



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2017 – 11:26 AM EDT

PDB ID : 3B6A
Title : Crystal structure of the Streptomyces coelicolor TetR family protein ActR in complex with actinorhodin
Authors : Willems, A.R.; Junop, M.S.
Deposited on : unknown
Resolution : 3.05 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 : rb-20030345
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) : rb-20030345

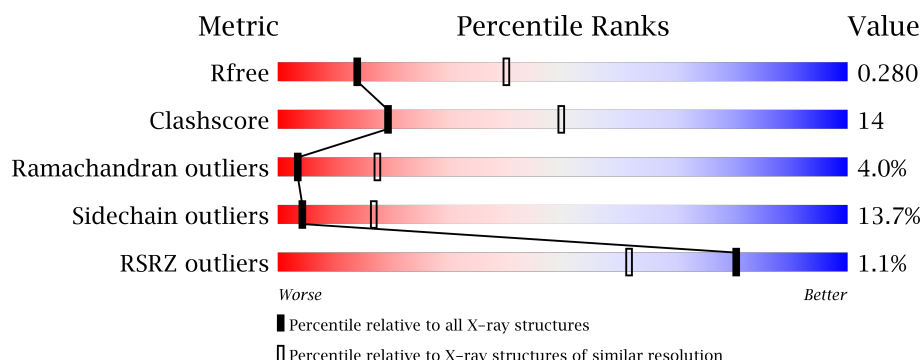
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1348 (3.10-3.02)
Clashscore	112137	1462 (3.10-3.02)
Ramachandran outliers	110173	1410 (3.10-3.02)
Sidechain outliers	110143	1410 (3.10-3.02)
RSRZ outliers	101464	1355 (3.10-3.02)

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	234	<div> <div>2%</div> <div> <div></div> <div>56%</div> <div>30%</div> <div>5%</div> <div>9%</div> </div> </div>
1	B	234	<div> <div>0%</div> <div> <div></div> <div>62%</div> <div>20%</div> <div>7%</div> <div>11%</div> </div> </div>
1	C	234	<div> <div></div> <div> <div></div> <div>56%</div> <div>29%</div> <div>6%</div> <div>9%</div> </div> </div>
1	D	234	<div> <div>0%</div> <div> <div></div> <div>62%</div> <div>21%</div> <div>6%</div> <div>11%</div> </div> </div>
1	E	234	<div> <div>2%</div> <div> <div></div> <div>58%</div> <div>29%</div> <div>5%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	234	
1	G	234	
1	H	234	

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	ZCT	A	1	-	-	-	X
2	ZCT	B	1	-	-	-	X
2	ZCT	C	1	-	-	-	X
2	ZCT	D	1	-	-	-	X
2	ZCT	E	1	-	-	-	X
2	ZCT	F	1	-	-	-	X
2	ZCT	G	1	-	-	-	X
2	ZCT	H	1	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13188 atoms, of which 32 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 ActR protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1616	1012	290	307	7			
1	B	209	Total	C	N	O	S	0	0	0
			1581	993	282	299	7			
1	C	213	Total	C	N	O	S	0	0	0
			1616	1012	290	307	7			
1	D	209	Total	C	N	O	S	0	0	0
			1581	993	282	299	7			
1	E	213	Total	C	N	O	S	0	0	0
			1616	1012	290	307	7			
1	F	209	Total	C	N	O	S	0	0	0
			1581	993	282	299	7			
1	G	213	Total	C	N	O	S	0	0	0
			1616	1012	290	307	7			
1	H	209	Total	C	N	O	S	0	0	0
			1581	993	282	299	7			

There are 32 discrepancies between the modelled and reference sequences:

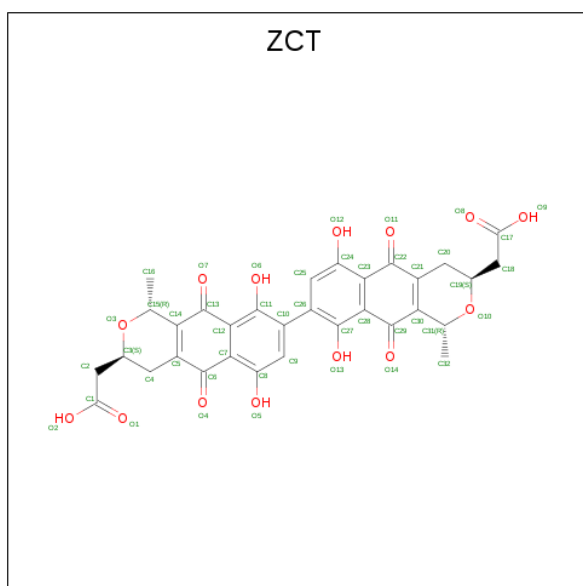
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	EXPRESSION TAG	UNP Q53901
A	27	ALA	-	EXPRESSION TAG	UNP Q53901
A	28	MET	-	EXPRESSION TAG	UNP Q53901
A	29	ALA	-	EXPRESSION TAG	UNP Q53901
B	26	GLY	-	EXPRESSION TAG	UNP Q53901
B	27	ALA	-	EXPRESSION TAG	UNP Q53901
B	28	MET	-	EXPRESSION TAG	UNP Q53901
B	29	ALA	-	EXPRESSION TAG	UNP Q53901
C	26	GLY	-	EXPRESSION TAG	UNP Q53901
C	27	ALA	-	EXPRESSION TAG	UNP Q53901
C	28	MET	-	EXPRESSION TAG	UNP Q53901
C	29	ALA	-	EXPRESSION TAG	UNP Q53901
D	26	GLY	-	EXPRESSION TAG	UNP Q53901

