12	2:D:518:LEU:HD11	1.91	0.50
1:A:434:VAL:HG13	1:A:435:LEU:N	2.26	0.50
1:B:452:ILE:HA	1:B:458:THR:HG22	1.93	0.50
1:A:77:GLY:HA2	1:B:117[B]:ARG:CD	2.41	0.50
1:B:240:SER:CB	1:B:321:LEU:HD22	2.42	0.50
1:A:268:LEU:CD2	1:A:272:ILE:HD11	2.42	0.50
1:A:77:GLY:O	1:A:81:ILE:HG13	2.12	0.50
1:B:60:ARG:HH11	1:B:60:ARG:HG3	1.74	0.50
1:A:350:ILE:HG23	1:A:463:MET:CE	2.42	0.50
2:C:509:THR:O	2:C:512:ALA:HB3	2.11	0.50
4:F:3:DT:C5	4:F:4:DC:N4	2.80	0.50
1:B:59:TYR:HB3	1:B:120:GLU:HB3	1.94	0.49
2:C:520:THR:CG2	2:C:622:MET:HG3	2.39	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:420:VAL:HG12	1:A:421:THR:HG23	1.94	0.49
1:B:220:GLN:HG2	1:B:483:GLU:HB2	1.94	0.49
2:C:597:ASN:C	2:C:599:GLU:H	2.15	0.49
1:B:79:SER:OG	8:H:101:1UV:O09	2.27	0.49
1:A:355:GLU:OE2	1:A:355:GLU:HA	2.11	0.49
1:A:425:TYR:CD1	1:B:398:LYS:HD2	2.47	0.49
1:A:169:GLY:CA	1:A:176:THR:HG22	2.38	0.49
1:A:95:ARG:HA	1:A:214:PRO:HB3	1.94	0.49
1:A:384:ILE:HB	1:A:387:GLU:HG3	1.94	0.49
1:A:397:ASN:O	1:A:398:LYS:C	2.50	0.49
4:F:8:DC:H2''	4:F:9:DA:H5'	1.94	0.49
1:A:6:ASN:OD1	1:A:6:ASN:N	2.38	0.49
1:B:126:ILE:CG2	1:B:127:ALA:N	2.75	0.49
1:B:194:ILE:CG1	1:B:350:ILE:CD1	2.79	0.49
1:A:256:ILE:HD13	1:A:321:LEU:CD2	2.26	0.49
1:A:70:MET:HE2	1:A:78:ASP:HA	1.95	0.49
1:A:117[B]:ARG:CD	1:B:77:GLY:HA2	2.39	0.49
1:B:70:MET:HE2	1:B:78:ASP:HA	1.93	0.49
2:C:536:TYR:N	2:C:536:TYR:CD2	2.81	0.49
1:A:44:ILE:HG12	1:A:69:ILE:HD13	1.94	0.49
1:A:40:VAL:HG23	1:A:74:HIS:CD2	2.48	0.49
2:C:627:GLU:N	2:C:628:PRO:CD	2.76	0.49
2:D:527:ARG:N	2:D:528:PRO:CD	2.76	0.49
1:B:77:GLY:O	1:B:81:ILE:HG13	2.12	0.48
2:C:591:LEU:HD22	2:C:596:MET:SD	2.53	0.48
1:A:290:GLU:HB2	1:A:297:ARG:HG2	1.95	0.48
2:C:433:GLU:HB2	2:C:505:THR:HG22	1.96	0.48
2:C:476:ILE:HD12	2:C:521:PHE:CD2	2.49	0.48
1:B:272:ILE:HG22	1:B:287:VAL:HG21	1.95	0.48
2:C:629:ARG:O	2:C:633:ILE:HG13	2.13	0.48
1:A:95:ARG:HB2	1:A:180:PRO:HB2	1.96	0.48
1:A:40:VAL:CG1	1:A:41:GLN:N	2.76	0.48
1:B:237:VAL:CG1	1:B:322:GLN:NE2	2.75	0.48
1:A:219:ILE:HB	1:A:482:LEU:HD23	1.95	0.48
1:A:84:ALA:O	1:A:88:MET:HG3	2.13	0.48
1:B:333:ASP:O	1:B:334:ASN:C	2.51	0.48
2:C:538:ALA:O	2:C:540:PRO:HD3	2.14	0.48
