



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:44 AM GMT

PDB ID : 3BYW
Title : Crystal structure of an extracellular domain of arabinofuranosyltransferase from *Corynebacterium diphtheriae*
Authors : Tan, K.; Hatzos, C.; Abdullah, J.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2008-01-16
Resolution : 2.35 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

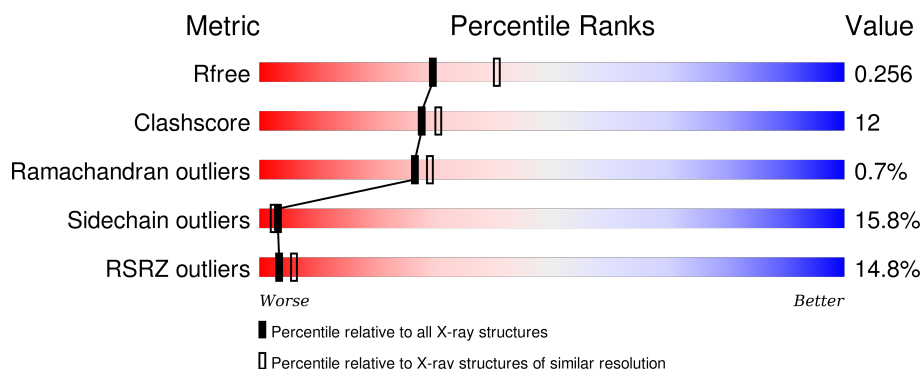
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.



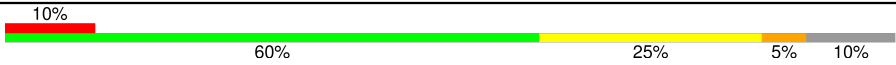


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	177	<div> <div>11%</div> <div> <div></div> <div>60%</div> <div>23%</div> <div>6%</div> <div>11%</div> </div> </div>
1	B	177	<div> <div>16%</div> <div> <div></div> <div>59%</div> <div>27%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	177	<div> <div>11%</div> <div> <div></div> <div>63%</div> <div>23%</div> <div>5%</div> <div>10%</div> </div> </div>
1	D	177	<div> <div>16%</div> <div> <div></div> <div>68%</div> <div>18%</div> <div>•</div> <div>11%</div> </div> </div>
1	E	177	<div> <div>16%</div> <div> <div></div> <div>63%</div> <div>22%</div> <div>5%</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	177	
1	G	177	
1	H	177	

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
3	ACT	E	5	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9635 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 Putative arabinofuranosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	Se	0	0	0
			1168	717	200	249	2			
1	B	159	Total	C	N	O	Se	0	1	0
			1191	734	202	252	3			
1	C	160	Total	C	N	O	Se	0	0	0
			1192	733	203	254	2			
1	D	157	Total	C	N	O	Se	0	0	0
			1164	716	197	249	2			
1	E	159	Total	C	N	O	Se	0	0	0
			1186	730	202	252	2			
1	F	160	Total	C	N	O	Se	0	0	0
			1193	735	203	253	2			
1	G	159	Total	C	N	O	Se	0	0	0
			1186	730	202	252	2			
1	H	158	Total	C	N	O	Se	0	0	0
			1175	722	201	250	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	SER	-	EXPRESSION TAG	UNP Q6NK78
A	32	ASN	-	EXPRESSION TAG	UNP Q6NK78
A	33	ALA	-	EXPRESSION TAG	UNP Q6NK78
B	31	SER	-	EXPRESSION TAG	UNP Q6NK78
B	32	ASN	-	EXPRESSION TAG	UNP Q6NK78
B	33	ALA	-	EXPRESSION TAG	UNP Q6NK78
C	31	SER	-	EXPRESSION TAG	UNP Q6NK78
C	32	ASN	-	EXPRESSION TAG	UNP Q6NK78
C	33	ALA	-	EXPRESSION TAG	UNP Q6NK78
D	31	SER	-	EXPRESSION TAG	UNP Q6NK78
D	32	ASN	-	EXPRESSION TAG	UNP Q6NK78
D	33	ALA	-	EXPRESSION TAG	UNP Q6NK78
E	31	SER	-	EXPRESSION TAG	UNP Q6NK78

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Chain	Residue	Modelled	Actual	Comment	Reference
E	32	ASN	-	EXPRESSION TAG	UNP Q6NK78
E	33	ALA	-	EXPRESSION TAG	UNP Q6NK78
F	31	SER	-	EXPRESSION TAG	UNP Q6NK78
F	32	ASN	-	EXPRESSION TAG	UNP Q6NK78
F	33	ALA	-	EXPRESSION TAG	UNP Q6NK78
G	31	SER	-	EXPRESSION TAG	UNP Q6NK78
G	32	ASN	-	EXPRESSION TAG	UNP Q6NK78
G	33	ALA	-	EXPRESSION TAG	UNP Q6NK78
H	31	SER	-	EXPRESSION TAG	UNP Q6NK78
H	32	ASN	-	EXPRESSION TAG	UNP Q6NK78
H	33	ALA	-	EXPRESSION TAG	UNP Q6NK78

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	D	4	Total Zn 4 4	0	0
2	E	4	Total Zn 4 4	0	0
2	B	3	Total Zn 3 3	0	0
2	C	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		

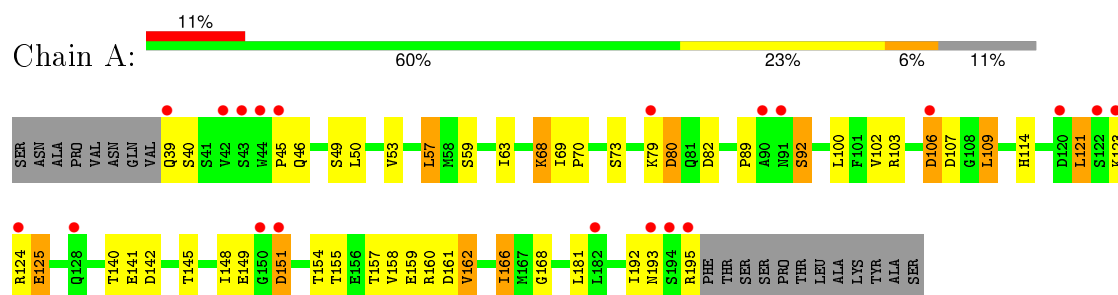
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total 4	O 4	0	0
4	B	14	Total 14	O 14	0	0
4	C	8	Total 8	O 8	0	0
4	D	18	Total 18	O 18	0	0
4	E	27	Total 27	O 27	0	0
4	F	13	Total 13	O 13	0	0
4	G	15	Total 15	O 15	0	0
4	H	10	Total 10	O 10	0	0