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Chain	Residue	Modelled	Actual	Comment	Reference
D	27	ALA	-	EXPRESSION TAG	UNP Q53901
D	28	MET	-	EXPRESSION TAG	UNP Q53901
D	29	ALA	-	EXPRESSION TAG	UNP Q53901
E	26	GLY	-	EXPRESSION TAG	UNP Q53901
E	27	ALA	-	EXPRESSION TAG	UNP Q53901
E	28	MET	-	EXPRESSION TAG	UNP Q53901
E	29	ALA	-	EXPRESSION TAG	UNP Q53901
F	26	GLY	-	EXPRESSION TAG	UNP Q53901
F	27	ALA	-	EXPRESSION TAG	UNP Q53901
F	28	MET	-	EXPRESSION TAG	UNP Q53901
F	29	ALA	-	EXPRESSION TAG	UNP Q53901
G	26	GLY	-	EXPRESSION TAG	UNP Q53901
G	27	ALA	-	EXPRESSION TAG	UNP Q53901
G	28	MET	-	EXPRESSION TAG	UNP Q53901
G	29	ALA	-	EXPRESSION TAG	UNP Q53901
H	26	GLY	-	EXPRESSION TAG	UNP Q53901
H	27	ALA	-	EXPRESSION TAG	UNP Q53901
H	28	MET	-	EXPRESSION TAG	UNP Q53901
H	29	ALA	-	EXPRESSION TAG	UNP Q53901

- Molecule 2 is 2,2'-[(1R,1'R,3S,3'S)-6,6',9,9'-tetrahydroxy-1,1'-dimethyl-5,5',10,10'-tetraoxo-3,3',4,4',5,5',10,10'-octahydro-1H,1'H-8,8'-bibenzo[g]isochromene-3,3'-diyl]diacetic acid (three-letter code: ZCT) (formula: C₃₂H₂₆O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			50	32	4	14		

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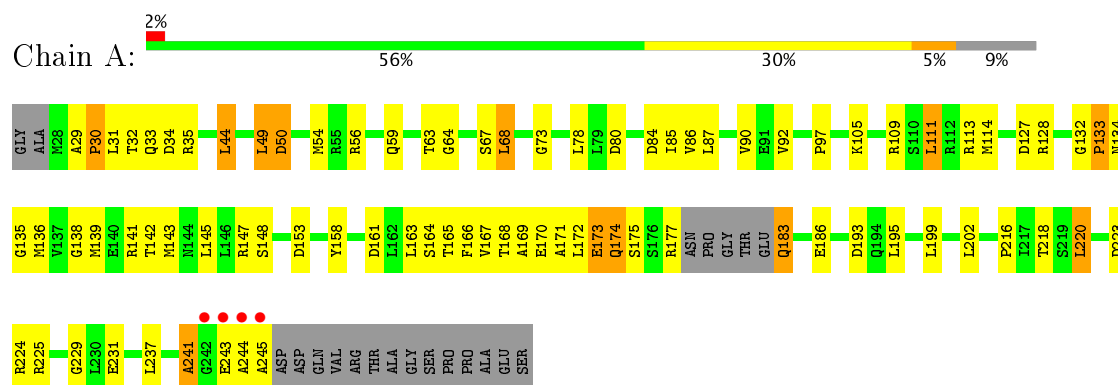
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			50	32	4	14		
2	C	1	Total	C	H	O	0	0
			50	32	4	14		
2	D	1	Total	C	H	O	0	0
			50	32	4	14		
2	E	1	Total	C	H	O	0	0
			50	32	4	14		
2	F	1	Total	C	H	O	0	0
			50	32	4	14		
2	G	1	Total	C	H	O	0	0
			50	32	4	14		
2	H	1	Total	C	H	O	0	0
			50	32	4	14		

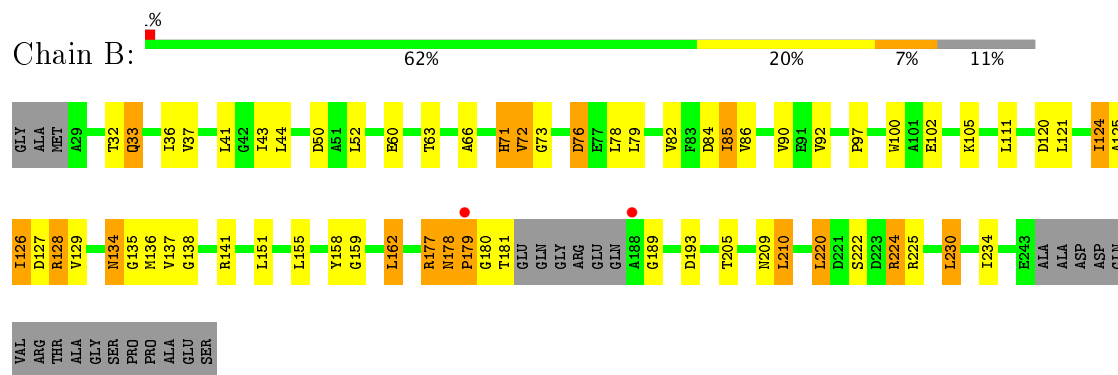
3 Residue-property plots [i](#)

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.