1:A:96:GLU:HG2	1:A:126:ILE:CD1	2.41	0.48
2:C:629:ARG:HD2	4:F:9:DA:OP1	2.13	0.48
1:B:417:GLU:O	1:B:421:THR:HG23	2.13	0.47
1:B:237:VAL:HG11	1:B:322:GLN:HE21	1.74	0.47
1:B:412:THR:HG23	1:B:415:GLN:OE1	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:13:MET:CE	2:D:520:THR:HG22	2.44	0.47
1:B:181:HIS:CD2	1:B:211:PRO:HA	2.50	0.47
1:B:292:ASP:O	1:B:294:ASP:N	2.47	0.47
1:B:37:LEU:CD1	1:B:155:LEU:HD12	2.44	0.47
1:B:429:ASN:O	1:B:429:ASN:CG	2.51	0.47
1:B:336:THR:HG22	1:B:337:PRO:HD2	1.96	0.47
1:B:66:VAL:O	1:B:69:ILE:HB	2.14	0.47
2:C:441:ALA:O	2:C:445:ARG:HB3	2.15	0.47
2:D:446:ASP:O	2:D:448:LYS:N	2.48	0.47
1:A:359:ALA:HA	1:A:362:ARG:NH1	2.29	0.47
1:B:139:VAL:HG11	1:B:154:VAL:O	2.15	0.47
2:C:462:THR:N	9:C:802:HOH:O	2.47	0.47
1:A:79:SER:OG	8:H:102:1UV:O09	2.26	0.47
1:A:217:ALA:N	1:A:258:GLU:OE1	2.43	0.47
2:D:483:ILE:HG22	2:D:483:ILE:O	2.15	0.47
2:D:592:TRP:HA	2:D:596:MET:HB2	1.97	0.47
1:B:10:GLU:HA	2:D:617:ARG:HG2	1.97	0.47
2:D:424:PRO:O	2:D:499:ASP:HB2	2.15	0.47
1:A:382:ILE:HD12	1:A:432:VAL:HG23	1.96	0.47
1:B:157:ALA:O	1:B:353:ARG:HD3	2.15	0.47
1:B:110:GLY:HA3	1:B:264:ASN:HD21	1.80	0.47
1:A:41:GLN:CG	1:A:88:MET:HE2	2.44	0.46
1:A:70:MET:CE	1:A:78:ASP:CB	2.81	0.46
1:B:10:GLU:C	1:B:12:ILE:H	2.17	0.46
1:B:167:SER:O	1:B:168:THR:CB	2.63	0.46
1:B:281:VAL:HG21	1:B:314:TYR:CD2	2.50	0.46
2:C:536:TYR:HB3	2:C:603:LEU:HD13	1.97	0.46
1:A:181:HIS:CD2	1:A:211:PRO:HA	2.50	0.46
1:A:412:THR:HG23	1:A:415:GLN:CD	2.35	0.46
1:B:51:ASP:O	1:B:60:ARG:NH2	2.48	0.46
1:B:60:ARG:NH1	1:B:60:ARG:CG	2.56	0.46
1:A:28:ARG:NH2	3:E:14:DA:H4'	2.30	0.46
2:C:455:LEU:CD1	2:C:518:LEU:HD11	2.46	0.46
2:D:483:ILE:HD13	2:D:501:ILE:CD1	2.46	0.46
2:D:615:GLU:O	2:D:619:ASN:HB2	2.15	0.46
1:A:51:ASP:O	1:A:52:SER:HB2	2.14	0.46
2:C:536:TYR:CB	2:C:603:LEU:CD1	2.92	0.46
2:D:483:ILE:HD13	2:D:501:ILE:HD11	1.97	0.46
1:A:459:MET:SD	1:A:459:MET:C	2.94	0.46
1:B:216:GLY:O	1:B:217:ALA:HB3	2.16	0.46
1:B:372:LEU:HD22	1:B:376:GLU:HG3	1.97	0.46
1:B:336:THR:HG23	1:B:337:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:110:GLY:HA3	1:B:264:ASN:ND2	2.31	0.45
1:B:41:GLN:CB	1:B:88:MET:HE2	2.45	0.45