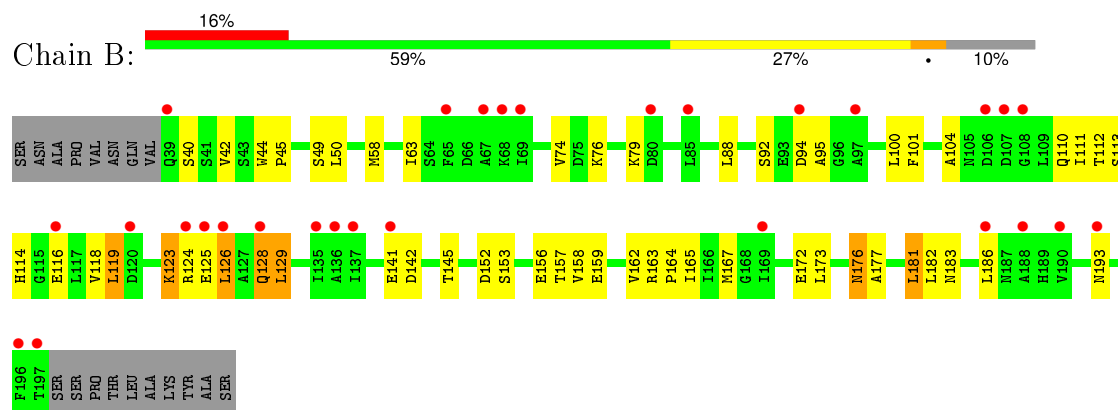
3 Residue-property plots [i](#)

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

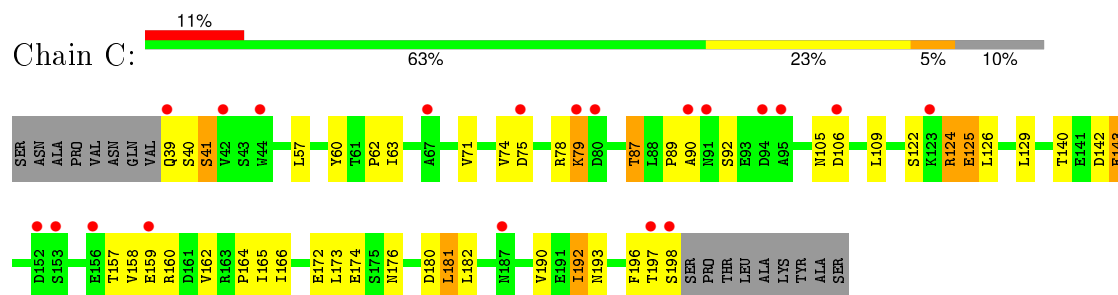
- Molecule 1: Putative arabinofuranosyltransferase



- Molecule 1: Putative arabinofuranosyltransferase

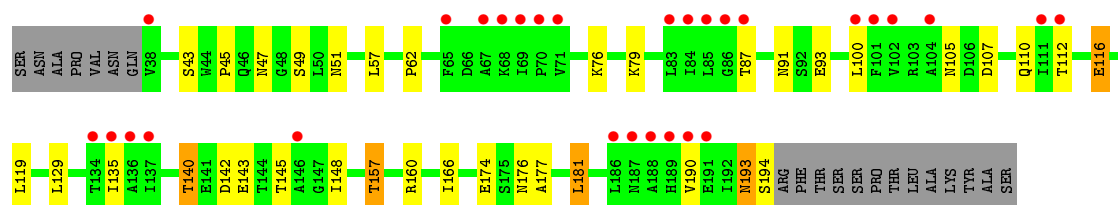


- Molecule 1: Putative arabinofuranosyltransferase

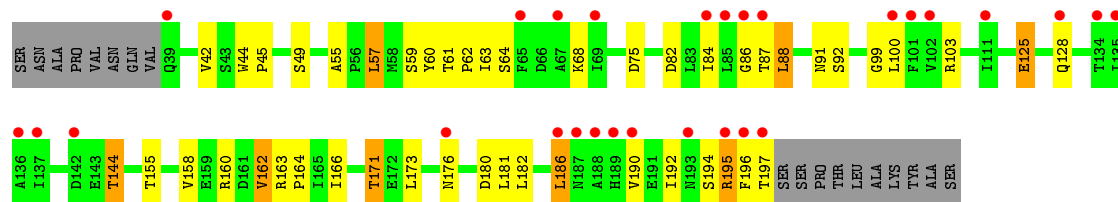


- Molecule 1: Putative arabinofuranosyltransferase

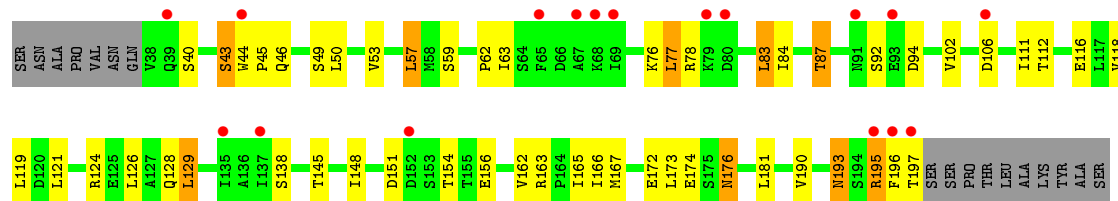




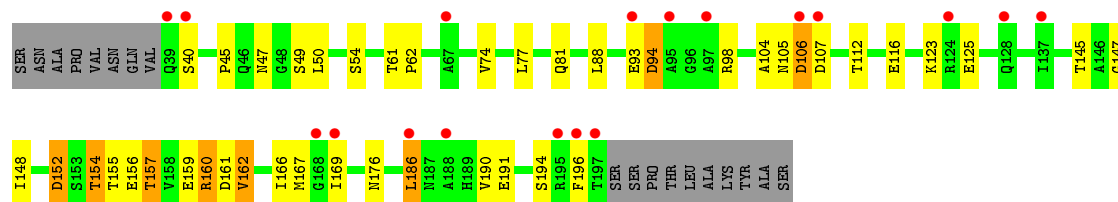
• Molecule 1: Putative arabinofuranosyltransferase



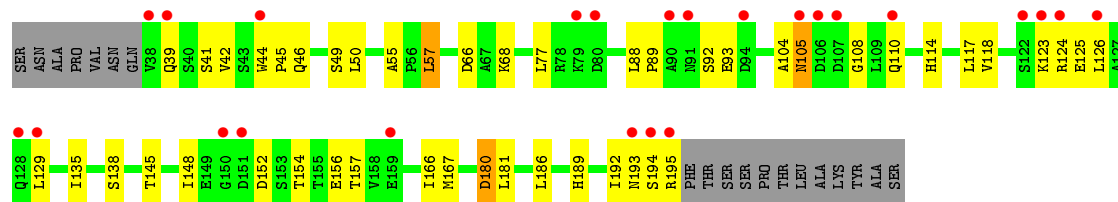
• Molecule 1: Putative arabinofuranosyltransferase



