



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:17 am GMT

PDB ID : 3ORX
Title : PDK1 mutant bound to allosteric disulfide fragment inhibitor 1F8
Authors : Sadowsky, J.D.; Wells, J.A.
Deposited on : 2010-09-08
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

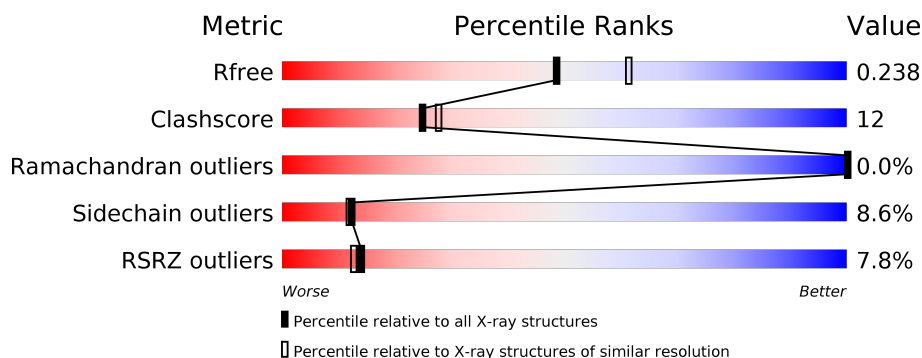
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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. 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	316	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	316	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>18%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	316	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>•</div> <div>10%</div> </div> </div>
1	D	316	<div> <div>8%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>•</div> <div>10%</div> </div> </div>
1	E	316	<div> <div>6%</div> <div> <div></div> <div>65%</div> <div>19%</div> <div>•</div> <div>13%</div> </div> </div>
1	F	316	<div> <div>10%</div> <div> <div></div> <div>66%</div> <div>18%</div> <div>•</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	316	
1	H	316	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	1F8	A	1	-	-	-	X
2	1F8	B	1	-	-	-	X
2	1F8	E	1	-	-	-	X
2	1F8	G	1	-	-	-	X
2	1F8	H	1	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19043 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 3-phosphoinositide-dependent protein kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	P	S	0	0	0
			2271	1476	374	412	1	8			
1	B	281	Total	C	N	O	P	S	0	0	0
			2262	1470	368	415	1	8			
1	C	284	Total	C	N	O	P	S	0	0	0
			2264	1469	369	417	1	8			
1	D	283	Total	C	N	O	P	S	0	0	0
			2256	1468	370	409	1	8			
1	E	274	Total	C	N	O	S		0	0	0
			2163	1415	354	386	8				
1	F	275	Total	C	N	O	P	S	0	0	0
			2132	1391	348	384	1	8			
1	G	275	Total	C	N	O	P	S	0	0	0
			2155	1406	352	388	1	8			
1	H	275	Total	C	N	O	P	S	0	0	0
			2114	1379	342	384	1	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	GLY	-	EXPRESSION TAG	UNP O15530
A	45	ALA	-	EXPRESSION TAG	UNP O15530
A	46	MET	-	EXPRESSION TAG	UNP O15530
A	47	ASP	-	EXPRESSION TAG	UNP O15530
A	48	PRO	-	EXPRESSION TAG	UNP O15530
A	49	GLU	-	EXPRESSION TAG	UNP O15530
A	50	PHE	-	EXPRESSION TAG	UNP O15530
A	148	CYS	THR	ENGINEERED MUTATION	UNP O15530
B	44	GLY	-	EXPRESSION TAG	UNP O15530
B	45	ALA	-	EXPRESSION TAG	UNP O15530
B	46	MET	-	EXPRESSION TAG	UNP O15530
B	47	ASP	-	EXPRESSION TAG	UNP O15530
B	48	PRO	-	EXPRESSION TAG	UNP O15530

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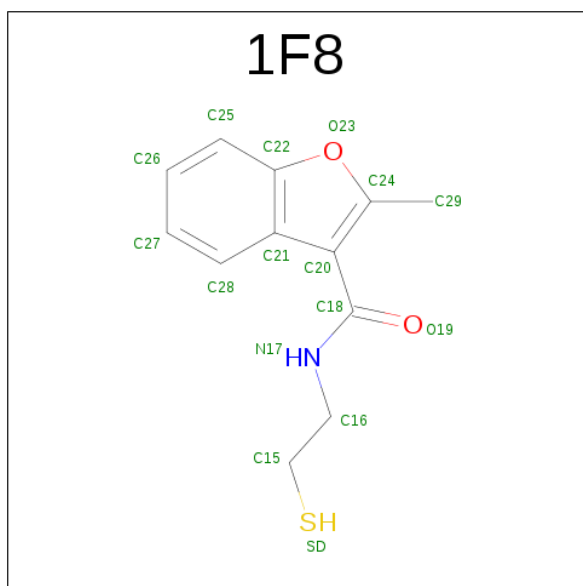
Chain	Residue	Modelled	Actual	Comment	Reference
B	49	GLU	-	EXPRESSION TAG	UNP O15530
B	50	PHE	-	EXPRESSION TAG	UNP O15530
B	148	CYS	THR	ENGINEERED MUTATION	UNP O15530
C	44	GLY	-	EXPRESSION TAG	UNP O15530
C	45	ALA	-	EXPRESSION TAG	UNP O15530
C	46	MET	-	EXPRESSION TAG	UNP O15530
C	47	ASP	-	EXPRESSION TAG	UNP O15530
C	48	PRO	-	EXPRESSION TAG	UNP O15530
C	49	GLU	-	EXPRESSION TAG	UNP O15530
C	50	PHE	-	EXPRESSION TAG	UNP O15530
C	148	CYS	THR	ENGINEERED MUTATION	UNP O15530
D	44	GLY	-	EXPRESSION TAG	UNP O15530
D	45	ALA	-	EXPRESSION TAG	UNP O15530
D	46	MET	-	EXPRESSION TAG	UNP O15530
D	47	ASP	-	EXPRESSION TAG	UNP O15530
D	48	PRO	-	EXPRESSION TAG	UNP O15530
D	49	GLU	-	EXPRESSION TAG	UNP O15530
D	50	PHE	-	EXPRESSION TAG	UNP O15530
D	148	CYS	THR	ENGINEERED MUTATION	UNP O15530
E	44	GLY	-	EXPRESSION TAG	UNP O15530
E	45	ALA	-	EXPRESSION TAG	UNP O15530
E	46	MET	-	EXPRESSION TAG	UNP O15530
E	47	ASP	-	EXPRESSION TAG	UNP O15530
E	48	PRO	-	EXPRESSION TAG	UNP O15530
E	49	GLU	-	EXPRESSION TAG	UNP O15530
E	50	PHE	-	EXPRESSION TAG	UNP O15530
E	148	CYS	THR	ENGINEERED MUTATION	UNP O15530
F	44	GLY	-	EXPRESSION TAG	UNP O15530
F	45	ALA	-	EXPRESSION TAG	UNP O15530
F	46	MET	-	EXPRESSION TAG	UNP O15530
F	47	ASP	-	EXPRESSION TAG	UNP O15530
F	48	PRO	-	EXPRESSION TAG	UNP O15530
F	49	GLU	-	EXPRESSION TAG	UNP O15530
F	50	PHE	-	EXPRESSION TAG	UNP O15530
F	148	CYS	THR	ENGINEERED MUTATION	UNP O15530
G	44	GLY	-	EXPRESSION TAG	UNP O15530
G	45	ALA	-	EXPRESSION TAG	UNP O15530
G	46	MET	-	EXPRESSION TAG	UNP O15530
G	47	ASP	-	EXPRESSION TAG	UNP O15530
G	48	PRO	-	EXPRESSION TAG	UNP O15530
G	49	GLU	-	EXPRESSION TAG	UNP O15530
G	50	PHE	-	EXPRESSION TAG	UNP O15530

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Chain	Residue	Modelled	Actual	Comment	Reference
G	148	CYS	THR	ENGINEERED MUTATION	UNP O15530
H	44	GLY	-	EXPRESSION TAG	UNP O15530
H	45	ALA	-	EXPRESSION TAG	UNP O15530
H	46	MET	-	EXPRESSION TAG	UNP O15530
H	47	ASP	-	EXPRESSION TAG	UNP O15530
H	48	PRO	-	EXPRESSION TAG	UNP O15530
H	49	GLU	-	EXPRESSION TAG	UNP O15530
H	50	PHE	-	EXPRESSION TAG	UNP O15530
H	148	CYS	THR	ENGINEERED MUTATION	UNP O15530

- Molecule 2 is 2-METHYL-N-(2-SULFANYLETHYL)-1-BENZOFURAN-3-CARBOXAMID E (three-letter code: 1F8) (formula: C₁₂H₁₃NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
2	B	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
2	C	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
2	D	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
2	E	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
2	F	1	Total	C	N	O	S	0	0
			16	12	1	2	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
2	H	1	Total	C	N	O	S	0	0
			16	12	1	2	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