1:B:95:ARG:HB2	1:B:180:PRO:HB2	1.97	0.45
6:H:3:DC:H4'	6:H:4:DT:OP1	2.16	0.45
1:A:194:ILE:HG12	1:A:463:MET:HE2	1.99	0.45
2:C:623:GLY:O	2:C:629:ARG:NH2	2.48	0.45
1:A:13:MET:CE	2:C:520:THR:HG22	2.46	0.45
1:A:424:LEU:HD23	1:B:424:LEU:HD23	1.98	0.45
1:A:139:VAL:HG13	1:A:140:PRO:HD2	1.98	0.45
1:B:10:GLU:O	1:B:12:ILE:N	2.50	0.45
1:B:459:MET:C	1:B:459:MET:SD	2.94	0.45
1:A:59:TYR:CD2	1:A:122:ARG:HG2	2.52	0.45
1:A:273:ASP:O	1:A:277:VAL:HG23	2.17	0.45
1:B:281:VAL:HG21	1:B:314:TYR:HB2	1.98	0.45
1:B:66:VAL:HG12	1:B:67:GLY:N	2.31	0.45
1:A:254:ILE:HD13	1:A:312:LEU:HD13	1.99	0.45
1:A:194:ILE:HG12	1:A:350:ILE:HD13	1.98	0.45
1:A:373:HIS:CE1	1:A:412:THR:HG21	2.52	0.45
1:B:240:SER:HB2	1:B:321:LEU:HD22	1.99	0.45
1:B:432:VAL:HG13	1:B:436:GLN:HG3	1.98	0.45
1:A:387:GLU:HG2	1:A:387:GLU:H	1.46	0.45
1:A:142:ALA:O	1:A:150:LYS:HA	2.18	0.44
1:A:391:LEU:HD22	1:A:405:LEU:HD23	1.98	0.44
1:B:132:GLN:O	1:B:133:ASP:HB2	2.17	0.44
1:B:372:LEU:O	1:B:372:LEU:HD22	2.18	0.44
1:B:59:TYR:CD2	1:B:122:ARG:HG2	2.52	0.44
1:B:338:ARG:HD2	1:B:340:VAL:CG1	2.47	0.44
2:D:516:THR:HG22	2:D:517:LEU:N	2.32	0.44
4:F:8:DC:H2''	4:F:9:DA:C5'	2.47	0.44
1:A:247:LEU:O	1:A:249:GLY:N	2.51	0.44
1:A:391:LEU:HD21	1:A:404:ASN:HB3	1.99	0.44
2:C:591:LEU:CD2	2:C:596:MET:HG3	2.47	0.44
1:B:293:ARG:NE	2:C:592:TRP:CD1	2.85	0.44
2:C:596:MET:O	2:C:598:PRO:HD3	2.18	0.44
1:A:161:ASN:ND2	9:A:601:HOH:O	2.50	0.44
1:B:159:PHE:HB2	1:B:160:PRO:CD	2.48	0.44
1:B:239:ARG:HG3	1:B:316:PHE:CE2	2.53	0.44
1:B:23:TYR:HB2	2:D:509:THR:HG21	1.99	0.44
1:B:44:ILE:HD12	1:B:88:MET:HE1	1.99	0.44
2:D:536:TYR:CB	2:D:603:LEU:HD11	2.48	0.44
1:A:157:ALA:O	1:A:353:ARG:HD3	2.18	0.44
2:C:491:PHE:HD1	2:C:528:PRO:HG2	1.83	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:611:LEU:HD13	2:C:611:LEU:O	2.17	0.44
1:B:194:ILE:CD1	1:B:463:MET:CE	2.96	0.43
1:B:23:TYR:HE1	1:B:28:ARG:HH21	1.66	0.43
2:D:580:TYR:CE1	2:D:586:MET:HG2	2.53	0.43
1:B:59:TYR:CE1	1:B:102:HIS:CE1	3.05	0.43
1:B:342:ILE:HD13	1:B:342:ILE:HA	1.60	0.43
1:A:132:GLN:O	1:A:133:ASP:HB2	2.18	0.43
1:A:27:ASP:C	1:A:39:PRO:HG2	2.38	0.43
1:B:40:VAL:CG1	1:B:41:GLN:N	2.80	0.43
1:A:415:GLN:O	1:A:419:ILE:HG13	2.18	0.43