• Molecule 1: Putative arabinofuranosyltransferase



• Molecule 1: Putative arabinofuranosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.89Å 80.62Å 115.83Å 90.00° 110.91° 90.00°	Depositor
Resolution (Å)	35.25 – 2.35 35.24 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.6 (35.25-2.35) 96.6 (35.24-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.209 , 0.263 0.208 , 0.256	Depositor DCC
R_{free} test set	2939 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.8	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 58219 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9635	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.42 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.8472e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.65	0/1180	0.76	0/1604
1	B	0.68	0/1207	0.82	0/1640
1	C	0.69	0/1205	0.80	0/1638
1	D	0.82	1/1176 (0.1%)	0.88	0/1600
1	E	0.91	0/1199	0.92	2/1630 (0.1%)
1	F	0.72	0/1206	0.87	1/1640 (0.1%)
1	G	0.72	0/1199	0.82	1/1630 (0.1%)
1	H	0.68	2/1187 (0.2%)	0.78	2/1614 (0.1%)
All	All	0.74	3/9559 (0.0%)	0.83	6/12996 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	125	GLU	CD-OE1	5.98	1.32	1.25
1	D	93	GLU	CG-CD	5.65	1.60	1.51
1	H	125	GLU	CD-OE2	5.35	1.31	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	180	ASP	CB-CG-OD1	-5.61	113.26	118.30
1	H	117	LEU	CA-CB-CG	5.45	127.84	115.30
1	F	83	LEU	CA-CB-CG	5.28	127.45	115.30
1	E	180	ASP	CB-CG-OD2	5.10	122.89	118.30
1	G	186	LEU	CA-CB-CG	5.09	127.02	115.30
1	H	180	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1168	0	1145	23	0
1	B	1191	0	1170	33	0
1	C	1192	0	1166	30	0
1	D	1164	0	1141	27	0
1	E	1186	0	1161	48	0
1	F	1193	0	1170	50	0
1	G	1186	0	1161	22	0
1	H	1175	0	1154	20	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
3	A	4	0	3	0	0
3	B	12	0	9	0	0
3	C	4	0	3	0	0
3	D	12	0	9	0	0
3	E	12	0	9	0	0
3	G	4	0	3	0	0
3	H	4	0	3	0	0
4	A	4	0	0	0	0
4	B	14	0	0	0	0
4	C	8	0	0	0	0
4	D	18	0	0	0	0
4	E	27	0	0	0	0
4	F	13	0	0	0	0
4	G	15	0	0	0	0
4	H	10	0	0	0	0
All	All	9635	0	9307	223	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 (223) 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:E:196:PHE:HE1	1:F:196:PHE:CD2	1.54	1.25
1:G:145:THR:HG22	1:G:157:THR:HB	1.22	1.15
1:B:58[A]:MSE:HE2	1:B:167:MSE:HE3	1.16	1.14
1:B:58[A]:MSE:HE2	1:B:167:MSE:CE	1.78	1.13
1:E:84:ILE:O	1:E:171:THR:HG23	1.49	1.10
1:D:79:LYS:HA	1:D:79:LYS:HE2	1.31	1.10
1:E:196:PHE:CE1	1:F:196:PHE:CD2	2.46	1.04
1:E:196:PHE:CE1	1:F:196:PHE:HD2	1.76	1.03
1:E:182:LEU:HD21	1:F:45:PRO:HG2	1.49	0.94
1:D:135:ILE:HD13	1:D:148:ILE:HD13	1.51	0.93
1:F:176:ASN:HD22	1:F:176:ASN:H	1.14	0.92
1:F:176:ASN:ND2	1:F:176:ASN:H	1.64	0.91
1:B:88:LEU:HD21	1:B:165:ILE:HG22	1.52	0.90
1:H:148:ILE:HG12	1:H:154:THR:HG21	1.53	0.90
1:C:122:SER:OG	1:C:125:GLU:HB2	1.72	0.88
1:E:144:THR:HG23	1:E:162:VAL:HG23	1.52	0.88
1:E:196:PHE:HE1	1:F:196:PHE:HD2	0.93	0.87
1:G:62:PRO:HG3	1:G:166:ILE:HD12	1.56	0.86
1:E:84:ILE:O	1:E:171:THR:CG2	2.26	0.84
1:F:151:ASP:O	1:F:154:THR:HG22	1.77	0.84
1:B:58[A]:MSE:CE	1:B:167:MSE:HE3	2.07	0.81
1:H:195:ARG:HB3	1:H:195:ARG:HH11	1.48	0.77
1:A:103:ARG:O	1:A:109:LEU:HD23	1.87	0.75
1:D:62:PRO:HG3	1:D:166:ILE:HD12	1.65	0.75
1:F:76:LYS:O	1:F:174:GLU:HG2	1.88	0.74
1:C:62:PRO:HG3	1:C:166:ILE:HD13	1.70	0.74
1:H:105:ASN:HD22	1:H:105:ASN:N	1.86	0.74
1:G:148:ILE:H	1:G:154:THR:CG2	2.00	0.73
1:H:66:ASP:OD1	1:H:189:HIS:HB3	1.89	0.72
1:A:106:ASP:O	1:A:123:LYS:HG2	1.89	0.72
1:A:121:LEU:HB3	1:A:125:GLU:HB3	1.72	0.72
1:D:79:LYS:CE	1:D:79:LYS:HA	2.14	0.70
1:E:171:THR:HG21	1:E:173:LEU:HD12	1.73	0.69
1:C:39:GLN:HA	1:D:193:ASN:CB	2.23	0.69
1:C:39:GLN:HA	1:D:193:ASN:HB3	1.73	0.68
1:H:105:ASN:H	1:H:105:ASN:HD22	1.41	0.67
1:G:148:ILE:HB	1:G:154:THR:HG21	1.76	0.66
1:C:63:ILE:HD11	1:C:193:ASN:HB2	1.77	0.66
1:E:62:PRO:HA	1:F:196:PHE:CE1	2.32	0.65
1:E:62:PRO:HA	1:F:196:PHE:CZ	2.32	0.64
1:B:124:ARG:HD2	1:B:124:ARG:H	1.62	0.64
1:F:111:ILE:HG12	1:F:119:LEU:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:HD11	1:A:193:ASN:HB2	1.79	0.64
1:A:151:ASP:O	1:A:154:THR:HG22	1.99	0.63
1:A:57:LEU:HD22	1:A:59:SER:O	1.98	0.63