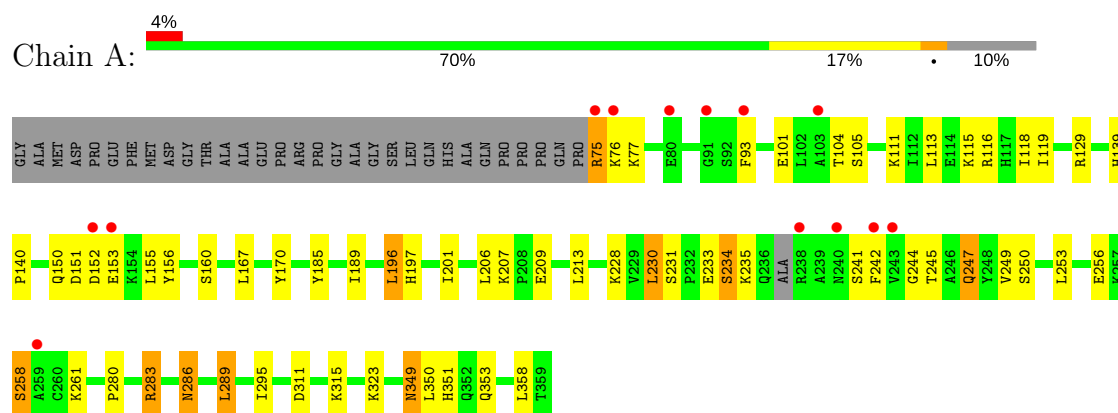
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	204	Total	O	0	0
			204	204		
4	B	213	Total	O	0	0
			213	213		
4	C	194	Total	O	0	0
			194	194		
4	D	187	Total	O	0	0
			187	187		
4	E	120	Total	O	0	0
			120	120		
4	F	121	Total	O	0	0
			121	121		
4	G	121	Total	O	0	0
			121	121		
4	H	134	Total	O	0	0
			134	134		

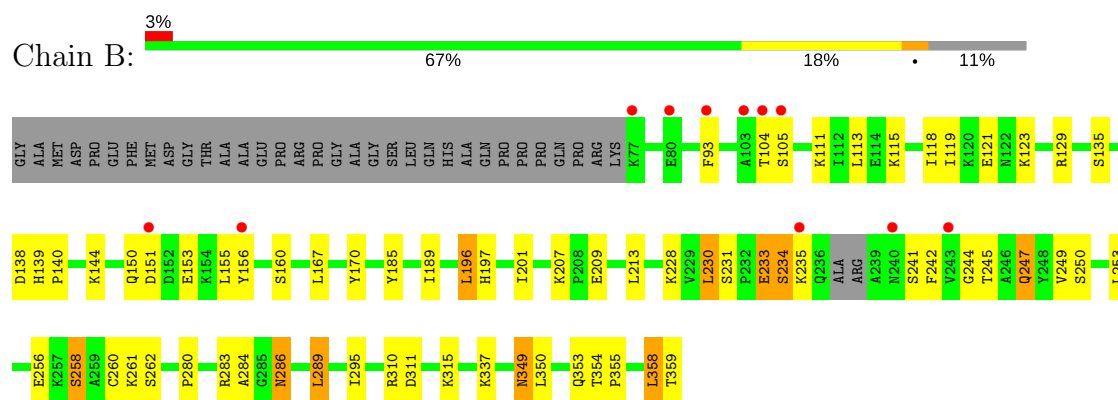
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

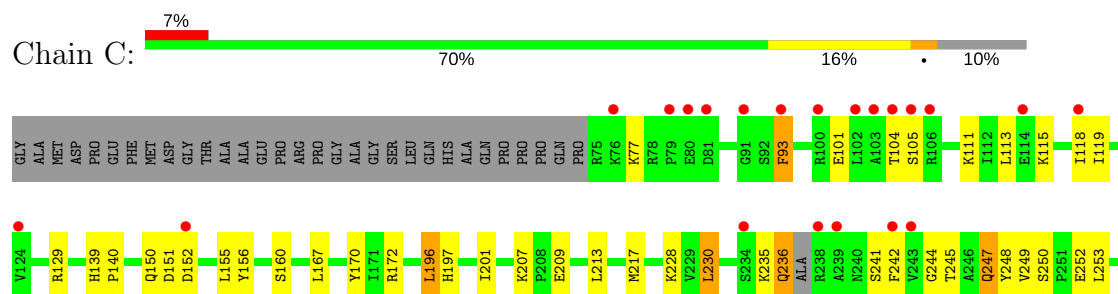
- Molecule 1: 3-phosphoinositide-dependent protein kinase 1

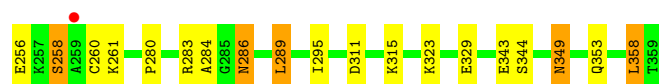


- Molecule 1: 3-phosphoinositide-dependent protein kinase 1

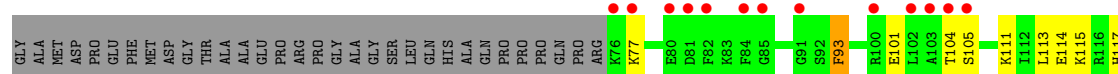


- Molecule 1: 3-phosphoinositide-dependent protein kinase 1

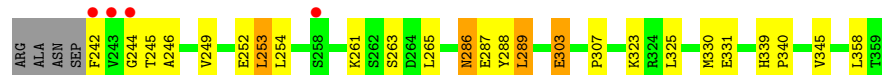
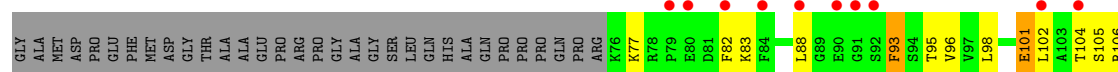




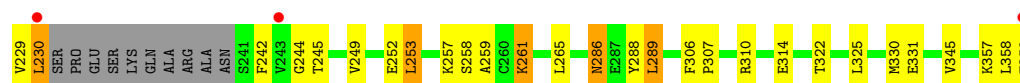
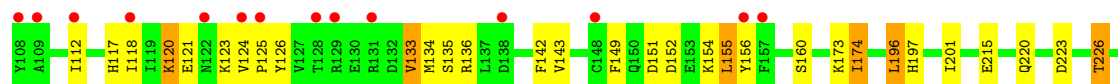
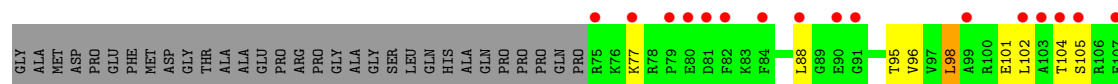
- Molecule 1: 3-phosphoinositide-dependent protein kinase 1



- Molecule 1: 3-phosphoinositide-dependent protein kinase 1

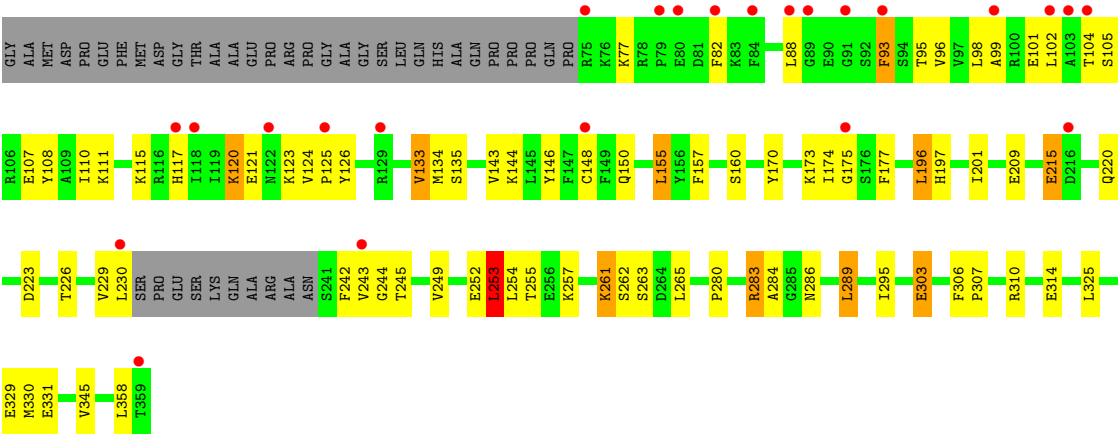


- Molecule 1: 3-phosphoinositide-dependent protein kinase 1

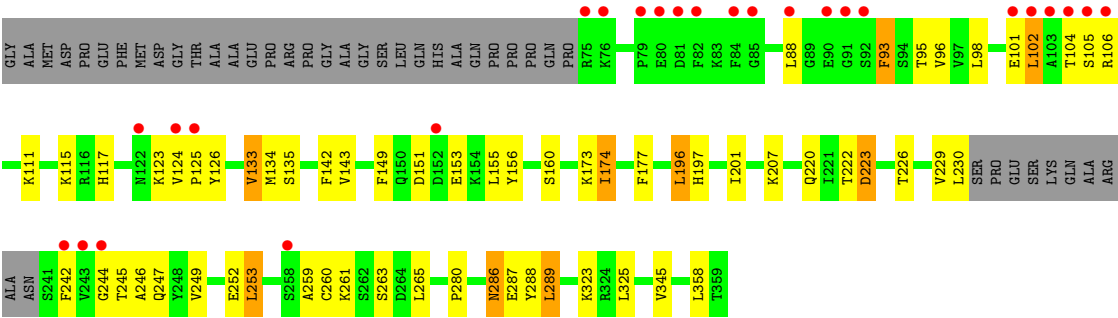


- Molecule 1: 3-phosphoinositide-dependent protein kinase 1





● Molecule 1: 3-phosphoinositide-dependent protein kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	40.29Å 115.87Å 145.72Å 91.76° 89.99° 95.41°	Depositor
Resolution (Å)	45.25 – 2.20 45.25 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (45.25-2.20) 96.1 (45.25-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 2010_01_09_2330)	Depositor
R, R_{free}	0.208 , 0.243 0.202 , 0.238	Depositor DCC
R_{free} test set	6438 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.073 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19043	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 1F8, SEP

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	0.61	0/2315	0.62	1/3125 (0.0%)
1	B	0.54	0/2306	0.62	0/3112
1	C	0.58	0/2308	0.61	0/3120
1	D	0.54	0/2300	0.61	2/3106 (0.1%)
1	E	0.75	0/2217	0.66	0/3003
1	F	0.69	0/2175	0.63	1/2950 (0.0%)
1	G	0.81	0/2199	0.66	2/2980 (0.1%)
1	H	0.70	0/2158	0.63	0/2932
All	All	0.66	0/17978	0.63	6/24328 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	136	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	D	136	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	G	253	LEU	CB-CG-CD2	-5.43	101.76	111.00
1	A	283	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	G	283	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	F	230	LEU	CA-CB-CG	-5.01	103.78	115.30

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	2271	0	2250	52	0
1	B	2262	0	2245	53	0
1	C	2264	0	2217	54	0
1	D	2256	0	2233	43	0
1	E	2163	0	2101	62	0
1	F	2132	0	2040	56	0
1	G	2155	0	2069	68	0
1	H	2114	0	1982	56	0
2	A	16	0	12	3	0
2	B	16	0	12	3	0
2	C	16	0	12	3	0
2	D	16	0	12	3	0
2	E	16	0	12	2	0
2	F	16	0	12	2	0
2	G	16	0	12	3	0
2	H	16	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	204	0	0	4	0
4	B	213	0	0	9	0
4	C	194	0	0	11	0
4	D	187	0	0	5	0
4	E	120	0	0	1	0
4	F	121	0	0	3	0
4	G	121	0	0	2	0
4	H	134	0	0	3	0
All	All	19043	0	17233	425	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 12.