1:B:237:VAL:HG13	1:B:322:GLN:HE21	1.83	0.43
2:C:511:GLY:O	2:C:515:GLN:HG3	2.19	0.43
1:B:259:ILE:HB	1:B:260:PRO:HD2	2.00	0.43
1:A:285:ALA:HB3	1:A:301:GLU:HG2	2.01	0.43
1:A:144:ASN:CA	9:A:602:HOH:O	2.66	0.43
1:B:160:PRO:HA	1:B:349:TYR:CE1	2.54	0.43
1:B:345:ILE:HG22	1:B:346:LEU:N	2.33	0.43
1:B:130:LEU:HD23	1:B:157:ALA:HA	2.00	0.43
2:C:464:LYS:HZ2	4:F:8:DC:P	2.42	0.43
6:H:5:DA:C2	6:H:6:DT:C2	3.06	0.43
2:C:460:ILE:O	9:C:802:HOH:O	2.20	0.43
1:A:371:ARG:HG2	1:A:442:LEU:HD11	2.00	0.43
2:C:633:ILE:O	2:C:637:VAL:HB	2.19	0.43
1:A:261:TYR:CD2	1:A:262:GLU:HG3	2.54	0.42
1:B:359:ALA:HA	1:B:362:ARG:HH11	1.84	0.42
1:B:41:GLN:CA	1:B:88:MET:HE1	2.42	0.42
1:A:194:ILE:CD1	1:A:463:MET:HE2	2.49	0.42
1:A:412:THR:HG23	1:A:415:GLN:CG	2.49	0.42
1:B:23:TYR:CG	2:D:509:THR:HG21	2.54	0.42
1:B:321:LEU:HA	1:B:321:LEU:HD23	1.77	0.42
2:C:442:LYS:O	2:C:445:ARG:HD3	2.19	0.42
1:B:162:LEU:HD21	1:B:178:ILE:HD12	2.00	0.42
1:B:296:LEU:C	1:B:296:LEU:HD23	2.39	0.42
1:B:442:LEU:HA	1:B:442:LEU:HD23	1.67	0.42
2:C:485:ALA:HB3	2:C:491:PHE:CE2	2.54	0.42
2:D:441:ALA:HB1	2:D:452:ILE:HD12	2.02	0.42
1:A:293:ARG:CD	2:D:589:ASP:HA	2.50	0.42
1:B:242:THR:HG22	1:B:256:ILE:HG12	2.02	0.42
1:B:13:MET:HE2	2:D:618:VAL:HG22	2.01	0.42
1:A:87:ARG:C	1:A:89:SER:H	2.23	0.42
1:B:440:ALA:O	1:B:441:GLU:C	2.57	0.42
1:A:268:LEU:HD22	1:A:272:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:320:ASP:C	1:A:322:GLN:N	2.69	0.42
1:B:167:SER:O	1:B:168:THR:CG2	2.66	0.42
1:B:34:ARG:HD2	1:B:352:HIS:ND1	2.34	0.42
1:B:89:SER:HA	1:B:99:VAL:O	2.20	0.42
2:C:529:LEU:HA	2:C:529:LEU:HD23	1.77	0.42
1:A:350:ILE:HG23	1:A:463:MET:HE2	2.02	0.42
1:B:146:ASP:O	1:B:147:ASP:HB2	2.20	0.42
2:C:597:ASN:O	2:C:599:GLU:N	2.52	0.42
2:C:423:ASN:O	2:C:427:ASN:HB2	2.19	0.41
2:C:430:TYR:CE2	2:C:502:ILE:HD12	2.55	0.41
2:C:529:LEU:HD22	2:C:534:HIS:CB	2.50	0.41
1:A:77:GLY:HA2	1:B:117[B]:ARG:HD3	2.03	0.41
1:B:60:ARG:HG3	1:B:60:ARG:NH1	2.32	0.41
1:A:28:ARG:NH1	2:C:510:ASP:OD1	2.37	0.41
2:D:525:TYR:O	2:D:526:MET:HG3	2.20	0.41
2:D:560:THR:C	2:D:562:GLY:N	2.73	0.41
1:B:350:ILE:CG2	1:B:463:MET:HE1	2.48	0.41
1:A:349:TYR:O	1:A:352:HIS:HB3	2.21	0.41