1:E:61:THR:HB	1:F:195:ARG:HA	1.81	0.63
1:C:162:VAL:O	1:C:162:VAL:CG1	2.47	0.62
1:F:162:VAL:HG12	1:F:162:VAL:O	2.01	0.61
1:B:124:ARG:N	1:B:124:ARG:HD2	2.15	0.61
1:G:62:PRO:HG3	1:G:166:ILE:CD1	2.29	0.61
1:B:45:PRO:HB3	1:B:49:SER:O	2.01	0.61
1:C:78:ARG:HG3	1:C:172:GLU:O	2.01	0.60
1:C:60:TYR:CE2	1:C:192:ILE:HD12	2.37	0.60
1:G:147:GLY:HA3	1:G:155:THR:HG22	1.84	0.59
1:C:89:PRO:HG2	1:C:92:SER:HB3	1.85	0.59
1:C:182:LEU:HD21	1:D:45:PRO:HG2	1.82	0.59
1:C:162:VAL:O	1:C:162:VAL:HG13	2.04	0.58
1:G:116:GLU:OE2	1:G:160:ARG:NH2	2.36	0.58
1:C:87:THR:CG2	1:C:165:ILE:O	2.51	0.58
1:C:122:SER:HG	1:C:125:GLU:HB2	1.68	0.58
1:E:144:THR:CG2	1:E:162:VAL:HG23	2.30	0.57
1:D:135:ILE:HD13	1:D:148:ILE:CD1	2.32	0.57
1:C:140:THR:HG22	1:C:142:ASP:H	1.70	0.57
1:D:135:ILE:CD1	1:D:148:ILE:HD13	2.31	0.57
1:E:190:VAL:HG12	1:E:192:ILE:CD1	2.35	0.57
1:A:57:LEU:CD2	1:A:59:SER:O	2.53	0.56
1:F:162:VAL:O	1:F:162:VAL:CG1	2.53	0.56
1:F:148:ILE:HB	1:F:154:THR:HG21	1.86	0.56
1:F:43:SER:O	1:F:46:GLN:NE2	2.35	0.56
1:E:192:ILE:HA	1:F:196:PHE:CE1	2.40	0.56
1:A:148:ILE:HB	1:A:154:THR:HG21	1.87	0.56
1:G:94:ASP:O	1:G:98:ARG:HG3	2.05	0.56
1:B:58[A]:MSE:HE2	1:B:167:MSE:HE1	1.77	0.56
1:E:190:VAL:CG1	1:E:192:ILE:HD11	2.35	0.56
1:E:171:THR:HG21	1:E:173:LEU:CD1	2.36	0.55
1:F:176:ASN:N	1:F:176:ASN:HD22	1.94	0.55
1:E:182:LEU:CD2	1:F:45:PRO:HG2	2.29	0.55
1:E:192:ILE:HG23	1:F:196:PHE:CZ	2.42	0.55
1:C:143:GLU:HB2	1:C:158:VAL:O	2.07	0.55
1:F:87:THR:HG23	1:F:166:ILE:HG13	1.88	0.55
1:D:177:ALA:HB1	1:D:181:LEU:HD22	1.89	0.54
1:F:87:THR:CG2	1:F:165:ILE:O	2.56	0.54
1:F:44:TRP:HZ2	1:F:50:LEU:O	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58[A]:MSE:CE	1:B:167:MSE:CE	2.70	0.54
1:F:102:VAL:HG13	1:F:111:ILE:CD1	2.38	0.54
1:G:88:LEU:HD23	1:G:167:MSE:HG3	1.90	0.53
1:E:68:LYS:O	1:E:186:LEU:HA	2.08	0.53
1:A:141:GLU:O	1:A:161:ASP:HB2	2.08	0.53
1:A:89:PRO:O	1:A:92:SER:HB2	2.07	0.53
1:G:191:GLU:OE2	1:H:41:SER:HB3	2.07	0.53
1:F:102:VAL:HG13	1:F:111:ILE:HD12	1.90	0.53
1:G:116:GLU:HG3	1:G:162:VAL:HG11	1.90	0.53
1:B:183:ASN:HD21	1:D:47:ASN:ND2	2.06	0.53
1:H:105:ASN:N	1:H:105:ASN:ND2	2.55	0.52
1:B:119:LEU:HD23	1:B:156:GLU:HG3	1.90	0.52
1:F:87:THR:HG23	1:F:166:ILE:HA	1.92	0.52
1:D:140:THR:HG22	1:D:143:GLU:H	1.75	0.52
1:E:181:LEU:HD12	1:F:50:LEU:HD21	1.91	0.52
1:A:46:GLN:HG3	1:A:53:VAL:HG11	1.92	0.52
1:D:51:ASN:HD22	1:D:51:ASN:N	2.06	0.52
1:G:148:ILE:H	1:G:154:THR:HG21	1.74	0.51
1:G:45:PRO:HB3	1:G:49:SER:O	2.11	0.51
1:E:190:VAL:HG12	1:E:192:ILE:HD11	1.92	0.51
1:G:148:ILE:CB	1:G:154:THR:HG21	2.41	0.51
1:G:116:GLU:HG3	1:G:162:VAL:CG1	2.41	0.51
1:D:76:LYS:O	1:D:174:GLU:HG3	2.10	0.51
1:E:63:ILE:H	1:F:196:PHE:HE1	1.60	0.50
1:E:158:VAL:HG12	1:E:160:ARG:HG2	1.94	0.50
1:D:145:THR:HG22	1:D:157:THR:HB	1.93	0.50
1:G:169:ILE:HG21	1:H:44:TRP:CD2	2.47	0.50
1:E:62:PRO:O	1:E:163:ARG:NH1	2.38	0.50
1:A:45:PRO:HG2	1:B:182:LEU:HD21	1.93	0.50
1:E:144:THR:HG23	1:E:162:VAL:CG2	2.34	0.50
1:F:148:ILE:H	1:F:154:THR:CG2	2.25	0.50
1:H:88:LEU:HD23	1:H:167:MSE:HG2	1.94	0.49
1:E:57:LEU:HD22	1:E:59:SER:O	2.11	0.49
1:E:171:THR:CG2	1:E:173:LEU:HG	2.43	0.49
1:D:87:THR:HB	1:D:166:ILE:HG12	1.92	0.49
1:B:126:LEU:HA	1:B:129:LEU:HD22	1.94	0.49
1:E:63:ILE:HG12	1:F:196:PHE:CE1	2.47	0.49
1:E:195:ARG:HB3	1:E:195:ARG:HH11	1.77	0.49
1:F:62:PRO:HG3	1:F:166:ILE:HD12	1.95	0.49
1:B:74:VAL:HG13	1:B:104:ALA:HB1	1.95	0.49
1:E:62:PRO:HD3	1:E:166:ILE:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:LEU:HA	1:F:129:LEU:HD22	1.95	0.48
1:A:68:LYS:HE3	1:A:149:GLU:OE2	2.13	0.48
1:B:125:GLU:HA	1:B:128:GLN:HE22	1.79	0.48
1:E:60:TYR:CE2	1:E:192:ILE:HD12	2.48	0.47
1:D:140:THR:HG23	1:D:142:ASP:H	1.80	0.47
1:F:78:ARG:HB2	1:F:172:GLU:O	2.14	0.47
1:B:76:LYS:HD2	1:B:177:ALA:HB2	1.96	0.47
1:F:45:PRO:HB3	1:F:49:SER:O	2.15	0.47
1:G:74:VAL:HG13	1:G:104:ALA:HB1	1.95	0.47
1:C:140:THR:HG22	1:C:142:ASP:N	2.29	0.47
1:H:45:PRO:HB3	1:H:49:SER:O	2.13	0.47
1:B:76:LYS:HD2	1:B:177:ALA:CB	2.45	0.47
1:B:63:ILE:HD11	1:B:193:ASN:HB2	1.96	0.47
1:C:196:PHE:CD1	1:D:193:ASN:ND2	2.83	0.47
1:H:89:PRO:HG2	1:H:92:SER:HB2	1.95	0.47
1:C:39:GLN:HA	1:D:193:ASN:HB2	1.96	0.47