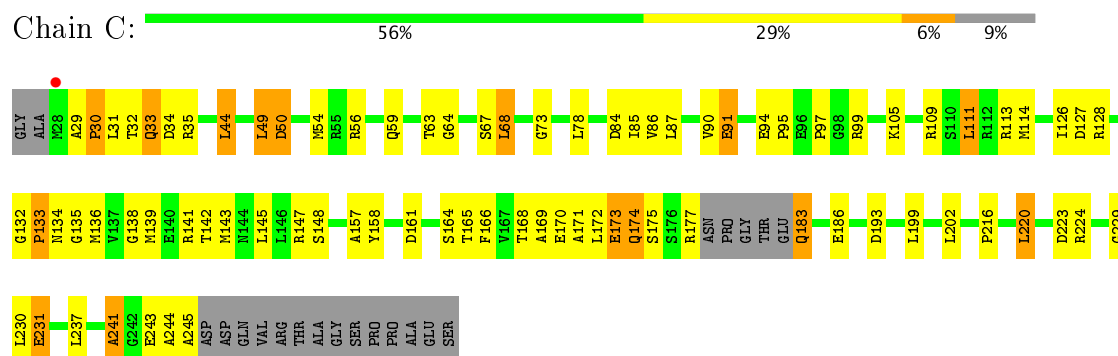
• Molecule 1: ActR protein



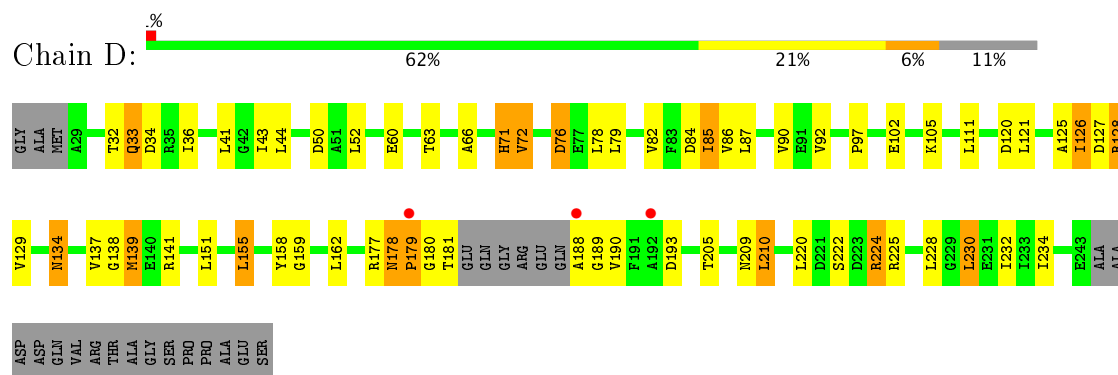
• Molecule 1: ActR protein



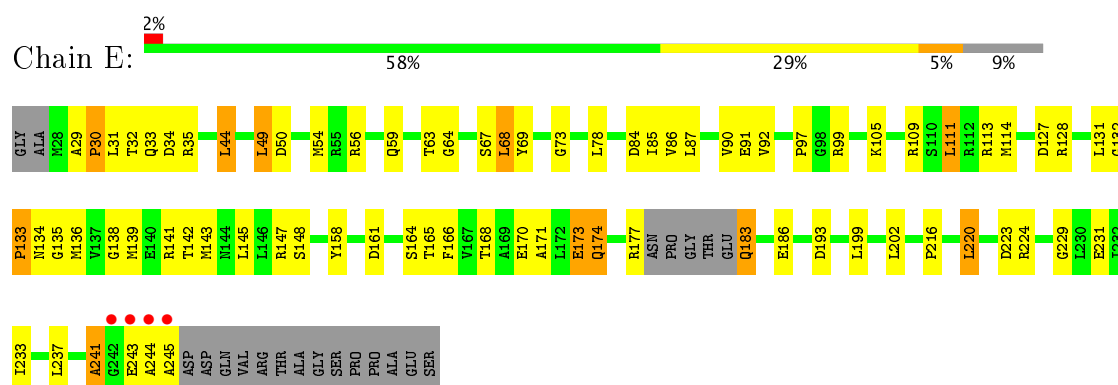
• Molecule 1: ActR protein



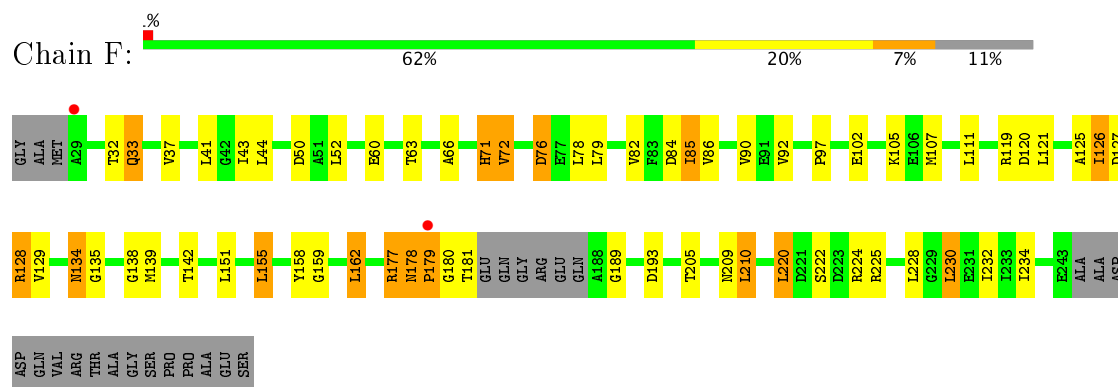
- Molecule 1: ActR protein



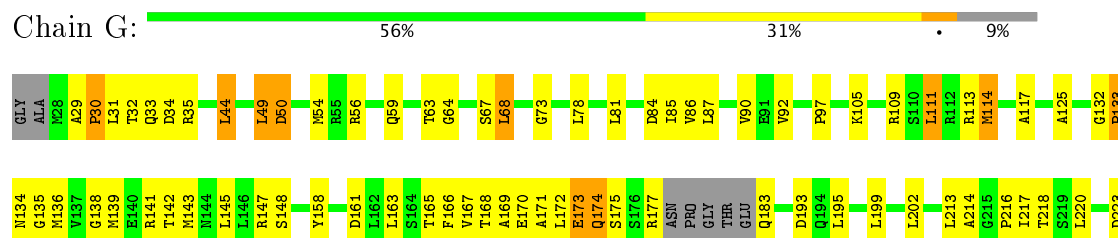
- Molecule 1: ActR protein



- Molecule 1: ActR protein

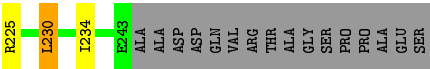


- Molecule 1: ActR protein





● Molecule 1: ActR protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.88Å 79.00Å 107.19Å 89.56° 89.92° 89.88°	Depositor
Resolution (Å)	37.12 – 3.05 31.23 – 3.05	Depositor EDS
% Data completeness (in resolution range)	85.1 (37.12-3.05) 83.9 (31.23-3.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.260 , 0.288 0.262 , 0.280	Depositor DCC
R_{free} test set	961 reflections (3.23%)	DCC
Wilson B-factor (Å ²)	82.7	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.438 for h,-k,-l 0.438 for -h,k,-l 0.439 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13188	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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