2:D:458:LYS:HB2	6:H:6:DT:O2	2.21	0.41
1:A:245:GLU:OE2	1:A:297:ARG:NH2	2.53	0.41
1:B:116:MET:HB3	1:B:116:MET:HE3	1.85	0.41
2:D:491:PHE:CE1	2:D:528:PRO:HB2	2.55	0.41
1:B:130:LEU:HA	1:B:130:LEU:HD23	1.88	0.41
1:B:13:MET:HE1	2:D:520:THR:CG2	2.50	0.41
1:B:320:ASP:C	1:B:322:GLN:N	2.74	0.41
2:C:416:LEU:HD12	2:C:482:THR:CB	2.50	0.41
1:A:173:GLY:C	1:A:174:TYR:CD2	2.94	0.41
1:A:358:LEU:HA	1:A:358:LEU:HD23	1.88	0.41
1:B:406:LYS:HE2	1:B:413:GLU:HA	2.03	0.41
2:C:516:THR:HG23	2:C:622:MET:CE	2.50	0.41
1:B:13:MET:HE2	2:D:520:THR:HG22	2.03	0.41
1:B:48:MET:CE	1:B:122:ARG:HA	2.50	0.41
1:B:302:LEU:HD12	1:B:302:LEU:H	1.85	0.41
1:B:435:LEU:HA	1:B:435:LEU:HD23	1.88	0.41
2:C:433:GLU:HG3	2:C:514:ILE:HD13	2.02	0.41
1:A:168:THR:HA	1:A:169:GLY:HA3	1.86	0.41
1:A:190:ALA:O	1:A:194:ILE:HG13	2.21	0.41
1:A:228:ALA:HA	1:A:233:LYS:O	2.20	0.41
1:A:90:GLN:HB3	1:A:92:TRP:CH2	2.56	0.41
1:A:393:ARG:NH1	1:B:386:ASP:OD2	2.54	0.41
1:B:385:LEU:HA	1:B:385:LEU:HD23	1.84	0.41
1:A:261:TYR:CE2	1:A:262:GLU:HG3	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:424:LEU:HA	1:A:424:LEU:HD23	1.74	0.40
1:A:397:ASN:HA	1:B:428:THR:OG1	2.22	0.40
1:A:452:ILE:CD1	1:A:462:LEU:HD12	2.47	0.40
1:B:139:VAL:HG13	1:B:140:PRO:HD2	2.02	0.40
1:B:462:LEU:HA	1:B:462:LEU:HD23	1.68	0.40
1:A:433:VAL:O	1:A:434:VAL:C	2.59	0.40
1:B:290:GLU:OE1	1:B:297:ARG:NH1	2.52	0.40
1:B:116:MET:HG2	1:B:116:MET:O	2.21	0.40
1:A:268:LEU:HD22	1:A:272:ILE:CD1	2.51	0.40
1:A:424:LEU:CD2	1:B:424:LEU:HD23	2.52	0.40
1:B:307:ASN:HD22	1:B:310:LEU:N	2.16	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	Distance(Å)	Clash(Å)
1:A:393:ARG:NH2	1:B:279:ASN:O[4_455]	2.06	0.14

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	481/496 (97%)	438 (91%)	35 (7%)	8 (2%)	14	63
1	B	481/496 (97%)	434 (90%)	37 (8%)	10 (2%)	11	58
2	C	202/268 (75%)	183 (91%)	17 (8%)	2 (1%)	22	75
2	D	204/268 (76%)	183 (90%)	17 (8%)	4 (2%)	11	59
All	All	1368/1528 (90%)	1238 (90%)	106 (8%)	24 (2%)	13	63

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	168	THR

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Mol	Chain	Res	Type
1	A	217	ALA
1	A	248	LYS