1:A:100:LEU:C	1:A:100:LEU:HD23	2.35	0.47
1:B:124:ARG:O	1:B:128:GLN:NE2	2.48	0.46
1:G:196:PHE:CD1	1:H:193:ASN:HB3	2.50	0.46
1:E:87:THR:HB	1:E:166:ILE:HD13	1.96	0.46
1:B:124:ARG:CD	1:B:124:ARG:H	2.27	0.46
1:G:106:ASP:N	1:G:106:ASP:OD1	2.49	0.46
1:E:171:THR:HG22	1:E:173:LEU:HG	1.98	0.46
1:B:176:ASN:OD1	1:B:176:ASN:N	2.45	0.46
1:C:71:VAL:O	1:C:74:VAL:HG13	2.15	0.46
1:E:63:ILE:HG12	1:F:196:PHE:CD1	2.50	0.46
1:E:86:GLY:HA2	1:E:100:LEU:O	2.16	0.46
1:D:135:ILE:CD1	1:D:148:ILE:CD1	2.93	0.46
1:B:141:GLU:HB3	1:B:163:ARG:CZ	2.46	0.45
1:A:69:ILE:HA	1:A:70:PRO:HD2	1.80	0.45
1:D:116:GLU:CD	1:D:160:ARG:HH22	2.20	0.45
1:C:164:PRO:HG2	1:C:166:ILE:HD11	1.98	0.45
1:E:42:VAL:HG21	1:E:55:ALA:HB1	1.99	0.45
1:D:45:PRO:HB3	1:D:49:SER:O	2.16	0.45
1:D:105:ASN:OD1	1:D:107:ASP:HB2	2.16	0.45
1:C:62:PRO:HG3	1:C:166:ILE:CD1	2.42	0.45
1:H:195:ARG:CB	1:H:195:ARG:HH11	2.26	0.44
1:E:171:THR:HG21	1:E:173:LEU:CG	2.47	0.44
1:B:100:LEU:HA	1:B:112:THR:O	2.16	0.44
1:E:88:LEU:HD22	1:E:99:GLY:CA	2.47	0.44
1:B:100:LEU:HB2	1:B:164:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:TRP:CG	1:E:45:PRO:HA	2.52	0.44
1:E:190:VAL:HG11	1:E:192:ILE:HD11	1.99	0.44
1:A:160:ARG:HG2	1:A:161:ASP:N	2.31	0.44
1:E:194:SER:HB3	1:F:57:LEU:HD21	2.00	0.44
1:F:87:THR:CG2	1:F:166:ILE:HG13	2.48	0.44
1:C:87:THR:HG23	1:C:165:ILE:O	2.17	0.43
1:F:138:SER:HB3	1:F:145:THR:HG22	2.00	0.43
1:H:42:VAL:HG21	1:H:55:ALA:HB1	2.00	0.43
1:A:102:VAL:HG12	1:A:109:LEU:HD21	1.99	0.43
1:G:152:ASP:OD2	1:G:152:ASP:N	2.50	0.43
1:F:176:ASN:N	1:F:176:ASN:ND2	2.44	0.43
1:D:62:PRO:HG3	1:D:166:ILE:CD1	2.43	0.42
1:F:59:SER:HB3	1:F:167:MSE:HG2	2.01	0.42
1:B:123:LYS:HG3	1:B:124:ARG:HH21	1.84	0.42
1:F:116:GLU:HG3	1:F:162:VAL:HG22	2.01	0.42
1:E:100:LEU:HB2	1:E:164:PRO:HB3	2.01	0.42
1:A:162:VAL:HG13	1:A:162:VAL:O	2.20	0.42
1:H:138:SER:HB3	1:H:145:THR:HG22	2.00	0.42
1:C:176:ASN:H	1:C:176:ASN:ND2	2.17	0.42
1:A:166:ILE:HD12	1:A:168:GLY:N	2.34	0.42
1:A:82:ASP:O	1:A:103:ARG:HA	2.20	0.42
1:D:107:ASP:HB3	1:D:110:GLN:NE2	2.34	0.42
1:C:174:GLU:HB3	1:C:176:ASN:HD21	1.84	0.42
1:E:125:GLU:HG2	1:E:125:GLU:H	1.74	0.42
1:D:100:LEU:HA	1:D:112:THR:O	2.20	0.42
1:F:63:ILE:HD11	1:F:193:ASN:CB	2.50	0.42
1:B:92:SER:HB2	1:B:95:ALA:HB2	2.01	0.41
1:E:82:ASP:OD1	1:E:103:ARG:NH1	2.53	0.41
1:C:181:LEU:HA	1:C:181:LEU:HD12	1.85	0.41
1:H:89:PRO:HD3	1:H:167:MSE:HG3	2.02	0.41
1:B:116:GLU:HG2	1:B:158:VAL:HG11	2.02	0.41
1:G:194:SER:HB3	1:H:57:LEU:HD21	2.01	0.41
1:F:53:VAL:O	1:F:53:VAL:HG23	2.19	0.41
1:C:40:SER:HB2	1:C:41:SER:H	1.69	0.41
1:E:63:ILE:N	1:F:196:PHE:CE1	2.87	0.41
1:C:79:LYS:H	1:C:79:LYS:HD3	1.85	0.41
1:A:145:THR:HG22	1:A:157:THR:OG1	2.21	0.41
1:F:77:LEU:CD1	1:F:84:ILE:HG13	2.51	0.41
1:H:195:ARG:HB3	1:H:195:ARG:NH1	2.25	0.41
1:B:123:LYS:CG	1:B:124:ARG:NH2	2.84	0.41
1:B:44:TRP:CG	1:B:45:PRO:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HD12	1:B:113:SER:HB3	2.02	0.41
1:C:124:ARG:HG3	1:C:124:ARG:H	1.65	0.41
1:E:196:PHE:O	1:F:163:ARG:NH1	2.43	0.41
1:E:45:PRO:HB3	1:E:49:SER:O	2.20	0.41
1:G:160:ARG:HB2	1:G:161:ASP:H	1.73	0.41
1:C:158:VAL:O	1:C:158:VAL:HG23	2.20	0.41
1:F:63:ILE:HD11	1:F:193:ASN:HB2	2.03	0.40
1:F:148:ILE:H	1:F:154:THR:HG23	1.86	0.40
1:F:44:TRP:CD1	1:F:45:PRO:HA	2.56	0.40
1:A:45:PRO:HB3	1:A:49:SER:O	2.22	0.40
1:B:181:LEU:HA	1:B:181:LEU:HD12	1.80	0.40
1:B:101:PHE:O	1:B:111:ILE:HA	2.21	0.40
1:C:57:LEU:HB2	1:D:57:LEU:HB3	2.04	0.40
1:B:159:GLU:HG3	1:B:159:GLU:O	2.21	0.40
1:H:104:ALA:HA	1:H:108:GLY:O	2.22	0.40
1:A:82:ASP:OD2	1:A:103:ARG:HD3	2.22	0.40
1:H:126:LEU:HD12	1:H:129:LEU:HD12	2.03	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	155/177 (88%)	147 (95%)	7 (4%)	1 (1%)	30	34
1	B	158/177 (89%)	152 (96%)	6 (4%)	0	100	100
1	C	158/177 (89%)	149 (94%)	7 (4%)	2 (1%)	15	13
1	D	155/177 (88%)	147 (95%)	7 (4%)	1 (1%)	30	34
1	E	157/177 (89%)	153 (98%)	3 (2%)	1 (1%)	30	34
1	F	158/177 (89%)	147 (93%)	9 (6%)	2 (1%)	15	13
1	G	157/177 (89%)	145 (92%)	11 (7%)	1 (1%)	30	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	156/177 (88%)	149 (96%)	6 (4%)	1 (1%)	30	34
All	All	1254/1416 (89%)	1189 (95%)	56 (4%)	9 (1%)	26	29