All (425) 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:A:230:LEU:HD21	1:A:235:LYS:HA	1.28	1.12
1:A:323:LYS:NZ	1:G:310:ARG:HH21	1.47	1.10
1:F:253:LEU:HD23	1:F:253:LEU:N	1.69	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:LEU:HD23	1:E:253:LEU:N	1.74	1.01
1:G:253:LEU:HD23	1:G:253:LEU:N	1.72	0.99
1:B:253:LEU:HD23	1:B:258:SER:O	1.66	0.96
1:A:253:LEU:HD23	1:A:258:SER:O	1.67	0.95
1:B:310:ARG:HH21	1:E:323:LYS:HE2	1.31	0.95
1:C:253:LEU:HD23	1:C:258:SER:O	1.68	0.94
1:E:253:LEU:CD2	1:E:253:LEU:N	2.30	0.94
1:C:323:LYS:NZ	1:F:310:ARG:HH21	1.64	0.94
1:A:323:LYS:HZ1	1:G:310:ARG:NH2	1.65	0.94
1:D:253:LEU:HD23	1:D:258:SER:O	1.67	0.94
1:G:253:LEU:CD2	1:G:253:LEU:N	2.30	0.93
1:F:253:LEU:HD23	1:F:253:LEU:H	1.32	0.93
1:F:253:LEU:N	1:F:253:LEU:CD2	2.30	0.92
1:F:230:LEU:C	1:F:230:LEU:HD12	1.91	0.91
1:G:253:LEU:HD23	1:G:253:LEU:H	1.36	0.89
1:A:230:LEU:HD21	1:A:235:LYS:CA	2.03	0.87
1:C:323:LYS:HZ1	1:F:310:ARG:HH21	1.16	0.87
1:D:310:ARG:HH21	1:H:323:LYS:HE2	1.41	0.84
1:F:229:VAL:HG12	1:F:230:LEU:HG	1.59	0.83
1:G:252:GLU:HG2	1:G:253:LEU:HD23	1.61	0.82
1:A:323:LYS:HZ1	1:G:310:ARG:HH21	0.83	0.82
1:H:104:THR:CB	1:H:106:ARG:HD3	2.11	0.81
1:B:151:ASP:HB2	1:B:156:TYR:HE1	1.46	0.80
1:B:310:ARG:NH2	1:E:323:LYS:HE2	1.96	0.80
1:D:151:ASP:HB2	1:D:156:TYR:HE1	1.47	0.80
1:C:151:ASP:HB2	1:C:156:TYR:HE1	1.47	0.79
1:H:101:GLU:OE1	1:H:104:THR:CB	2.30	0.79
1:A:151:ASP:HB2	1:A:156:TYR:HE1	1.47	0.79
1:F:226:THR:HG23	4:F:895:HOH:O	1.82	0.79
1:C:236:GLN:HA	1:C:236:GLN:HE21	1.48	0.79
1:G:104:THR:O	1:G:105:SER:CB	2.31	0.78
1:E:253:LEU:HD23	1:E:253:LEU:H	1.48	0.78
1:H:174:ILE:HD11	1:H:177:PHE:CD1	2.19	0.78
1:B:155:LEU:HD22	2:B:1:1F8:H28	1.65	0.77
1:A:155:LEU:HD22	2:A:1:1F8:H28	1.67	0.76
1:E:101:GLU:HG2	1:E:104:THR:OG1	1.86	0.76
1:D:155:LEU:HD22	2:D:1:1F8:H28	1.67	0.76
1:C:155:LEU:HD22	2:C:1:1F8:H28	1.67	0.75
1:G:144:LYS:HD2	4:G:564:HOH:O	1.86	0.75
1:E:104:THR:O	1:E:105:SER:CB	2.31	0.74
1:F:136:ARG:HD3	4:F:1418:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:245:THR:O	1:G:249:VAL:HG23	1.87	0.73
1:H:245:THR:O	1:H:249:VAL:HG23	1.89	0.72
1:G:99:ALA:HB2	1:G:110:ILE:HG13	1.72	0.72
1:C:344:SER:HB3	1:G:307:PRO:HG2	1.71	0.72
1:A:323:LYS:NZ	1:G:310:ARG:NH2	2.29	0.71
1:C:155:LEU:HD22	2:C:1:1F8:C28	2.21	0.71
1:G:155:LEU:HD11	2:G:1:1F8:C28	2.20	0.71
1:E:252:GLU:HG2	1:E:253:LEU:HD23	1.72	0.71
1:A:155:LEU:HD22	2:A:1:1F8:C28	2.21	0.70
1:H:102:LEU:N	1:H:102:LEU:HD23	2.06	0.70
1:B:207:LYS:HE3	1:B:209:GLU:HG2	1.73	0.70
1:B:155:LEU:HD22	2:B:1:1F8:C28	2.21	0.70
1:D:93:PHE:HB2	4:D:1364:HOH:O	1.91	0.70
1:F:252:GLU:HB2	1:F:258:SER:HB3	1.74	0.70
1:D:207:LYS:HE3	1:D:209:GLU:HG2	1.74	0.69
1:C:349:ASN:ND2	1:C:353:GLN:HE21	1.91	0.69
1:D:286:ASN:ND2	1:D:289:LEU:H	1.91	0.69
1:D:155:LEU:HD22	2:D:1:1F8:C28	2.22	0.69
1:A:349:ASN:ND2	1:A:353:GLN:HE21	1.91	0.69
1:A:286:ASN:ND2	1:A:289:LEU:H	1.90	0.69
1:G:155:LEU:HD11	2:G:1:1F8:H28	1.75	0.69
1:E:155:LEU:HD11	2:E:1:1F8:H28	1.75	0.68
1:E:151:ASP:OD1	1:E:151:ASP:C	2.30	0.68
1:E:115:LYS:O	1:E:119:ILE:HG12	1.93	0.68
1:F:245:THR:O	1:F:249:VAL:HG23	1.94	0.68
1:C:311:ASP:OD2	1:C:315:LYS:HE2	1.93	0.68
1:F:197:HIS:HB3	1:F:261:LYS:HD2	1.74	0.68
1:G:229:VAL:HG12	1:G:230:LEU:N	2.09	0.67
1:G:174:ILE:HD11	1:G:177:PHE:CD1	2.30	0.67
1:H:151:ASP:OD1	1:H:153:GLU:HG2	1.94	0.67
1:A:249:VAL:HG13	1:A:253:LEU:HD12	1.75	0.67
1:C:283:ARG:HG2	4:C:1371:HOH:O	1.94	0.67
1:B:311:ASP:OD2	1:B:315:LYS:HE2	1.94	0.67
1:F:252:GLU:HG2	1:F:253:LEU:HD23	1.77	0.67
1:B:286:ASN:ND2	1:B:289:LEU:H	1.93	0.66
1:D:310:ARG:NH2	1:H:323:LYS:HE2	2.11	0.66
1:A:207:LYS:HE3	1:A:209:GLU:HG2	1.78	0.66
1:A:311:ASP:OD2	1:A:315:LYS:HE2	1.95	0.66
1:G:252:GLU:HG2	1:G:253:LEU:CD2	2.25	0.66
1:C:286:ASN:ND2	1:C:289:LEU:H	1.93	0.66
1:D:349:ASN:ND2	1:D:353:GLN:HE21	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:151:ASP:OD1	1:H:151:ASP:C	2.33	0.66
1:A:280:PRO:O	1:A:283:ARG:HD3	1.96	0.65
1:B:349:ASN:ND2	1:B:353:GLN:HE21	1.94	0.65
1:D:311:ASP:OD2	1:D:315:LYS:HE2	1.96	0.65
1:C:230:LEU:HD21	1:C:235:LYS:HA	1.79	0.65
1:D:245:THR:O	1:D:249:VAL:HG23	1.95	0.65
1:C:249:VAL:HG13	1:C:253:LEU:HD12	1.77	0.65
1:C:286:ASN:C	1:C:286:ASN:HD22	2.00	0.65
1:F:229:VAL:HG12	1:F:230:LEU:N	2.11	0.65
1:G:280:PRO:O	1:G:283:ARG:NH1	2.30	0.65
1:C:245:THR:O	1:C:249:VAL:HG23	1.96	0.65
1:G:170:TYR:O	1:G:174:ILE:HG12	1.97	0.65
1:F:151:ASP:C	1:F:151:ASP:OD1	2.33	0.64
1:C:207:LYS:HE3	1:C:209:GLU:HG2	1.80	0.64
1:C:196:LEU:HD22	1:C:201:ILE:HB	1.79	0.64
1:C:323:LYS:NZ	1:F:310:ARG:NH2	2.43	0.64
1:G:124:VAL:N	1:G:125:PRO:HD2	2.13	0.64
1:E:229:VAL:HG12	1:E:230:LEU:N	2.12	0.64
1:A:196:LEU:HD22	1:A:201:ILE:HB	1.79	0.64
1:D:249:VAL:HG13	1:D:253:LEU:HD12	1.78	0.64
1:H:96:VAL:CG2	1:H:111:LYS:HD2	2.28	0.63
1:H:253:LEU:N	1:H:253:LEU:HD23	2.12	0.63
1:E:104:THR:CB	1:E:106:ARG:HD2	2.29	0.63
1:G:196:LEU:HD22	1:G:201:ILE:HB	1.81	0.63
1:G:197:HIS:HB3	1:G:261:LYS:HD2	1.79	0.63
1:H:229:VAL:HG12	1:H:230:LEU:N	2.12	0.63
1:H:253:LEU:CD2	1:H:253:LEU:N	2.61	0.63
1:H:196:LEU:HD22	1:H:201:ILE:HB	1.81	0.63
1:B:196:LEU:HD22	1:B:201:ILE:HB	1.80	0.63
1:G:229:VAL:HG12	1:G:230:LEU:H	1.63	0.63
1:B:115:LYS:O	1:B:119:ILE:HG12	1.99	0.62
1:E:96:VAL:CG2	1:E:111:LYS:HD2	2.29	0.62
1:G:96:VAL:CG2	1:G:111:LYS:HD2	2.29	0.62
1:D:196:LEU:HD22	1:D:201:ILE:HB	1.81	0.62
1:F:124:VAL:N	1:F:125:PRO:HD2	2.14	0.62
1:A:115:LYS:O	1:A:119:ILE:HG12	1.99	0.62
1:A:245:THR:O	1:A:249:VAL:HG23	1.99	0.62
1:A:351:HIS:HB2	4:A:1005:HOH:O	1.99	0.62
1:A:350:LEU:HD22	4:A:651:HOH:O	2.00	0.61
1:A:286:ASN:HD22	1:A:286:ASN:C	2.04	0.61
1:C:323:LYS:HZ1	1:F:310:ARG:NH2	1.94	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:VAL:HG12	1:E:230:LEU:H	1.65	0.61
1:E:124:VAL:N	1:E:125:PRO:HD2	2.14	0.61
1:E:174:ILE:HD11	1:E:177:PHE:CD1	2.35	0.61
1:E:196:LEU:HD22	1:E:201:ILE:HB	1.83	0.61
1:B:249:VAL:HG13	1:B:253:LEU:HD12	1.81	0.61
1:E:151:ASP:OD1	1:E:153:GLU:HG2	2.00	0.61
1:F:196:LEU:HD22	1:F:201:ILE:HB	1.83	0.60
1:D:115:LYS:O	1:D:119:ILE:HG12	2.01	0.60
1:H:124:VAL:N	1:H:125:PRO:HD2	2.15	0.60
1:C:115:LYS:O	1:C:119:ILE:HG12	2.00	0.60
1:G:99:ALA:CB	1:G:110:ILE:HG13	2.31	0.60
1:B:245:THR:O	1:B:249:VAL:HG23	2.00	0.60
1:B:286:ASN:HD22	1:B:286:ASN:C	2.05	0.60
1:G:93:PHE:N	1:G:93:PHE:CD1	2.62	0.60
1:C:252:GLU:HG3	4:C:683:HOH:O	2.01	0.60
1:F:120:LYS:HG3	1:F:121:GLU:N	2.16	0.60
1:H:229:VAL:HG12	1:H:230:LEU:H	1.66	0.60
1:E:246:ALA:HB3	1:E:287:GLU:OE1	2.03	0.59
1:E:245:THR:O	1:E:249:VAL:HG23	2.02	0.59
1:B:242:PHE:CZ	1:B:244:GLY:HA2	2.38	0.59
1:D:242:PHE:CZ	1:D:244:GLY:HA2	2.38	0.59