1	B	11	ASP
1	B	293	ARG
2	C	496	ALA
2	D	467	MET
2	D	600	THR
1	A	116	MET
1	A	397	ASN
1	B	157	ALA
2	D	447	ARG
1	A	249	GLY
1	B	217	ALA
1	A	221	GLY
1	B	169	GLY
1	B	334	ASN
1	A	4	ILE
1	B	345	ILE
1	B	221	GLY
2	C	598	PRO
1	A	169	GLY
1	B	4	ILE
2	D	423	ASN

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	378/431 (88%)	345 (91%)	33 (9%)	15	53
1	B	376/431 (87%)	334 (89%)	42 (11%)	9	38
2	C	117/224 (52%)	101 (86%)	16 (14%)	5	27
2	D	109/224 (49%)	99 (91%)	10 (9%)	13	49
All	All	980/1310 (75%)	879 (90%)	101 (10%)	10	42

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	9	LEU
1	A	28	ARG
1	A	34	ARG
1	A	58	SER
1	A	90	GLN
1	A	91	ASN
1	A	97	ILE
1	A	102	HIS
1	A	111	ASP
1	A	136	LYS
1	A	162	LEU
1	A	168	THR
1	A	208	LEU
1	A	236	VAL
1	A	293	ARG
1	A	297	ARG
1	A	308	THR
1	A	321	LEU
1	A	338	ARG
1	A	342	ILE
1	A	347	SER
1	A	371	ARG
1	A	385	LEU
1	A	387	GLU
1	A	412	THR
1	A	414	GLU
1	A	415	GLN
1	A	420	VAL
1	A	428	THR
1	A	432	VAL
1	A	462	LEU
1	A	476	THR
1	B	4	ILE
1	B	6	ASN
1	B	9	LEU
1	B	12	ILE
1	B	16	ARG
1	B	60	ARG
1	B	70	MET
1	B	96	GLU
1	B	102	HIS
1	B	116	MET

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Mol	Chain	Res	Type
1	B	122	ARG
1	B	139	VAL
1	B	162	LEU
1	B	167	SER
1	B	168	THR
1	B	177	ASP
1	B	198	THR
1	B	208	LEU
1	B	268	LEU
1	B	274	ASP
1	B	293	ARG
1	B	297	ARG
1	B	301	GLU
1	B	302	LEU
1	B	308	THR
1	B	310	LEU
1	B	321	LEU
1	B	338	ARG
1	B	347	SER
1	B	371	ARG
1	B	372	LEU
1	B	381	VAL
1	B	385	LEU
1	B	393	ARG
1	B	414	GLU
1	B	420	VAL
1	B	432	VAL
1	B	434	VAL
1	B	452	ILE
1	B	462	LEU
1	B	476	THR
1	B	478	ARG
2	C	429	LEU
2	C	435	ASP
2	C	436	SER
2	C	445	ARG
2	C	453	LEU
2	C	475	GLU
2	C	509	THR
2	C	514	ILE
2	C	516	THR
2	C	524	ARG

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Mol	Chain	Res	Type
2	C	534	HIS
2	C	536	TYR
2	C	586	MET
2	C	595	THR
2	C	603	LEU
2	C	605	ARG
2	D	429	LEU
2	D	436	SER
2	D	445	ARG
2	D	453	LEU
2	D	514	ILE
2	D	516	THR
2	D	524	ARG
2	D	595	THR
2	D	603	LEU
2	D	619	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	307	ASN
1	B	322	GLN
2	C	636	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	1UV	H	101	7	31,31,31	2.04	8 (25%)	45,48,48	3.28	24 (53%)