5.1 Standard geometry

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

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	0/1640	0.77	1/2220 (0.0%)
1	B	0.62	0/1606	0.75	0/2177
1	C	0.61	0/1640	0.76	1/2220 (0.0%)
1	D	0.60	0/1606	0.75	0/2177
1	E	0.61	0/1640	0.77	1/2220 (0.0%)
1	F	0.61	0/1606	0.75	0/2177
1	G	0.61	0/1640	0.76	0/2220
1	H	0.62	0/1606	0.74	0/2177
All	All	0.61	0/12984	0.76	3/17588 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	LEU	CA-CB-CG	5.33	127.55	115.30
1	C	220	LEU	CA-CB-CG	5.11	127.04	115.30
1	E	111	LEU	CA-CB-CG	5.10	127.04	115.30

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	1616	0	1615	61	0
1	B	1581	0	1584	39	0
1	C	1616	0	1615	62	0
1	D	1581	0	1584	37	0
1	E	1616	0	1615	57	0
1	F	1581	0	1584	34	0
1	G	1616	0	1615	63	0
1	H	1581	0	1584	38	0
2	A	46	4	23	13	0
2	B	46	4	23	9	0
2	C	46	4	23	14	0
2	D	46	4	23	9	0
2	E	46	4	23	12	0
2	F	46	4	23	5	0
2	G	46	4	23	12	0
2	H	46	4	24	6	0
All	All	13156	32	12981	377	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 14.