1:E:93:PHE:CD1	1:E:93:PHE:N	2.63	0.59
1:C:242:PHE:CZ	1:C:244:GLY:HA2	2.37	0.58
1:F:229:VAL:HG12	1:F:230:LEU:H	1.68	0.58
1:H:93:PHE:CD1	1:H:93:PHE:N	2.64	0.58
1:E:155:LEU:HD11	2:E:1:1F8:C28	2.34	0.58
1:D:104:THR:O	1:D:105:SER:HB2	2.04	0.57
1:D:280:PRO:HB2	4:D:39:HOH:O	2.04	0.57
1:E:118:ILE:HG22	1:E:124:VAL:HG23	1.86	0.57
1:B:138:ASP:HB3	4:B:1402:HOH:O	2.05	0.57
1:A:242:PHE:CZ	1:A:244:GLY:HA2	2.39	0.57
1:C:170:TYR:CE2	1:C:213:LEU:HD12	2.39	0.57
1:B:280:PRO:HB2	4:B:11:HOH:O	2.05	0.57
1:H:246:ALA:HB3	1:H:287:GLU:OE1	2.05	0.57
1:E:245:THR:HG22	4:E:1094:HOH:O	2.04	0.57
1:A:323:LYS:NZ	1:G:314:GLU:OE2	2.38	0.57
1:D:286:ASN:HD22	1:D:286:ASN:C	2.09	0.56
1:F:230:LEU:CD1	1:F:230:LEU:C	2.60	0.56
1:H:155:LEU:HD11	2:H:1:1F8:H28	1.86	0.56
1:D:231:SER:H	1:D:234:SER:HB2	1.70	0.56
1:F:118:ILE:HG22	1:F:124:VAL:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:259:ALA:O	1:H:260:CYS:HB3	2.05	0.56
1:H:93:PHE:HD1	1:H:93:PHE:H	1.53	0.56
1:H:102:LEU:H	1:H:102:LEU:CD2	2.18	0.56
1:E:104:THR:HB	1:E:106:ARG:HD2	1.88	0.56
1:B:104:THR:O	1:B:105:SER:HB2	2.06	0.56
1:A:104:THR:O	1:A:105:SER:HB2	2.06	0.55
1:G:242:PHE:CZ	1:G:244:GLY:HA2	2.41	0.55
1:D:337:LYS:HE2	4:D:1315:HOH:O	2.06	0.55
1:D:344:SER:HB3	1:E:307:PRO:HG2	1.87	0.55
1:B:337:LYS:HE2	4:B:1323:HOH:O	2.07	0.55
1:F:286:ASN:ND2	1:F:289:LEU:H	2.05	0.55
1:E:104:THR:OG1	1:E:106:ARG:HD2	2.06	0.55
1:C:280:PRO:HB2	4:C:23:HOH:O	2.06	0.55
1:F:104:THR:O	1:F:105:SER:CB	2.55	0.55
1:D:113:LEU:HB3	1:D:118:ILE:HD11	1.90	0.54
1:B:121:GLU:HB2	1:B:123:LYS:HE2	1.88	0.54
1:G:148:CYS:SG	1:G:157:PHE:CE1	3.00	0.54
1:H:286:ASN:HD22	1:H:288:TYR:H	1.53	0.54
1:C:344:SER:HB3	1:G:307:PRO:CG	2.37	0.54
1:H:252:GLU:HG2	1:H:253:LEU:HD23	1.90	0.54
1:B:230:LEU:HD21	1:B:235:LYS:HA	1.89	0.54
1:H:286:ASN:HD22	1:H:288:TYR:N	2.06	0.54
1:F:98:LEU:HG	1:F:98:LEU:O	2.07	0.54
1:B:113:LEU:HB3	1:B:118:ILE:HD11	1.91	0.53
1:B:350:LEU:HD22	4:B:979:HOH:O	2.08	0.53
1:D:170:TYR:CE2	1:D:213:LEU:HD12	2.43	0.53
1:D:350:LEU:HD22	4:D:553:HOH:O	2.08	0.53
1:E:286:ASN:ND2	1:E:289:LEU:H	2.06	0.53
1:A:113:LEU:HB3	1:A:118:ILE:HD11	1.91	0.53
1:B:155:LEU:CD2	2:B:1:1F8:H28	2.36	0.53
1:C:104:THR:O	1:C:105:SER:HB2	2.07	0.53
1:C:155:LEU:CD2	2:C:1:1F8:H28	2.35	0.53
1:A:349:ASN:HD21	1:A:353:GLN:HE21	1.56	0.53
1:C:113:LEU:HB3	1:C:118:ILE:HD11	1.91	0.53
1:G:243:VAL:O	1:G:243:VAL:HG12	2.08	0.53
1:A:155:LEU:CD2	2:A:1:1F8:H28	2.36	0.53
1:B:260:CYS:HB3	4:B:874:HOH:O	2.08	0.53
1:D:230:LEU:HD21	1:D:235:LYS:HA	1.91	0.52
1:E:101:GLU:CG	1:E:104:THR:OG1	2.57	0.52
1:H:88:LEU:HD12	1:H:96:VAL:HG12	1.89	0.52
1:C:93:PHE:HB2	4:C:1210:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:GLU:OE2	1:D:117:HIS:HB2	2.08	0.52
1:H:247:GLN:NE2	4:H:387:HOH:O	2.42	0.52
1:H:286:ASN:ND2	1:H:289:LEU:H	2.07	0.52
1:C:349:ASN:HD21	1:C:353:GLN:HE21	1.57	0.52
1:F:265:LEU:HD13	1:F:325:LEU:O	2.10	0.52
1:G:120:LYS:CG	1:G:121:GLU:N	2.73	0.52
1:A:75:ARG:HG2	1:A:76:LYS:N	2.25	0.52
1:F:88:LEU:HD12	1:F:96:VAL:HG12	1.90	0.52
1:G:120:LYS:HG3	1:G:121:GLU:N	2.23	0.52
1:A:170:TYR:CE2	1:A:213:LEU:HD12	2.44	0.51
1:D:155:LEU:CD2	2:D:1:1F8:H28	2.38	0.51
1:B:170:TYR:CE2	1:B:213:LEU:HD12	2.45	0.51
1:E:88:LEU:HD12	1:E:96:VAL:HG12	1.90	0.51
1:H:102:LEU:H	1:H:102:LEU:HD23	1.71	0.51
1:H:123:LYS:O	1:H:126:TYR:HB3	2.10	0.51
1:C:172:ARG:HD2	4:C:813:HOH:O	2.11	0.51
1:F:123:LYS:O	1:F:126:TYR:HB3	2.11	0.51
1:C:230:LEU:HD21	1:C:235:LYS:CA	2.41	0.51
1:C:242:PHE:CE1	1:C:244:GLY:HA2	2.46	0.50
1:G:88:LEU:HD12	1:G:96:VAL:HG12	1.91	0.50
1:B:242:PHE:CE1	1:B:244:GLY:HA2	2.46	0.50
1:H:174:ILE:HD11	1:H:177:PHE:CE1	2.47	0.50
1:F:252:GLU:HG2	1:F:253:LEU:CD2	2.41	0.50
1:D:111:LYS:HE2	1:D:113:LEU:HD21	1.93	0.50
1:D:230:LEU:HD23	1:D:234:SER:HB3	1.93	0.50
1:G:99:ALA:CB	1:G:110:ILE:CG1	2.90	0.50
1:A:250:SER:OG	1:A:253:LEU:HG	2.12	0.49
1:D:242:PHE:CE1	1:D:244:GLY:HA2	2.47	0.49
1:C:129:ARG:NH2	1:C:241:SEP:O3P	2.45	0.49
1:G:93:PHE:HD1	1:G:93:PHE:N	2.09	0.49
1:A:234:SER:O	1:A:235:LYS:C	2.49	0.49
1:E:123:LYS:O	1:E:126:TYR:HB3	2.12	0.49
1:G:123:LYS:O	1:G:126:TYR:HB3	2.13	0.49
1:C:217:MET:HG3	4:C:597:HOH:O	2.12	0.49
1:C:260:CYS:SG	4:C:683:HOH:O	2.60	0.49
1:E:101:GLU:CG	1:E:101:GLU:O	2.60	0.49
1:H:155:LEU:HD11	2:H:1:1F8:C28	2.42	0.49
1:B:359:THR:HG22	4:B:473:HOH:O	2.11	0.49
1:C:250:SER:OG	1:C:253:LEU:HG	2.13	0.49
1:B:250:SER:OG	1:B:253:LEU:HG	2.13	0.49
1:A:242:PHE:CE1	1:A:244:GLY:HA2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:GLU:O	1:D:114:GLU:HG3	2.10	0.49
1:D:286:ASN:HD22	1:D:289:LEU:H	1.60	0.49
1:G:209:GLU:HG3	4:G:833:HOH:O	2.12	0.49
1:C:329:GLU:HA	4:C:1200:HOH:O	2.14	0.48
1:H:115:LYS:NZ	1:H:151:ASP:O	2.42	0.48
1:E:286:ASN:HD22	1:E:288:TYR:N	2.11	0.48
1:B:111:LYS:HE2	1:B:113:LEU:HD21	1.95	0.48
1:G:115:LYS:NZ	1:G:150:GLN:OE1	2.32	0.48
1:G:229:VAL:CG1	1:G:230:LEU:N	2.77	0.48
1:E:77:LYS:HD3	1:E:82:PHE:CZ	2.49	0.48
1:G:93:PHE:HD1	1:G:93:PHE:H	1.50	0.48
1:A:111:LYS:HE2	1:A:113:LEU:HD21	1.95	0.48
1:H:222:THR:OG1	1:H:223:ASP:N	2.45	0.48
1:C:111:LYS:HE2	1:C:113:LEU:HD21	1.96	0.47
1:B:129:ARG:HD2	4:B:1239:HOH:O	2.15	0.47
1:G:174:ILE:HG13	1:G:175:GLY:N	2.28	0.47
1:A:129:ARG:NH2	1:A:241:SEP:O3P	2.44	0.47
1:B:197:HIS:CG	1:B:261:LYS:HG2	2.49	0.47
1:E:93:PHE:HD1	1:E:93:PHE:N	2.10	0.47
1:G:108:TYR:HE1	1:G:146:TYR:CD2	2.32	0.47
1:E:197:HIS:HB3	1:E:261:LYS:HD2	1.96	0.47
1:H:104:THR:O	1:H:105:SER:CB	2.63	0.47
1:D:250:SER:OG	1:D:253:LEU:HG	2.15	0.47
1:F:286:ASN:HD22	1:F:288:TYR:N	2.13	0.47
1:B:129:ARG:NH2	1:B:241:SEP:O3P	2.45	0.47
1:B:233:GLU:HA	1:B:233:GLU:OE2	2.14	0.47
1:B:286:ASN:HD22	1:B:289:LEU:H	1.62	0.47
1:E:303:GLU:HG3	1:E:303:GLU:H	1.45	0.46
1:G:77:LYS:HD3	1:G:82:PHE:CZ	2.50	0.46
1:B:247:GLN:HE21	1:B:280:PRO:HG2	1.80	0.46
1:B:310:ARG:HE	1:E:323:LYS:HE3	1.80	0.46
1:E:265:LEU:HD13	1:E:325:LEU:O	2.16	0.46
1:H:93:PHE:HD1	1:H:93:PHE:N	2.11	0.46
1:B:144:LYS:HD3	4:B:634:HOH:O	2.15	0.46
1:E:174:ILE:HD11	1:E:177:PHE:CE1	2.50	0.46
1:G:155:LEU:CD1	2:G:1:1F8:C28	2.92	0.46
1:H:88:LEU:HD12	1:H:96:VAL:CG1	2.45	0.46
1:H:242:PHE:CZ	1:H:244:GLY:HA2	2.51	0.46
1:F:229:VAL:CG1	1:F:230:LEU:N	2.79	0.46
1:B:207:LYS:HE3	1:B:209:GLU:CG	2.45	0.46
1:E:330:MET:C	1:E:331:GLU:HG2	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:265:LEU:HD13	1:H:325:LEU:O	2.16	0.46
1:B:260:CYS:SG	1:B:262:SER:HB3	2.56	0.46
1:F:88:LEU:HD12	1:F:96:VAL:CG1	2.46	0.46
1:E:93:PHE:H	1:E:93:PHE:HD1	1.52	0.46
1:F:306:PHE:HA	1:F:307:PRO:HD3	1.85	0.46
1:E:286:ASN:C	1:E:286:ASN:HD22	2.20	0.45
1:F:174:ILE:HB	1:F:359:THR:OXT	2.16	0.45