8	1UV	H	102	7	31,31,31	2.00	9 (29%)	45,48,48	3.47	24 (53%)

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
8	1UV	H	101	7	-	0/8/33/33	1/4/5/5
8	1UV	H	102	7	-	0/8/33/33	1/4/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	101	1UV	O16-C15	-4.92	1.38	1.44
8	H	101	1UV	O16-C17	-4.83	1.37	1.42
8	H	102	1UV	O16-C17	-4.43	1.37	1.42
8	H	102	1UV	O16-C15	-4.29	1.38	1.44
8	H	102	1UV	C14-C13	3.70	1.46	1.43
8	H	102	1UV	C06-C07	3.63	1.57	1.50
8	H	101	1UV	C27-C25	3.55	1.38	1.35
8	H	102	1UV	C27-C25	3.45	1.38	1.35
8	H	101	1UV	C14-C13	3.39	1.46	1.43
8	H	101	1UV	C18-N19	3.19	1.51	1.47
8	H	101	1UV	C06-C07	3.05	1.55	1.50
8	H	102	1UV	C18-N19	2.84	1.51	1.47
8	H	101	1UV	C10-C06	-2.61	1.37	1.41
8	H	101	1UV	C02-N01	-2.46	1.45	1.49
8	H	102	1UV	C21-C22	-2.14	1.49	1.53
8	H	102	1UV	C10-C06	-2.05	1.38	1.41
8	H	102	1UV	C17-C18	-2.02	1.48	1.50

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	102	1UV	C03-C02-N01	14.59	139.41	118.92
8	H	101	1UV	C03-C02-N01	13.43	137.78	118.92
8	H	102	1UV	C22-C18-N19	6.52	105.51	100.49
8	H	101	1UV	C20-N19-C24	6.48	140.07	115.97
8	H	102	1UV	C20-N19-C24	6.44	139.90	115.97
8	H	102	1UV	C20-N19-C18	-6.16	101.53	111.55
8	H	101	1UV	C20-N19-C18	-6.12	101.59	111.55
8	H	101	1UV	C22-C18-N19	6.11	105.19	100.49
8	H	101	1UV	C05-N01-C02	-4.48	114.25	119.16
8	H	102	1UV	C05-N01-C02	-4.18	114.58	119.16
8	H	102	1UV	C21-C20-N19	3.98	107.28	103.38
8	H	101	1UV	C15-C14-C13	3.88	125.86	121.01
8	H	102	1UV	C15-C14-C24	-3.85	113.16	121.35
8	H	102	1UV	C14-C24-N19	3.84	124.67	118.57
8	H	102	1UV	C15-C14-C13	3.78	125.74	121.01
8	H	102	1UV	C10-C12-C13	3.68	122.79	119.67
8	H	101	1UV	C15-C14-C24	-3.66	113.55	121.35
8	H	102	1UV	C25-C27-C12	3.41	122.46	119.82
8	H	101	1UV	C14-C24-N19	3.36	123.91	118.57
8	H	102	1UV	C14-C13-N01	3.32	127.65	122.21
8	H	101	1UV	O16-C17-C18	-3.04	108.74	114.85
8	H	101	1UV	C21-C20-N19	2.97	106.29	103.38
8	H	102	1UV	C27-C12-C10	-2.93	117.65	122.12
8	H	102	1UV	C02-N01-C13	2.89	124.49	121.15
8	H	102	1UV	O16-C17-C18	-2.88	109.07	114.85
8	H	101	1UV	C14-C13-N01	2.83	126.84	122.21
8	H	101	1UV	C17-C18-N19	-2.82	108.06	113.00