All (377) 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:87:LEU:HB3	2:E:1:ZCT:C16	1.97	0.94
1:A:87:LEU:HB3	2:A:1:ZCT:C16	1.98	0.92
1:F:90:VAL:O	2:F:1:ZCT:H4	1.69	0.91
1:D:90:VAL:O	2:D:1:ZCT:H2	1.72	0.87
1:G:87:LEU:HB3	2:G:1:ZCT:C16	2.04	0.87
1:C:138:GLY:CA	2:C:1:ZCT:H2A	2.10	0.81
1:B:92:VAL:HG23	2:B:1:ZCT:H4A	1.62	0.79
1:F:151:LEU:HD23	1:F:155:LEU:HB3	1.65	0.79
1:A:29:ALA:HB1	1:A:30:PRO:HD2	1.66	0.78
1:C:84:ASP:OD1	1:C:134:ASN:HB2	1.84	0.78
1:D:151:LEU:HD23	1:D:155:LEU:HB3	1.66	0.77
1:A:87:LEU:HD13	2:A:1:ZCT:H16	1.67	0.77
1:C:138:GLY:HA3	2:C:1:ZCT:H2A	1.64	0.77
1:E:29:ALA:HB1	1:E:30:PRO:HD2	1.67	0.76
1:G:84:ASP:OD1	1:G:134:ASN:HB2	1.86	0.76
1:H:151:LEU:HD23	1:H:155:LEU:HB3	1.68	0.76
1:C:126:ILE:HA	2:C:1:ZCT:H32	1.68	0.75
1:A:142:THR:HG22	1:A:143:MET:CE	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LEU:HD23	1:B:155:LEU:HB3	1.70	0.74
1:D:92:VAL:HG23	2:D:1:ZCT:H4A	1.68	0.74
1:A:141:ARG:HG2	1:A:141:ARG:HH11	1.53	0.74
1:G:29:ALA:HB1	1:G:30:PRO:HD2	1.69	0.73
1:E:84:ASP:OD1	1:E:134:ASN:HB2	1.87	0.73
1:C:142:THR:HG22	1:C:143:MET:CE	2.19	0.73
1:G:142:THR:HG22	1:G:143:MET:CE	2.19	0.73
1:C:29:ALA:HB1	1:C:30:PRO:HD2	1.69	0.72
1:C:111:LEU:HG	2:C:1:ZCT:H16	1.72	0.71
1:G:141:ARG:HH11	1:G:141:ARG:HG2	1.55	0.71
1:D:84:ASP:OD2	1:D:134:ASN:HB2	1.90	0.71
1:F:105:LYS:HD3	1:F:230:LEU:HD13	1.73	0.70
1:B:105:LYS:HD3	1:B:230:LEU:HD13	1.73	0.70
1:B:90:VAL:HB	2:B:1:ZCT:H4	1.74	0.70
1:H:92:VAL:HG23	2:H:1:ZCT:H4A	1.73	0.70
1:H:105:LYS:HD3	1:H:230:LEU:HD13	1.73	0.70
1:A:84:ASP:OD1	1:A:134:ASN:HB2	1.91	0.70
1:F:84:ASP:OD2	1:F:134:ASN:HB2	1.92	0.70
1:H:84:ASP:OD2	1:H:134:ASN:HB2	1.92	0.69
1:B:84:ASP:OD2	1:B:134:ASN:HB2	1.92	0.68
1:E:141:ARG:HG2	1:E:141:ARG:HH11	1.58	0.68
1:C:105:LYS:HD3	1:C:109:ARG:HH11	1.59	0.68
1:D:105:LYS:HD3	1:D:230:LEU:HD13	1.76	0.67
1:C:141:ARG:HG2	1:C:141:ARG:HH11	1.58	0.67
1:H:135:GLY:HA2	2:H:1:ZCT:O7	1.94	0.67
1:G:87:LEU:HB3	2:G:1:ZCT:H16	1.76	0.67
1:E:87:LEU:HD13	2:E:1:ZCT:H16	1.77	0.65
1:C:138:GLY:HA2	2:C:1:ZCT:H2A	1.79	0.64
1:A:105:LYS:HD3	1:A:109:ARG:HH11	1.62	0.64
1:A:44:LEU:HD21	1:A:49:LEU:HA	1.80	0.64
1:E:142:THR:HG22	1:E:143:MET:CE	2.28	0.64
1:A:92:VAL:HG23	2:A:1:ZCT:H4A	1.80	0.64
1:A:90:VAL:HB	2:A:1:ZCT:H4	1.77	0.64
1:A:168:THR:O	1:A:171:ALA:N	2.32	0.63
1:E:105:LYS:HD3	1:E:109:ARG:HH11	1.63	0.63
1:G:92:VAL:HG23	2:G:1:ZCT:H4A	1.80	0.63
1:A:142:THR:HG22	1:A:143:MET:HE1	1.80	0.62
1:H:125:ALA:O	2:H:1:ZCT:H32	1.98	0.62
1:E:87:LEU:HB3	2:E:1:ZCT:H16	1.79	0.62
1:G:90:VAL:HB	2:G:1:ZCT:H4	1.80	0.62
1:A:87:LEU:HB3	2:A:1:ZCT:H16B	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:VAL:HB	2:D:1:ZCT:H4	1.82	0.61
1:B:179:PRO:C	1:B:181:THR:HA	2.21	0.61
1:D:178:ASN:N	1:D:179:PRO:HD3	2.15	0.61
1:G:138:GLY:HA3	2:G:1:ZCT:C15	2.31	0.61