1:C:284:ALA:HB1	1:C:289:LEU:HB3	1.98	0.45
1:G:253:LEU:HD22	1:G:253:LEU:N	2.21	0.45
1:G:284:ALA:HB1	1:G:289:LEU:HB3	1.98	0.45
1:F:155:LEU:HD11	2:F:1:1F8:H28	1.98	0.45
1:G:197:HIS:CB	1:G:261:LYS:HD2	2.46	0.45
1:G:330:MET:C	1:G:331:GLU:HG2	2.37	0.45
1:D:129:ARG:NH2	1:D:241:SEP:O3P	2.47	0.45
1:E:83:LYS:HB2	1:E:102:LEU:HD21	1.97	0.45
1:E:108:TYR:HE1	1:E:146:TYR:CD2	2.35	0.45
1:E:214:ASN:OD1	1:E:214:ASN:C	2.55	0.45
1:B:135:SER:HA	4:B:1348:HOH:O	2.15	0.45
1:C:323:LYS:NZ	1:F:314:GLU:OE2	2.50	0.45
1:F:149:PHE:CE1	1:F:156:TYR:CD1	3.04	0.45
1:A:231:SER:OG	1:A:234:SER:HB2	2.17	0.45
1:E:88:LEU:HD12	1:E:96:VAL:CG1	2.46	0.45
1:F:242:PHE:CZ	1:F:244:GLY:HA2	2.52	0.45
1:F:286:ASN:HD22	1:F:286:ASN:C	2.20	0.45
1:G:229:VAL:CG1	1:G:230:LEU:H	2.29	0.45
1:A:230:LEU:HD23	1:A:231:SER:N	2.32	0.45
1:H:143:VAL:HG23	1:H:220:GLN:HG2	1.99	0.45
1:E:286:ASN:HD22	1:E:288:TYR:H	1.64	0.45
1:A:323:LYS:CE	1:G:310:ARG:NH2	2.79	0.44
1:B:349:ASN:HD21	1:B:353:GLN:HE21	1.61	0.44
1:H:207:LYS:NZ	4:H:945:HOH:O	2.51	0.44
1:D:197:HIS:CG	1:D:261:LYS:HG2	2.52	0.44
1:A:197:HIS:CG	1:A:261:LYS:HG2	2.52	0.44
1:F:112:ILE:HA	1:F:155:LEU:O	2.17	0.44
1:A:280:PRO:HB2	4:A:369:HOH:O	2.16	0.44
1:E:196:LEU:HD23	1:E:196:LEU:HA	1.85	0.44
1:F:120:LYS:CG	1:F:121:GLU:N	2.81	0.44
1:G:102:LEU:HD23	1:G:102:LEU:HA	1.48	0.44
1:G:88:LEU:HD12	1:G:96:VAL:CG1	2.47	0.44
1:F:102:LEU:N	1:F:102:LEU:HD23	2.33	0.44
1:G:253:LEU:HD22	1:G:253:LEU:HA	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:LEU:CD2	1:B:258:SER:O	2.52	0.44
1:E:124:VAL:N	1:E:125:PRO:CD	2.81	0.44
1:E:253:LEU:HD22	1:E:253:LEU:HA	1.43	0.43
1:H:196:LEU:HA	1:H:196:LEU:HD23	1.86	0.43
1:H:229:VAL:CG1	1:H:230:LEU:N	2.80	0.43
1:A:249:VAL:CG1	1:A:253:LEU:HD12	2.48	0.43
1:D:217:MET:HG3	4:D:521:HOH:O	2.18	0.43
1:H:142:PHE:CZ	1:H:196:LEU:HG	2.53	0.43
1:E:252:GLU:HG2	1:E:253:LEU:CD2	2.44	0.43
1:G:124:VAL:N	1:G:125:PRO:CD	2.80	0.43
1:H:96:VAL:HG22	1:H:111:LYS:HD2	2.01	0.43
1:A:139:HIS:CG	1:A:140:PRO:HD2	2.54	0.43
1:C:197:HIS:CG	1:C:261:LYS:HG2	2.53	0.43
1:G:252:GLU:OE1	1:G:263:SER:HB3	2.18	0.43
1:A:247:GLN:HE21	1:A:280:PRO:HG2	1.84	0.43
1:E:222:THR:OG1	1:E:223:ASP:N	2.52	0.43
1:H:197:HIS:CG	1:H:261:LYS:HD2	2.54	0.43
1:F:258:SER:OG	1:F:259:ALA:N	2.51	0.43
1:G:196:LEU:HD23	1:G:196:LEU:HA	1.88	0.43
1:H:149:PHE:CE1	1:H:156:TYR:CG	3.07	0.43
1:H:88:LEU:HD21	1:H:98:LEU:HB2	2.00	0.43
1:D:253:LEU:CD2	1:D:258:SER:O	2.55	0.43
1:F:143:VAL:HG23	1:F:220:GLN:HG2	2.00	0.43
1:G:306:PHE:HA	1:G:307:PRO:HD3	1.86	0.43
1:H:124:VAL:N	1:H:125:PRO:CD	2.82	0.43
1:D:139:HIS:CG	1:D:140:PRO:HD2	2.54	0.42
1:G:265:LEU:HD13	1:G:325:LEU:O	2.19	0.42
1:H:253:LEU:HA	1:H:253:LEU:HD22	1.59	0.42
1:C:139:HIS:CG	1:C:140:PRO:HD2	2.54	0.42
1:D:260:CYS:SG	1:D:262:SER:HB3	2.60	0.42
1:A:139:HIS:ND1	1:A:140:PRO:HD2	2.34	0.42
1:G:303:GLU:H	1:G:303:GLU:HG3	1.43	0.42
1:F:142:PHE:CZ	1:F:196:LEU:HG	2.54	0.42
1:G:101:GLU:HG2	1:G:104:THR:H	1.83	0.42
1:G:143:VAL:HG22	1:G:220:GLN:HE21	1.84	0.42
1:H:197:HIS:HB3	1:H:261:LYS:HD2	2.01	0.42
1:B:231:SER:H	1:B:234:SER:HB2	1.85	0.42
1:C:77:LYS:HE3	1:C:101:GLU:OE2	2.20	0.42
1:C:236:GLN:CA	1:C:236:GLN:HE21	2.17	0.42
1:H:259:ALA:O	1:H:260:CYS:CB	2.62	0.42
1:H:286:ASN:C	1:H:286:ASN:HD22	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:TYR:O	1:A:189:ILE:HG13	2.19	0.42
1:B:280:PRO:O	1:B:283:ARG:HD3	2.19	0.42
1:C:248:TYR:HB2	4:C:759:HOH:O	2.20	0.42
1:C:249:VAL:CG1	1:C:253:LEU:HD12	2.49	0.42
1:C:284:ALA:CB	1:C:289:LEU:HB3	2.50	0.42
1:C:358:LEU:HD12	1:C:358:LEU:HA	1.87	0.42
1:F:253:LEU:HD22	1:F:253:LEU:HA	1.62	0.42
1:A:253:LEU:CD2	1:A:258:SER:O	2.55	0.42
1:C:172:ARG:HD2	4:C:400:HOH:O	2.20	0.42
1:E:142:PHE:CZ	1:E:196:LEU:HG	2.55	0.42
1:H:133:VAL:CG1	1:H:134:MET:N	2.83	0.42
1:E:88:LEU:HD21	1:E:98:LEU:HB2	2.02	0.42
1:F:124:VAL:N	1:F:125:PRO:CD	2.81	0.42
1:A:207:LYS:HE3	1:A:209:GLU:CG	2.48	0.41
1:A:230:LEU:HD23	1:A:231:SER:H	1.85	0.41
1:E:96:VAL:HG22	1:E:111:LYS:HD2	2.02	0.41
1:G:255:THR:C	1:G:257:LYS:H	2.21	0.41
1:B:115:LYS:NZ	1:B:150:GLN:HG2	2.34	0.41
1:B:284:ALA:HB1	1:B:289:LEU:HB3	2.02	0.41
1:D:349:ASN:HD21	1:D:353:GLN:HE21	1.64	0.41
1:G:98:LEU:HD11	1:G:107:GLU:HB3	2.02	0.41
1:G:215:GLU:HG3	1:G:215:GLU:H	1.51	0.41
1:G:254:LEU:HD12	1:G:295:ILE:CD1	2.50	0.41
1:B:139:HIS:CG	1:B:140:PRO:HD2	2.56	0.41
1:E:229:VAL:CG1	1:E:230:LEU:N	2.79	0.41
1:F:155:LEU:HD11	2:F:1:1F8:C28	2.51	0.41
1:D:77:LYS:HE3	1:D:101:GLU:OE2	2.20	0.41
1:C:343:GLU:HG3	4:C:963:HOH:O	2.20	0.41
1:E:339:HIS:CG	1:E:340:PRO:HD2	2.55	0.41
1:F:322:THR:HA	4:F:601:HOH:O	2.20	0.41
1:F:288:TYR:HD2	1:F:289:LEU:HD13	1.86	0.41
1:F:330:MET:C	1:F:331:GLU:HG2	2.41	0.41
1:A:115:LYS:NZ	1:A:150:GLN:HG2	2.35	0.41
1:A:77:LYS:HE3	1:A:101:GLU:OE2	2.21	0.41
1:C:115:LYS:NZ	1:C:150:GLN:HG2	2.35	0.41
1:E:254:LEU:HA	1:E:254:LEU:HD23	1.77	0.41
1:C:247:GLN:HE21	1:C:280:PRO:HG2	1.86	0.41
1:B:358:LEU:HD12	1:B:358:LEU:HA	1.94	0.41
1:F:126:TYR:C	1:F:126:TYR:CD2	2.94	0.40
1:F:229:VAL:CG1	1:F:230:LEU:H	2.32	0.40
1:B:185:TYR:O	1:B:189:ILE:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:LYS:HE3	1:D:209:GLU:CG	2.46	0.40
1:E:77:LYS:HD3	1:E:82:PHE:HZ	1.86	0.40
1:F:253:LEU:HD22	1:F:253:LEU:N	2.25	0.40
1:G:133:VAL:HG12	1:G:134:MET:N	2.36	0.40
1:B:354:THR:HA	1:B:355:PRO:HD3	1.89	0.40
1:F:133:VAL:HG12	1:F:134:MET:N	2.37	0.40
1:H:280:PRO:HB2	4:H:13:HOH:O	2.21	0.40
1:A:233:GLU:OE2	4:A:424:HOH:O	2.22	0.40
1:A:286:ASN:HD22	1:A:289:LEU:H	1.63	0.40
1:B:349:ASN:H	1:B:349:ASN:HD22	1.69	0.40
1:E:242:PHE:CZ	1:E:244:GLY:HA2	2.57	0.40
1:H:133:VAL:HG12	1:H:134:MET:N	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	279/316 (88%)	274 (98%)	5 (2%)	0	100	100
1	B	276/316 (87%)	271 (98%)	5 (2%)	0	100	100
1	C	279/316 (88%)	273 (98%)	6 (2%)	0	100	100
1	D	278/316 (88%)	272 (98%)	5 (2%)	1 (0%)	38	41
1	E	270/316 (85%)	260 (96%)	10 (4%)	0	100	100
1	F	271/316 (86%)	260 (96%)	11 (4%)	0	100	100
1	G	271/316 (86%)	261 (96%)	10 (4%)	0	100	100
1	H	271/316 (86%)	261 (96%)	10 (4%)	0	100	100
All	All	2195/2528 (87%)	2132 (97%)	62 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	244	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	239/273 (88%)	219 (92%)	20 (8%)	13	12
1	B	241/273 (88%)	224 (93%)	17 (7%)	17	18
1	C	238/273 (87%)	222 (93%)	16 (7%)	19	21
1	D	237/273 (87%)	221 (93%)	16 (7%)	18	20
1	E	220/273 (81%)	200 (91%)	20 (9%)	11	11
1	F	211/273 (77%)	185 (88%)	26 (12%)	5	4
1	G	215/273 (79%)	193 (90%)	22 (10%)	8	8
1	H	205/273 (75%)	187 (91%)	18 (9%)	12	11
All	All	1806/2184 (83%)	1651 (91%)	155 (9%)	12	12