8	H	102	1UV	C25-C24-N19	-2.77	115.45	121.62
8	H	101	1UV	C25-C27-C12	2.68	121.90	119.82
8	H	101	1UV	C05-C06-C10	2.66	120.12	116.85
8	H	101	1UV	C10-C12-C13	2.61	121.88	119.67
8	H	102	1UV	C17-C18-N19	-2.56	108.52	113.00
8	H	101	1UV	C02-N01-C13	2.54	124.09	121.15
8	H	101	1UV	C25-C24-N19	-2.50	116.05	121.62
8	H	101	1UV	C14-C24-C25	2.46	120.03	117.28
8	H	102	1UV	O08-C07-C06	2.37	120.95	114.35
8	H	102	1UV	C14-C24-C25	2.32	119.88	117.28
8	H	102	1UV	C06-C10-C12	-2.27	118.16	121.93
8	H	101	1UV	C27-C12-C10	-2.26	118.68	122.12
8	H	101	1UV	O09-C07-C06	-2.24	116.58	122.23
8	H	101	1UV	O08-C07-C06	2.20	120.49	114.35
8	H	101	1UV	C06-C10-C12	-2.20	118.28	121.93
8	H	101	1UV	C04-C02-N01	-2.19	115.83	118.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	102	1UV	C27-C25-C24	-2.10	120.23	123.31
8	H	101	1UV	C20-C21-C22	2.10	106.58	102.87
8	H	102	1UV	C14-C13-C12	-2.08	116.78	119.00
8	H	102	1UV	C20-C21-C22	2.05	106.49	102.87
8	H	102	1UV	C05-C06-C10	2.01	119.32	116.85

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	102	1UV	C14-C15-C17-C18-C24-N19-O16
8	H	101	1UV	C14-C15-C17-C18-C24-N19-O16

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	482/496 (97%)	-0.47	0 100 100	53, 73, 110, 153	0
1	B	482/496 (97%)	-0.47	0 100 100	52, 73, 107, 160	0
2	C	208/268 (77%)	-0.36	0 100 100	85, 117, 155, 183	0
2	D	210/268 (78%)	-0.31	0 100 100	79, 117, 157, 176	0
3	E	7/7 (100%)	-0.65	0 100 100	79, 82, 111, 143	0
4	F	11/11 (100%)	-0.61	0 100 100	84, 101, 120, 136	0
5	G	7/7 (100%)	-0.44	0 100 100	72, 82, 114, 137	0
6	H	11/11 (100%)	-0.52	0 100 100	81, 96, 112, 137	0
All	All	1418/1564 (90%)	-0.43	0 100 100	52, 82, 140, 183	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	MG	G	100	1/1	0.37	12.40	117,117,117,117	0
7	MG	C	701	1/1	0.69	8.05	100,100,100,100	0
7	MG	D	701	1/1	0.69	7.14	73,73,73,73	0
7	MG	A	502	1/1	0.36	6.20	112,112,112,112	0
8	1UV	H	102	27/27	0.24	1.58	103,128,152,159	0
8	1UV	H	101	27/27	0.21	0.99	107,130,156,163	0
7	MG	A	501	1/1	0.06	-2.21	77,77,77,77	0
7	MG	B	700	1/1	0.08	-2.36	92,92,92,92	0

6.5 Other polymers ⓘ

There are no such residues in this entry.