1:E:90:VAL:HB	2:E:1:ZCT:H4	1.83	0.61
1:C:126:ILE:HA	2:C:1:ZCT:C32	2.31	0.60
1:G:132:GLY:O	1:G:135:GLY:N	2.34	0.60
1:C:142:THR:HG22	1:C:143:MET:HE2	1.82	0.60
1:F:178:ASN:N	1:F:179:PRO:HD3	2.16	0.60
1:H:138:GLY:HA3	2:H:1:ZCT:C14	2.31	0.60
1:G:134:ASN:O	2:G:1:ZCT:H15	2.01	0.60
1:E:44:LEU:HD21	1:E:49:LEU:HA	1.83	0.60
1:C:168:THR:O	1:C:171:ALA:N	2.34	0.59
1:E:87:LEU:HB3	2:E:1:ZCT:H16B	1.83	0.59
1:G:139:MET:HB3	1:H:210:LEU:HD11	1.84	0.59
1:G:44:LEU:HD21	1:G:49:LEU:HA	1.85	0.59
1:B:178:ASN:N	1:B:179:PRO:HD3	2.17	0.59
1:F:179:PRO:C	1:F:181:THR:HA	2.23	0.59
1:C:139:MET:HB3	1:D:210:LEU:HD11	1.84	0.59
1:H:178:ASN:N	1:H:179:PRO:HD3	2.18	0.59
1:C:132:GLY:O	1:C:135:GLY:N	2.36	0.59
1:F:82:VAL:O	1:F:86:VAL:HG22	2.03	0.59
1:G:142:THR:HG22	1:G:143:MET:HE3	1.85	0.59
1:G:29:ALA:HB3	1:G:35:ARG:HH12	1.68	0.58
1:D:179:PRO:C	1:D:181:THR:HA	2.23	0.58
1:C:44:LEU:HD21	1:C:49:LEU:HA	1.85	0.58
1:H:179:PRO:C	1:H:181:THR:HA	2.23	0.58
1:G:168:THR:O	1:G:171:ALA:N	2.35	0.58
1:A:145:LEU:O	1:A:148:SER:HB3	2.04	0.58
1:G:142:THR:HG22	1:G:143:MET:HE2	1.85	0.58
1:E:29:ALA:HB3	1:E:35:ARG:HH12	1.68	0.57
1:A:142:THR:HG22	1:A:143:MET:HE2	1.86	0.57
1:E:92:VAL:HG23	2:E:1:ZCT:H4A	1.85	0.57
1:C:29:ALA:HB3	1:C:35:ARG:HH12	1.70	0.57
1:G:105:LYS:HD3	1:G:109:ARG:HH11	1.68	0.57
1:G:87:LEU:HD13	2:G:1:ZCT:H16	1.87	0.57
1:H:82:VAL:O	1:H:86:VAL:HG22	2.04	0.57
1:A:87:LEU:HB3	2:A:1:ZCT:H16	1.86	0.56
1:C:142:THR:HG22	1:C:143:MET:HE3	1.87	0.56
1:E:138:GLY:HA3	2:E:1:ZCT:H15	1.87	0.56
1:G:138:GLY:HA3	2:G:1:ZCT:H15	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:LEU:CD2	1:C:67:SER:HB3	2.35	0.56
1:E:168:THR:O	1:E:171:ALA:N	2.39	0.56
1:A:138:GLY:HA3	2:A:1:ZCT:H15	1.88	0.56
1:B:224:ARG:HD2	1:B:224:ARG:O	2.06	0.56
1:G:147:ARG:HD3	1:H:209:ASN:OD1	2.07	0.55
1:B:128:ARG:O	2:B:1:ZCT:C32	2.54	0.55
1:G:145:LEU:O	1:G:148:SER:HB3	2.05	0.55
1:G:31:LEU:CD2	1:G:67:SER:HB3	2.36	0.55
1:E:166:PHE:CZ	1:E:229:GLY:HA3	2.42	0.55
1:C:165:THR:O	1:C:168:THR:OG1	2.23	0.55
1:G:141:ARG:HG2	1:G:141:ARG:NH1	2.22	0.54
1:A:177:ARG:NH2	1:A:220:LEU:HA	2.23	0.54
1:C:199:LEU:O	1:C:202:LEU:HB2	2.08	0.54
1:E:142:THR:HG22	1:E:143:MET:HE2	1.88	0.54
1:D:71:HIS:N	1:D:71:HIS:CD2	2.76	0.54
1:D:82:VAL:O	1:D:86:VAL:HG22	2.08	0.54
1:G:166:PHE:CZ	1:G:229:GLY:HA3	2.43	0.54
1:A:132:GLY:O	1:A:135:GLY:N	2.41	0.53
1:G:199:LEU:O	1:G:202:LEU:HB2	2.09	0.53
1:A:199:LEU:O	1:A:202:LEU:HB2	2.08	0.53
1:E:145:LEU:O	1:E:148:SER:HB3	2.09	0.53
1:E:31:LEU:CD2	1:E:67:SER:HB3	2.38	0.53
1:E:139:MET:HB3	1:F:210:LEU:HD11	1.89	0.53
1:H:47:GLU:OE2	1:H:56:ARG:NH2	2.31	0.53
1:H:90:VAL:HB	2:H:1:ZCT:H4	1.91	0.53
1:C:166:PHE:CZ	1:C:229:GLY:HA3	2.44	0.53
1:A:31:LEU:CD2	1:A:67:SER:HB3	2.39	0.53
1:E:54:MET:HE2	1:E:73:GLY:O	2.09	0.53
1:C:174:GLN:OE1	1:C:177:ARG:HB2	2.10	0.52
1:F:92:VAL:HG23	2:F:1:ZCT:O4	2.09	0.52