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ARG
1	A	93	PHE
1	A	116	ARG
1	A	152	ASP
1	A	153	GLU
1	A	160	SER
1	A	167	LEU
1	A	196	LEU
1	A	206	LEU
1	A	228	LYS
1	A	230	LEU
1	A	234	SER
1	A	247	GLN
1	A	256	GLU
1	A	258	SER

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Mol	Chain	Res	Type
1	A	286	ASN
1	A	289	LEU
1	A	295	ILE
1	A	349	ASN
1	A	358	LEU
1	B	93	PHE
1	B	153	GLU
1	B	160	SER
1	B	167	LEU
1	B	196	LEU
1	B	228	LYS
1	B	230	LEU
1	B	233	GLU
1	B	234	SER
1	B	247	GLN
1	B	256	GLU
1	B	258	SER
1	B	286	ASN
1	B	289	LEU
1	B	295	ILE
1	B	349	ASN
1	B	358	LEU
1	C	93	PHE
1	C	152	ASP
1	C	160	SER
1	C	167	LEU
1	C	196	LEU
1	C	228	LYS
1	C	230	LEU
1	C	236	GLN
1	C	247	GLN
1	C	256	GLU
1	C	258	SER
1	C	286	ASN
1	C	289	LEU
1	C	295	ILE
1	C	349	ASN
1	C	358	LEU
1	D	93	PHE
1	D	160	SER
1	D	167	LEU
1	D	172	ARG