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	ASP
1	G	93	GLU
1	C	90	ALA
1	D	176	ASN
1	F	92	SER
1	C	159	GLU
1	F	94	ASP
1	E	91	ASN
1	H	118	VAL

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	129/144 (90%)	102 (79%)	27 (21%)	1	1
1	B	132/144 (92%)	108 (82%)	24 (18%)	2	1
1	C	132/144 (92%)	111 (84%)	21 (16%)	3	2
1	D	129/144 (90%)	118 (92%)	11 (8%)	13	14
1	E	131/144 (91%)	116 (88%)	15 (12%)	7	6
1	F	132/144 (92%)	111 (84%)	21 (16%)	3	2
1	G	131/144 (91%)	107 (82%)	24 (18%)	2	1
1	H	130/144 (90%)	108 (83%)	22 (17%)	2	2
All	All	1046/1152 (91%)	881 (84%)	165 (16%)	3	2

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	40	SER
1	A	50	LEU
1	A	57	LEU
1	A	68	LYS
1	A	73	SER
1	A	79	LYS
1	A	80	ASP
1	A	92	SER
1	A	106	ASP
1	A	107	ASP
1	A	109	LEU
1	A	114	HIS
1	A	121	LEU
1	A	124	ARG
1	A	125	GLU
1	A	140	THR
1	A	142	ASP
1	A	151	ASP
1	A	155	THR
1	A	158	VAL
1	A	159	GLU
1	A	162	VAL
1	A	166	ILE
1	A	181	LEU
1	A	192	ILE
1	A	195	ARG
1	B	40	SER
1	B	42	VAL
1	B	50	LEU
1	B	79	LYS
1	B	94	ASP
1	B	110	GLN
1	B	114	HIS
1	B	118	VAL
1	B	119	LEU
1	B	123	LYS
1	B	126	LEU
1	B	128	GLN
1	B	129	LEU
1	B	142	ASP
1	B	145	THR
1	B	152	ASP

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Mol	Chain	Res	Type
1	B	153	SER
1	B	157	THR
1	B	162	VAL
1	B	172	GLU
1	B	173	LEU
1	B	176	ASN
1	B	181	LEU
1	B	186	LEU
1	C	41	SER
1	C	75	ASP
1	C	79	LYS
1	C	87	THR
1	C	105	ASN
1	C	106	ASP
1	C	109	LEU
1	C	124	ARG
1	C	125	GLU
1	C	126	LEU
1	C	129	LEU
1	C	143	GLU
1	C	157	THR
1	C	160	ARG
1	C	173	LEU
1	C	180	ASP
1	C	181	LEU
1	C	190	VAL
1	C	192	ILE
1	C	197	THR
1	C	198	SER
1	D	43	SER
1	D	91	ASN
1	D	116	GLU
1	D	119	LEU
1	D	129	LEU
1	D	140	THR
1	D	157	THR
1	D	181	LEU
1	D	190	VAL
1	D	193	ASN
1	D	194	SER
1	E	57	LEU
1	E	64	SER

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Mol	Chain	Res	Type
1	E	75	ASP
1	E	88	LEU
1	E	92	SER
1	E	125	GLU
1	E	128	GLN
1	E	144	THR
1	E	155	THR
1	E	162	VAL
1	E	171	THR
1	E	176	ASN
1	E	186	LEU
1	E	195	ARG
1	E	197	THR
1	F	40	SER
1	F	43	SER
1	F	57	LEU
1	F	77	LEU
1	F	83	LEU
1	F	87	THR
1	F	106	ASP
1	F	112	THR
1	F	118	VAL
1	F	121	LEU
1	F	124	ARG
1	F	128	GLN
1	F	129	LEU
1	F	156	GLU
1	F	173	LEU
1	F	176	ASN
1	F	181	LEU
1	F	190	VAL
1	F	193	ASN
1	F	195	ARG
1	F	197	THR
1	G	40	SER
1	G	47	ASN
1	G	50	LEU
1	G	54	SER
1	G	61	THR
1	G	77	LEU
1	G	81	GLN
1	G	94	ASP