1:A:29:ALA:HB3	1:A:35:ARG:HH12	1.74	0.52
1:B:82:VAL:O	1:B:86:VAL:HG22	2.10	0.52
1:E:199:LEU:O	1:E:202:LEU:HB2	2.09	0.52
1:F:125:ALA:C	1:F:127:ASP:H	2.13	0.52
1:B:71:HIS:N	1:B:71:HIS:CD2	2.77	0.52
1:C:145:LEU:O	1:C:148:SER:HB3	2.09	0.52
1:C:111:LEU:HG	2:C:1:ZCT:C16	2.39	0.52
1:E:158:TYR:CE1	1:F:225:ARG:HB2	2.45	0.52
1:C:63:THR:OG1	1:C:64:GLY:N	2.43	0.52
1:D:138:GLY:HA3	2:D:1:ZCT:C15	2.39	0.52
1:E:177:ARG:NH2	1:E:220:LEU:HA	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:LEU:O	1:C:241:ALA:N	2.33	0.52
1:C:54:MET:HE1	1:C:68:LEU:HD11	1.92	0.51
1:G:32:THR:C	1:G:34:ASP:H	2.14	0.51
1:A:165:THR:O	1:A:168:THR:OG1	2.29	0.51
1:C:147:ARG:HD3	1:D:209:ASN:OD1	2.11	0.51
1:F:71:HIS:N	1:F:71:HIS:CD2	2.79	0.50
1:A:166:PHE:CZ	1:A:229:GLY:HA3	2.47	0.50
1:E:158:TYR:HE1	1:F:225:ARG:HB2	1.77	0.50
1:E:90:VAL:CG1	2:E:1:ZCT:H4	2.42	0.50
1:G:177:ARG:NH2	1:G:220:LEU:HA	2.27	0.50
1:A:87:LEU:CD1	2:A:1:ZCT:H16	2.38	0.50
1:E:54:MET:HE3	1:E:68:LEU:HD21	1.94	0.50
1:G:170:GLU:O	1:G:173:GLU:HB2	2.12	0.49
1:C:141:ARG:NH1	1:C:141:ARG:HG2	2.27	0.49
1:B:125:ALA:C	1:B:127:ASP:H	2.16	0.49
1:B:79:LEU:HB2	1:B:128:ARG:NH1	2.27	0.49
1:C:90:VAL:HG11	2:C:1:ZCT:H16A	1.94	0.49
1:G:132:GLY:O	1:G:133:PRO:C	2.51	0.49
1:G:87:LEU:HB3	2:G:1:ZCT:H16B	1.91	0.49
1:A:63:THR:OG1	1:A:64:GLY:N	2.46	0.48
1:H:71:HIS:CD2	1:H:71:HIS:N	2.81	0.48
1:B:180:GLY:N	1:B:181:THR:HA	2.28	0.48
1:D:137:VAL:O	1:D:141:ARG:HG3	2.12	0.48
1:A:158:TYR:CE1	1:B:225:ARG:HB2	2.48	0.48
1:C:54:MET:CE	1:C:68:LEU:HD11	2.43	0.48
1:E:170:GLU:O	1:E:173:GLU:HB2	2.13	0.48
1:C:113:ARG:HB2	1:C:113:ARG:NH2	2.28	0.48
1:E:174:GLN:OE1	1:E:177:ARG:HB2	2.13	0.48
1:D:79:LEU:HB2	1:D:128:ARG:NH1	2.28	0.48
1:H:230:LEU:HD22	1:H:234:ILE:HD11	1.95	0.48
1:B:138:GLY:HA3	2:B:1:ZCT:C15	2.43	0.48
1:G:158:TYR:O	1:G:161:ASP:HB3	2.14	0.48
1:A:164:SER:HB3	2:A:1:ZCT:H9	1.96	0.48
1:D:125:ALA:C	1:D:127:ASP:H	2.17	0.48
1:E:32:THR:C	1:E:34:ASP:H	2.17	0.48
1:A:113:ARG:NH2	1:A:113:ARG:HB2	2.28	0.48
1:A:174:GLN:OE1	1:A:177:ARG:HB2	2.14	0.48
1:A:237:LEU:O	1:A:241:ALA:N	2.34	0.48
1:H:158:TYR:CE2	1:H:162:LEU:HG	2.49	0.48
1:A:139:MET:HB3	1:B:210:LEU:HD11	1.95	0.47
2:D:1:ZCT:O14	2:D:1:ZCT:H32B	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:ALA:O	2:G:1:ZCT:H32	2.14	0.47
1:C:177:ARG:NH2	1:C:220:LEU:HA	2.29	0.47
1:E:237:LEU:O	1:E:241:ALA:N	2.32	0.47
1:F:138:GLY:HA3	2:F:1:ZCT:C13	2.44	0.47
1:F:139:MET:HB2	1:F:139:MET:HE3	1.81	0.47
1:F:135:GLY:HA2	2:F:1:ZCT:O7	2.14	0.47
1:C:138:GLY:HA2	2:C:1:ZCT:C2	2.43	0.47
1:D:230:LEU:HD22	1:D:234:ILE:HD11	1.95	0.47
1:D:180:GLY:N	1:D:181:THR:HA	2.29	0.47
1:G:54:MET:HE2	1:G:73:GLY:O	2.14	0.47
1:A:32:THR:C	1:A:34:ASP:H	2.17	0.47
1:A:34:ASP:OD2	1:D:34:ASP:HB2	2.14	0.47
1:G:134:ASN:HB3	2:G:1:ZCT:H16A	1.97	0.47
1:G:84:ASP:O	1:G:134:ASN:ND2	2.47	0.47