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Mol	Chain	Res	Type
1	D	196	LEU
1	D	228	LYS
1	D	230	LEU
1	D	234	SER
1	D	247	GLN
1	D	256	GLU
1	D	258	SER
1	D	286	ASN
1	D	289	LEU
1	D	295	ILE
1	D	349	ASN
1	D	358	LEU
1	E	93	PHE
1	E	95	THR
1	E	101	GLU
1	E	117	HIS
1	E	133	VAL
1	E	135	SER
1	E	155	LEU
1	E	160	SER
1	E	172	ARG
1	E	173	LYS
1	E	196	LEU
1	E	223	ASP
1	E	226	THR
1	E	253	LEU
1	E	263	SER
1	E	286	ASN
1	E	289	LEU
1	E	303	GLU
1	E	345	VAL
1	E	358	LEU
1	F	77	LYS
1	F	95	THR
1	F	98	LEU
1	F	101	GLU
1	F	117	HIS
1	F	120	LYS
1	F	133	VAL
1	F	135	SER
1	F	152	ASP
1	F	154	LYS

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Mol	Chain	Res	Type
1	F	155	LEU
1	F	160	SER
1	F	173	LYS
1	F	174	ILE
1	F	196	LEU
1	F	215	GLU
1	F	223	ASP
1	F	226	THR
1	F	253	LEU
1	F	257	LYS
1	F	261	LYS
1	F	286	ASN
1	F	289	LEU
1	F	345	VAL
1	F	357	LYS
1	F	358	LEU
1	G	93	PHE
1	G	95	THR
1	G	117	HIS
1	G	120	LYS
1	G	133	VAL
1	G	135	SER
1	G	155	LEU
1	G	160	SER
1	G	173	LYS
1	G	196	LEU
1	G	215	GLU
1	G	223	ASP
1	G	226	THR
1	G	253	LEU
1	G	261	LYS
1	G	262	SER
1	G	286	ASN
1	G	289	LEU
1	G	303	GLU
1	G	329	GLU
1	G	345	VAL
1	G	358	LEU
1	H	93	PHE
1	H	95	THR
1	H	102	LEU
1	H	117	HIS

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Mol	Chain	Res	Type
1	H	133	VAL
1	H	135	SER
1	H	160	SER
1	H	173	LYS
1	H	174	ILE
1	H	196	LEU
1	H	223	ASP
1	H	226	THR
1	H	253	LEU
1	H	263	SER
1	H	286	ASN
1	H	289	LEU
1	H	345	VAL
1	H	358	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	247	GLN
1	A	286	ASN
1	A	292	GLN
1	A	349	ASN
1	B	150	GLN
1	B	286	ASN
1	B	349	ASN
1	C	150	GLN
1	C	236	GLN
1	C	247	GLN
1	C	286	ASN
1	C	349	ASN
1	D	150	GLN
1	D	247	GLN
1	D	286	ASN
1	D	292	GLN
1	D	349	ASN
1	E	220	GLN
1	E	286	ASN
1	F	286	ASN
1	G	220	GLN
1	G	286	ASN
1	H	247	GLN

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Mol	Chain	Res	Type
1	H	286	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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	SEP	A	241	1	9,9,10	1.54	1 (11%)	9,12,14	1.47	2 (22%)
1	SEP	B	241	1	9,9,10	1.49	1 (11%)	9,12,14	1.40	1 (11%)
1	SEP	C	241	1	9,9,10	1.19	1 (11%)	9,12,14	1.88	3 (33%)
1	SEP	D	241	1	9,9,10	1.53	1 (11%)	9,12,14	1.45	2 (22%)
1	SEP	F	241	1	9,9,10	1.63	2 (22%)	9,12,14	1.39	2 (22%)
1	SEP	G	241	1	9,9,10	1.65	2 (22%)	9,12,14	1.53	2 (22%)
1	SEP	H	241	1	9,9,10	1.74	2 (22%)	9,12,14	1.31	1 (11%)

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	SEP	A	241	1	-	0/5/8/10	0/0/0/0
1	SEP	B	241	1	-	0/5/8/10	0/0/0/0
1	SEP	C	241	1	-	0/5/8/10	0/0/0/0
1	SEP	D	241	1	-	0/5/8/10	0/0/0/0
1	SEP	F	241	1	-	0/5/8/10	0/0/0/0
1	SEP	G	241	1	-	0/5/8/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	H	241	1	-	0/5/8/10	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	241	SEP	CA-C	-2.44	1.47	1.50
1	G	241	SEP	CA-C	2.46	1.53	1.50
1	F	241	SEP	CA-C	2.47	1.53	1.50
1	H	241	SEP	CA-C	3.02	1.54	1.50
1	B	241	SEP	P-O1P	3.23	1.61	1.50
1	G	241	SEP	P-O1P	3.24	1.61	1.50
1	A	241	SEP	P-O1P	3.26	1.61	1.50
1	F	241	SEP	P-O1P	3.27	1.61	1.50
1	H	241	SEP	P-O1P	3.31	1.62	1.50
1	D	241	SEP	P-O1P	3.33	1.62	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	241	SEP	P-OG-CB	-2.41	111.64	118.30
1	H	241	SEP	P-OG-CB	-2.39	111.71	118.30
1	G	241	SEP	P-OG-CB	-2.37	111.76	118.30
1	C	241	SEP	P-OG-CB	-2.24	112.12	118.30
1	D	241	SEP	O2P-P-OG	2.07	112.25	106.73
1	F	241	SEP	OG-CB-CA	2.24	110.38	108.17
1	A	241	SEP	O2P-P-OG	2.39	113.08	106.73
1	D	241	SEP	OG-CB-CA	2.50	110.63	108.17
1	B	241	SEP	OG-CB-CA	2.52	110.65	108.17
1	A	241	SEP	OG-CB-CA	2.60	110.73	108.17
1	C	241	SEP	O2P-P-OG	2.64	113.77	106.73
1	G	241	SEP	OG-CB-CA	2.90	111.03	108.17
1	C	241	SEP	OG-CB-CA	3.58	111.70	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	241	SEP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	241	SEP	1	0
1	C	241	SEP	1	0
1	D	241	SEP	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z > 2$
2	1F8	A	1	-	11,17,17	1.12	0	12,23,23	1.99	5 (41%)
2	1F8	B	1	-	11,17,17	1.17	0	12,23,23	2.00	5 (41%)
2	1F8	C	1	-	11,17,17	1.15	1 (9%)	12,23,23	1.97	5 (41%)
2	1F8	D	1	-	11,17,17	1.15	0	12,23,23	1.98	5 (41%)
2	1F8	E	1	-	11,17,17	1.19	1 (9%)	12,23,23	1.89	5 (41%)
2	1F8	F	1	-	11,17,17	1.14	0	12,23,23	1.92	5 (41%)
2	1F8	G	1	-	11,17,17	1.18	0	12,23,23	1.93	4 (33%)
2	1F8	H	1	-	11,17,17	1.17	0	12,23,23	1.99	5 (41%)

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	1F8	A	1	-	-	0/4/8/8	0/1/2/2
2	1F8	B	1	-	-	0/4/8/8	0/1/2/2
2	1F8	C	1	-	-	0/4/8/8	0/1/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1F8	D	1	-	-	0/4/8/8	0/1/2/2
2	1F8	E	1	-	-	0/4/8/8	0/1/2/2
2	1F8	F	1	-	-	0/4/8/8	0/1/2/2
2	1F8	G	1	-	-	0/4/8/8	0/1/2/2
2	1F8	H	1	-	-	0/4/8/8	0/1/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	1F8	C29-C24	2.00	1.51	1.48
2	E	1	1F8	C29-C24	2.06	1.51	1.48

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	1F8	C15-C16-N17	-4.00	103.80	112.50
2	A	1	1F8	C15-C16-N17	-3.95	103.90	112.50
2	C	1	1F8	C15-C16-N17	-3.87	104.08	112.50
2	D	1	1F8	C15-C16-N17	-3.85	104.12	112.50
2	B	1	1F8	C20-C21-C22	-3.17	102.57	107.76
2	A	1	1F8	C20-C21-C22	-3.16	102.59	107.76
2	F	1	1F8	C20-C21-C22	-3.15	102.60	107.76
2	C	1	1F8	C20-C21-C22	-3.14	102.62	107.76
2	H	1	1F8	C20-C21-C22	-3.11	102.67	107.76
2	G	1	1F8	C20-C21-C22	-3.10	102.67	107.76
2	D	1	1F8	C20-C21-C22	-3.10	102.68	107.76
2	E	1	1F8	C20-C21-C22	-3.05	102.76	107.76
2	F	1	1F8	C15-C16-N17	-3.01	105.96	112.50
2	G	1	1F8	C15-C16-N17	-2.98	106.02	112.50
2	H	1	1F8	C15-C16-N17	-2.91	106.17	112.50
2	E	1	1F8	C15-C16-N17	-2.75	106.51	112.50
2	H	1	1F8	C27-C28-C21	-2.55	117.24	120.88
2	C	1	1F8	C27-C28-C21	-2.46	117.36	120.88
2	D	1	1F8	C27-C28-C21	-2.38	117.48	120.88
2	G	1	1F8	C27-C28-C21	-2.37	117.48	120.88
2	E	1	1F8	C27-C28-C21	-2.36	117.51	120.88
2	B	1	1F8	C27-C28-C21	-2.35	117.52	120.88
2	A	1	1F8	C27-C28-C21	-2.32	117.57	120.88
2	F	1	1F8	C27-C28-C21	-2.28	117.61	120.88
2	H	1	1F8	C20-C18-N17	2.04	119.30	115.52
2	E	1	1F8	C20-C18-N17	2.06	119.34	115.52
2	F	1	1F8	C20-C18-N17	2.09	119.39	115.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	1F8	C28-C21-C22	2.58	122.01	120.38
2	D	1	1F8	C28-C21-C22	2.62	122.03	120.38
2	C	1	1F8	C28-C21-C22	2.63	122.04	120.38
2	B	1	1F8	C28-C21-C22	2.68	122.07	120.38
2	C	1	1F8	C16-N17-C18	2.81	128.52	122.11
2	B	1	1F8	C16-N17-C18	2.88	128.70	122.11
2	A	1	1F8	C16-N17-C18	3.00	128.96	122.11
2	D	1	1F8	C16-N17-C18	3.08	129.13	122.11
2	E	1	1F8	C28-C21-C22	3.11	122.34	120.38
2	F	1	1F8	C28-C21-C22	3.15	122.37	120.38
2	G	1	1F8	C28-C21-C22	3.33	122.48	120.38
2	H	1	1F8	C28-C21-C22	3.52	122.61	120.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	1F8	3	0
2	B	1	1F8	3	0
2	C	1	1F8	3	0
2	D	1	1F8	3	0
2	E	1	1F8	2	0
2	F	1	1F8	2	0
2	G	1	1F8	3	0
2	H	1	1F8	2	0