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Mol	Chain	Res	Type
1	G	105	ASN
1	G	106	ASP
1	G	107	ASP
1	G	112	THR
1	G	123	LYS
1	G	125	GLU
1	G	152	ASP
1	G	154	THR
1	G	156	GLU
1	G	157	THR
1	G	159	GLU
1	G	160	ARG
1	G	162	VAL
1	G	176	ASN
1	G	186	LEU
1	G	190	VAL
1	H	39	GLN
1	H	46	GLN
1	H	50	LEU
1	H	57	LEU
1	H	68	LYS
1	H	77	LEU
1	H	93	GLU
1	H	105	ASN
1	H	110	GLN
1	H	114	HIS
1	H	123	LYS
1	H	124	ARG
1	H	135	ILE
1	H	152	ASP
1	H	156	GLU
1	H	157	THR
1	H	166	ILE
1	H	180	ASP
1	H	181	LEU
1	H	186	LEU
1	H	192	ILE
1	H	194	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	B	51	ASN
1	B	110	GLN
1	B	128	GLN
1	C	176	ASN
1	C	193	ASN
1	D	47	ASN
1	D	51	ASN
1	D	91	ASN
1	D	193	ASN
1	E	46	GLN
1	E	51	ASN
1	E	110	GLN
1	E	176	ASN
1	E	193	ASN
1	F	39	GLN
1	F	51	ASN
1	F	91	ASN
1	F	128	GLN
1	F	176	ASN
1	G	47	ASN
1	G	81	GLN
1	G	176	ASN
1	H	39	GLN
1	H	81	GLN
1	H	105	ASN
1	H	110	GLN
1	H	128	GLN
1	H	189	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 19 are monoatomic - leaving 13 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
3	ACT	A	12	-	1,3,3	1.96	0	0,3,3	0.00	-
3	ACT	B	1	-	1,3,3	1.41	0	0,3,3	0.00	-
3	ACT	B	13	-	1,3,3	1.20	0	0,3,3	0.00	-
3	ACT	B	9	-	1,3,3	1.34	0	0,3,3	0.00	-
3	ACT	C	6	-	1,3,3	1.56	0	0,3,3	0.00	-
3	ACT	D	11	-	1,3,3	1.87	0	0,3,3	0.00	-
3	ACT	D	2	-	1,3,3	1.84	0	0,3,3	0.00	-
3	ACT	D	8	-	1,3,3	1.91	0	0,3,3	0.00	-
3	ACT	E	14	-	1,3,3	1.49	0	0,3,3	0.00	-
3	ACT	E	4	-	1,3,3	2.21	1 (100%)	0,3,3	0.00	-
3	ACT	E	5	-	1,3,3	1.59	0	0,3,3	0.00	-
3	ACT	G	3	-	1,3,3	1.26	0	0,3,3	0.00	-
3	ACT	H	10	-	1,3,3	1.75	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	A	12	-	-	0/0/0/0	0/0/0/0
3	ACT	B	1	-	-	0/0/0/0	0/0/0/0
3	ACT	B	13	-	-	0/0/0/0	0/0/0/0
3	ACT	B	9	-	-	0/0/0/0	0/0/0/0
3	ACT	C	6	-	-	0/0/0/0	0/0/0/0
3	ACT	D	11	-	-	0/0/0/0	0/0/0/0
3	ACT	D	2	-	-	0/0/0/0	0/0/0/0
3	ACT	D	8	-	-	0/0/0/0	0/0/0/0
3	ACT	E	14	-	-	0/0/0/0	0/0/0/0
3	ACT	E	4	-	-	0/0/0/0	0/0/0/0
3	ACT	E	5	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	G	3	-	-	0/0/0/0	0/0/0/0
3	ACT	H	10	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	ACT	CH3-C	2.21	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	155/177 (87%)	0.83	20 (12%) 5 9	27, 36, 48, 61	0
1	B	157/177 (88%)	1.01	29 (18%) 2 3	26, 37, 47, 54	0
1	C	158/177 (89%)	0.76	20 (12%) 5 9	28, 37, 47, 60	0
1	D	155/177 (87%)	1.09	29 (18%) 2 3	28, 35, 45, 60	0
1	E	157/177 (88%)	1.03	28 (17%) 2 3	28, 37, 48, 57	0
1	F	158/177 (89%)	0.79	17 (10%) 8 13	29, 37, 46, 64	0
1	G	157/177 (88%)	0.90	18 (11%) 6 11	26, 37, 47, 52	0
1	H	156/177 (88%)	0.92	24 (15%) 3 5	28, 37, 49, 64	0
All	All	1253/1416 (88%)	0.92	185 (14%) 3 6	26, 37, 48, 64	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	197	THR	9.3
1	B	197	THR	6.6
1	H	106	ASP	6.0
1	C	39	GLN	5.2
1	C	90	ALA	5.2
1	H	124	ARG	5.0
1	H	38	VAL	4.9
1	B	106	ASP	4.8
1	B	108	GLY	4.8
1	B	196	PHE	4.8
1	D	137	ILE	4.7
1	B	39	GLN	4.7
1	C	106	ASP	4.6
1	H	107	ASP	4.6
1	G	39	GLN	4.6
1	D	102	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	124	ARG	4.5
1	A	39	GLN	4.4
1	D	85	LEU	4.4
1	E	196	PHE	4.4
1	B	128	GLN	4.3
1	G	197	THR	4.2
1	D	135	ILE	4.2
1	A	91	ASN	4.2
1	B	124	ARG	4.1
1	D	100	LEU	4.0
1	D	65	PHE	4.0
1	H	195	ARG	4.0
1	D	136	ALA	3.9
1	D	84	ILE	3.9
1	D	67	ALA	3.9
1	D	101	PHE	3.7
1	H	126	LEU	3.6
1	E	137	ILE	3.6
1	B	107	ASP	3.6
1	G	40	SER	3.5
1	D	186	LEU	3.5
1	A	90	ALA	3.5
1	A	193	ASN	3.5
1	A	195	ARG	3.3
1	G	107	ASP	3.3
1	E	69	ILE	3.3
1	C	91	ASN	3.3
1	G	67	ALA	3.3
1	F	79	LYS	3.3
1	F	196	PHE	3.2
1	D	111	ILE	3.2
1	A	106	ASP	3.2
1	F	197	THR	3.2
1	E	67	ALA	3.2
1	E	65	PHE	3.1
1	D	86	GLY	3.1
1	H	80	ASP	3.1
1	H	159	GLU	3.1
1	E	190	VAL	3.1
1	D	87	THR	3.1
1	C	153	SER	3.1
1	D	69	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	188	ALA	3.0
1	C	197	THR	3.0
1	D	38	VAL	3.0
1	B	65	PHE	3.0
1	E	188	ALA	3.0
1	E	85	LEU	3.0
1	H	105	ASN	3.0
1	B	94	ASP	3.0
1	B	137	ILE	3.0
1	F	137	ILE	3.0
1	B	169	ILE	3.0
1	E	135	ILE	2.9
1	E	193	ASN	2.9
1	A	44	TRP	2.9
1	E	102	VAL	2.9
1	C	95	ALA	2.9
1	H	79	LYS	2.9
1	C	44	TRP	2.9
1	A	123	LYS	2.9
1	G	169	ILE	2.9
1	H	150	GLY	2.9
1	B	80	ASP	2.8
1	F	195	ARG	2.8
1	C	198	SER	2.8
1	D	187	ASN	2.8
1	H	94	ASP	2.8
1	F	39	GLN	2.8
1	B	85	LEU	2.7
1	G	106	ASP	2.7
1	E	39	GLN	2.7
1	F	67	ALA	2.7
1	H	90	ALA	2.7
1	B	190	VAL	2.6
1	A	120	ASP	2.6
1	E	142	ASP	2.6
1	B	97	ALA	2.6
1	D	83	LEU	2.6
1	H	194	SER	2.6
1	H	39	GLN	2.6
1	D	68	LYS	2.6
1	H	123	LYS	2.6
1	G	195	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	159	GLU	2.5
1	E	176	ASN	2.5
1	E	86	GLY	2.5
1	B	141	GLU	2.5
1	F	106	ASP	2.5
1	C	67	ALA	2.5
1	H	122	SER	2.5
1	E	84	ILE	2.5
1	G	128	GLN	2.5
1	E	101	PHE	2.5
1	G	124	ARG	2.4
1	E	136	ALA	2.4
1	E	186	LEU	2.4
1	B	116	GLU	2.4
1	F	80	ASP	2.4
1	B	188	ALA	2.4
1	C	75	ASP	2.4
1	F	65	PHE	2.4
1	H	129	LEU	2.4
1	G	93	GLU	2.4
1	B	67	ALA	2.4
1	D	134	THR	2.4
1	G	97	ALA	2.4
1	E	195	ARG	2.4
1	E	100	LEU	2.3
1	B	126	LEU	2.3
1	G	186	LEU	2.3
1	H	193	ASN	2.3
1	B	68	LYS	2.3
1	A	42	VAL	2.3
1	G	137	ILE	2.3
1	B	193	ASN	2.3
1	B	69	ILE	2.2
1	A	79	LYS	2.2
1	C	94	ASP	2.2
1	F	93	GLU	2.2
1	B	125	GLU	2.2
1	A	122	SER	2.2
1	D	146	ALA	2.2
1	H	110	GLN	2.2
1	E	111	ILE	2.2
1	H	151	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	43	SER	2.2
1	F	91	ASN	2.2
1	D	191	GLU	2.2
1	F	152	ASP	2.2
1	G	168	GLY	2.2
1	G	196	PHE	2.2
1	B	136	ALA	2.2
1	C	152	ASP	2.1
1	D	190	VAL	2.1
1	H	128	GLN	2.1
1	E	187	ASN	2.1
1	F	44	TRP	2.1
1	F	68	LYS	2.1
1	C	80	ASP	2.1
1	D	112	THR	2.1
1	C	187	ASN	2.1
1	A	45	PRO	2.1
1	C	42	VAL	2.1
1	C	79	LYS	2.1
1	D	71	VAL	2.1
1	A	151	ASP	2.1
1	E	128	GLN	2.1
1	A	150	GLY	2.1
1	G	95	ALA	2.1
1	F	69	ILE	2.1
1	D	189	HIS	2.1
1	E	189	HIS	2.1
1	A	128	GLN	2.1
1	B	186	LEU	2.1
1	B	120	ASP	2.1
1	A	194	SER	2.1
1	D	70	PRO	2.1
1	E	87	THR	2.0
1	G	188	ALA	2.0
1	C	123	LYS	2.0
1	H	44	TRP	2.0
1	C	156	GLU	2.0
1	H	91	ASN	2.0
1	D	104	ALA	2.0
1	B	135	ILE	2.0
1	F	135	ILE	2.0
1	E	134	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	182	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
3	ACT	E	5	4/4	0.85	0.36	2.13	71,72,72,72	0
3	ACT	D	8	4/4	0.92	0.18	0.37	51,51,51,51	0
3	ACT	C	6	4/4	0.78	0.23	0.31	68,68,68,68	0
3	ACT	G	3	4/4	0.89	0.13	-1.40	68,68,68,69	0
2	ZN	D	18	1/1	0.81	0.09	-	61,61,61,61	1
2	ZN	D	17	1/1	0.92	0.05	-	59,59,59,59	1
2	ZN	G	5	1/1	0.98	0.16	-	35,35,35,35	0
2	ZN	C	2	1/1	0.99	0.17	-	32,32,32,32	0
3	ACT	D	2	4/4	0.88	0.12	-	50,50,51,51	0
2	ZN	B	8	1/1	0.85	0.08	-	65,65,65,65	0
2	ZN	G	12	1/1	0.97	0.07	-	57,57,57,57	1
3	ACT	H	10	4/4	0.96	0.21	-	52,53,53,53	0
3	ACT	B	1	4/4	0.82	0.20	-	72,73,73,73	0
2	ZN	A	14	1/1	0.84	0.06	-	61,61,61,61	1
2	ZN	D	13	1/1	0.97	0.06	-	65,65,65,65	0
3	ACT	A	12	4/4	0.69	0.22	-	58,58,59,59	0
2	ZN	A	7	1/1	0.98	0.04	-	42,42,42,42	0
2	ZN	D	1	1/1	0.97	0.15	-	29,29,29,29	0
3	ACT	B	13	4/4	0.86	0.19	-	64,65,65,65	0
3	ACT	E	4	4/4	0.76	0.27	-	60,60,60,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ACT	B	9	4/4	0.71	0.28	-	72,72,72,73	0
2	ZN	C	16	1/1	0.85	0.06	-	68,68,68,68	1
2	ZN	E	10	1/1	0.94	0.05	-	53,53,53,53	0
3	ACT	E	14	4/4	0.92	0.11	-	60,61,61,62	0
2	ZN	E	3	1/1	0.99	0.16	-	27,27,27,27	0
2	ZN	F	11	1/1	0.94	0.06	-	48,48,48,48	1
2	ZN	E	19	1/1	0.66	0.12	-	44,44,44,44	1
3	ACT	D	11	4/4	0.81	0.33	-	64,64,65,65	0
2	ZN	F	4	1/1	0.99	0.11	-	35,35,35,35	0
2	ZN	B	15	1/1	0.96	0.06	-	71,71,71,71	0
2	ZN	B	6	1/1	0.98	0.14	-	34,34,34,34	0
2	ZN	E	9	1/1	0.98	0.10	-	45,45,45,45	1

6.5 Other polymers [i](#)

There are no such residues in this entry.