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	283/316 (89%)	0.09	13 (4%)	33	32	16, 32, 69, 100	0
1	B	280/316 (88%)	0.17	11 (3%)	40	38	17, 32, 70, 88	0
1	C	283/316 (89%)	0.19	22 (7%)	14	13	16, 32, 73, 98	0
1	D	282/316 (89%)	0.27	24 (8%)	11	10	17, 33, 72, 96	0
1	E	274/316 (86%)	0.30	20 (7%)	16	15	17, 41, 85, 109	0
1	F	274/316 (86%)	0.49	33 (12%)	5	4	18, 41, 86, 108	0
1	G	274/316 (86%)	0.37	24 (8%)	11	9	17, 42, 85, 109	0
1	H	274/316 (86%)	0.45	26 (9%)	9	8	17, 42, 86, 109	0
All	All	2224/2528 (87%)	0.29	173 (7%)	14	13	16, 37, 82, 109	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	82	PHE	7.7
1	E	243	VAL	7.3
1	H	124	VAL	7.3
1	H	102	LEU	6.5
1	H	82	PHE	6.5
1	D	102	LEU	6.2
1	D	103	ALA	5.6
1	H	258	SER	5.3
1	H	243	VAL	5.1
1	C	93	PHE	5.0
1	F	84	PHE	5.0
1	H	125	PRO	4.9
1	A	242	PHE	4.9
1	C	243	VAL	4.7
1	E	242	PHE	4.6
1	C	152	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	G	243	VAL	4.6
1	H	106	ARG	4.5
1	F	102	LEU	4.4
1	E	80	GLU	4.3
1	D	105	SER	4.3
1	H	84	PHE	4.2
1	C	102	LEU	4.2
1	D	76	LYS	4.1
1	H	76	LYS	4.0
1	F	125	PRO	4.0
1	F	88	LEU	3.9
1	F	124	VAL	3.9
1	F	99	ALA	3.8
1	D	77	LYS	3.7
1	H	122	ASN	3.6
1	A	152	ASP	3.6
1	F	91	GLY	3.6
1	A	76	LYS	3.5
1	G	122	ASN	3.5
1	D	242	PHE	3.4
1	F	230	LEU	3.4
1	F	122	ASN	3.3
1	C	76	LYS	3.3
1	G	230	LEU	3.3
1	E	258	SER	3.3
1	H	79	PRO	3.2
1	H	85	GLY	3.2
1	C	91	GLY	3.2
1	C	103	ALA	3.2
1	G	99	ALA	3.2
1	G	125	PRO	3.2
1	C	105	SER	3.2
1	H	80	GLU	3.2
1	G	88	LEU	3.1
1	G	104	THR	3.1
1	E	84	PHE	3.1
1	E	104	THR	3.0
1	C	234	SER	3.0
1	H	92	SER	3.0
1	B	243	VAL	3.0
1	F	80	GLU	2.9
1	F	103	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	105	SER	2.9
1	E	82	PHE	2.9
1	H	103	ALA	2.9
1	B	77	LYS	2.9
1	E	117	HIS	2.9
1	E	124	VAL	2.9
1	E	90	GLU	2.9
1	E	88	LEU	2.9
1	D	148	CYS	2.9
1	G	82	PHE	2.8
1	F	105	SER	2.8
1	D	104	THR	2.8
1	H	81	ASP	2.8
1	C	118	ILE	2.8
1	E	102	LEU	2.8
1	C	104	THR	2.8
1	A	238	ARG	2.8
1	F	77	LYS	2.8
1	D	156	TYR	2.8
1	A	153	GLU	2.8
1	C	242	PHE	2.7
1	G	80	GLU	2.7
1	D	81	ASP	2.7
1	E	122	ASN	2.7
1	A	93	PHE	2.7
1	F	138	ASP	2.7
1	B	93	PHE	2.7
1	G	148	CYS	2.6
1	F	104	THR	2.6
1	H	104	THR	2.6
1	B	105	SER	2.6
1	D	240	ASN	2.6
1	C	238	ARG	2.6
1	A	91	GLY	2.6
1	G	89	GLY	2.6
1	H	152	ASP	2.6
1	C	124	VAL	2.6
1	F	108	TYR	2.6
1	H	75	ARG	2.6
1	E	125	PRO	2.6
1	H	88	LEU	2.6
1	H	101	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	128	THR	2.6
1	F	148	CYS	2.6
1	C	106	ARG	2.5
1	A	103	ALA	2.5
1	B	104	THR	2.5
1	G	359	THR	2.5
1	D	91	GLY	2.5
1	G	129	ARG	2.5
1	G	117	HIS	2.5
1	C	81	ASP	2.5
1	D	238	ARG	2.5
1	H	91	GLY	2.5
1	C	80	GLU	2.4
1	C	114	GLU	2.4
1	D	85	GLY	2.4
1	E	91	GLY	2.4
1	F	75	ARG	2.4
1	E	119	ILE	2.4
1	G	175	GLY	2.4
1	D	243	VAL	2.4
1	G	216	ASP	2.4
1	B	235	LYS	2.4
1	C	239	ALA	2.4
1	H	242	PHE	2.4
1	D	154	LYS	2.4
1	D	151	ASP	2.4
1	F	109	ALA	2.4
1	D	84	PHE	2.4
1	H	90	GLU	2.3
1	E	92	SER	2.3
1	H	244	GLY	2.3
1	F	107	GLU	2.3
1	F	157	PHE	2.3
1	F	90	GLU	2.3
1	C	79	PRO	2.3
1	G	75	ARG	2.3
1	A	243	VAL	2.3
1	E	118	ILE	2.3
1	G	102	LEU	2.2
1	B	80	GLU	2.2
1	D	157	PHE	2.2
1	D	100	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	79	PRO	2.2
1	G	91	GLY	2.2
1	C	100	ARG	2.2
1	D	152	ASP	2.2
1	D	80	GLU	2.2
1	F	129	ARG	2.2
1	F	79	PRO	2.2
1	A	240	ASN	2.2
1	A	259	ALA	2.2
1	G	79	PRO	2.2
1	C	259	ALA	2.1
1	B	240	ASN	2.1
1	G	84	PHE	2.1
1	F	118	ILE	2.1
1	G	118	ILE	2.1
1	B	103	ALA	2.1
1	B	156	TYR	2.1
1	G	103	ALA	2.1
1	D	149	PHE	2.1
1	A	80	GLU	2.1
1	F	131	ARG	2.1
1	G	93	PHE	2.1
1	F	359	THR	2.1
1	D	82	PHE	2.1
1	E	244	GLY	2.0
1	F	156	TYR	2.0
1	F	243	VAL	2.0
1	F	112	ILE	2.0
1	A	75	ARG	2.0
1	B	151	ASP	2.0
1	F	81	ASP	2.0

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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	SEP	F	241	10/11	0.83	0.36	-	70,81,94,96	0
1	SEP	D	241	10/11	0.91	0.15	-	45,60,82,85	0
1	SEP	C	241	10/11	0.91	0.18	-	48,64,81,86	0
1	SEP	B	241	10/11	0.93	0.12	-	46,61,81,86	0
1	SEP	A	241	10/11	0.93	0.16	-	45,61,78,84	0
1	SEP	H	241	10/11	0.75	0.29	-	64,81,89,93	0
1	SEP	G	241	10/11	0.71	0.35	-	66,78,100,109	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	1F8	H	1	16/16	0.65	0.39	5.17	87,98,109,112	0
2	1F8	G	1	16/16	0.64	0.31	3.81	87,98,108,110	0
2	1F8	B	1	16/16	0.80	0.34	3.56	72,89,110,121	0
2	1F8	E	1	16/16	0.65	0.34	2.47	87,96,108,111	0
2	1F8	A	1	16/16	0.71	0.37	2.31	72,88,110,120	0
2	1F8	F	1	16/16	0.66	0.35	1.95	87,97,109,111	0
2	1F8	C	1	16/16	0.73	0.29	1.06	71,88,109,120	0
2	1F8	D	1	16/16	0.78	0.30	0.86	73,88,110,120	0
3	CL	A	2	1/1	0.97	0.22	-	45,45,45,45	0
3	CL	C	6	1/1	0.99	0.16	-	46,46,46,46	0
3	CL	B	5	1/1	0.94	0.17	-	44,44,44,44	0
3	CL	D	360	1/1	0.96	0.21	-	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.