1:D:76:ASP:HA	1:D:79:LEU:HD12	1.97	0.47
1:E:164:SER:HB3	2:E:1:ZCT:H9	1.96	0.47
1:F:180:GLY:N	1:F:181:THR:HA	2.29	0.47
1:F:79:LEU:HB2	1:F:128:ARG:NH1	2.29	0.47
1:A:141:ARG:HG2	1:A:141:ARG:NH1	2.21	0.47
1:C:32:THR:C	1:C:34:ASP:H	2.18	0.47
1:E:132:GLY:O	1:E:135:GLY:N	2.47	0.47
1:G:138:GLY:HA3	2:G:1:ZCT:C14	2.45	0.47
1:B:78:LEU:O	1:B:82:VAL:HG23	2.15	0.47
1:C:158:TYR:O	1:C:161:ASP:HB3	2.15	0.47
1:E:141:ARG:HG2	1:E:141:ARG:NH1	2.27	0.46
1:A:163:LEU:O	1:A:167:VAL:HG23	2.15	0.46
1:F:228:LEU:O	1:F:232:ILE:HD12	2.15	0.46
1:A:138:GLY:HA3	2:A:1:ZCT:C15	2.45	0.46
1:B:76:ASP:HA	1:B:79:LEU:HD12	1.97	0.46
1:G:54:MET:HE1	1:G:68:LEU:HD11	1.96	0.46
1:F:105:LYS:HE2	1:F:234:ILE:CD1	2.46	0.46
1:H:125:ALA:C	1:H:127:ASP:H	2.18	0.46
1:E:54:MET:CE	1:E:68:LEU:HD11	2.46	0.46
1:G:63:THR:OG1	1:G:64:GLY:N	2.49	0.46
1:A:158:TYR:HE1	1:B:225:ARG:HB2	1.81	0.46
1:A:80:ASP:OD1	1:A:128:ARG:NE	2.42	0.46
1:C:170:GLU:O	1:C:173:GLU:HB2	2.16	0.46
1:C:158:TYR:CE1	1:D:225:ARG:HB2	2.51	0.46
1:H:158:TYR:O	1:H:159:GLY:C	2.52	0.46
1:H:180:GLY:N	1:H:181:THR:HA	2.30	0.46
1:A:134:ASN:HB3	2:A:1:ZCT:H16A	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:GLN:HG2	1:E:33:GLN:O	2.16	0.45
1:E:147:ARG:HD3	1:F:209:ASN:OD1	2.16	0.45
1:D:43:ILE:HD11	1:D:52:LEU:HD13	1.99	0.45
1:E:113:ARG:NH2	1:E:113:ARG:HB2	2.30	0.45
1:A:54:MET:CE	1:A:68:LEU:HD11	2.47	0.45
1:D:86:VAL:HG21	1:D:121:LEU:HD21	1.99	0.45
1:G:111:LEU:O	1:G:114:MET:HB3	2.17	0.45
1:G:174:GLN:OE1	1:G:177:ARG:HB2	2.17	0.45
1:A:195:LEU:HD23	1:A:218:THR:HG22	1.99	0.45
1:G:163:LEU:O	1:G:167:VAL:HG23	2.17	0.45
1:B:71:HIS:O	1:B:73:GLY:N	2.45	0.45
1:C:87:LEU:HD23	1:C:87:LEU:HA	1.77	0.45
1:B:128:ARG:O	2:B:1:ZCT:H32A	2.16	0.45
1:A:54:MET:HE1	1:A:68:LEU:HD11	1.99	0.45
1:C:164:SER:HG	2:C:1:ZCT:C27	2.30	0.44
1:H:78:LEU:O	1:H:82:VAL:HG23	2.17	0.44
1:B:90:VAL:O	2:B:1:ZCT:H2	2.17	0.44
1:A:147:ARG:HD3	1:B:209:ASN:OD1	2.17	0.44
1:E:127:ASP:O	1:E:128:ARG:HG2	2.18	0.44
1:G:50:ASP:OD2	1:G:50:ASP:N	2.50	0.44
1:G:56:ARG:O	1:G:59:GLN:HB3	2.17	0.44
1:B:86:VAL:HG21	1:B:121:LEU:HD21	1.99	0.44
1:A:54:MET:HE2	1:A:73:GLY:O	2.17	0.44
1:A:56:ARG:O	1:A:59:GLN:HB3	2.18	0.44
1:B:33:GLN:HA	1:B:36:ILE:HD12	2.00	0.44
1:C:132:GLY:O	1:C:133:PRO:C	2.55	0.44
1:C:230:LEU:O	1:C:231:GLU:C	2.55	0.44
1:F:43:ILE:HD11	1:F:52:LEU:HD13	1.99	0.44
1:H:82:VAL:O	1:H:85:ILE:HG22	2.17	0.44
1:B:230:LEU:HD22	1:B:234:ILE:HD11	1.99	0.44
1:G:165:THR:O	1:G:168:THR:OG1	2.33	0.44
2:D:1:ZCT:C32	2:D:1:ZCT:O14	2.65	0.44
1:A:44:LEU:CD2	1:A:49:LEU:HA	2.47	0.44
1:F:230:LEU:HD22	1:F:234:ILE:HD11	2.00	0.44
1:C:56:ARG:O	1:C:59:GLN:HB3	2.18	0.44
1:H:137:VAL:O	1:H:141:ARG:HG3	2.18	0.44
1:C:33:GLN:HG2	1:C:33:GLN:O	2.18	0.44
1:G:158:TYR:CE1	1:H:225:ARG:HB2	2.53	0.44
1:B:125:ALA:O	2:B:1:ZCT:H32	2.18	0.43
1:E:158:TYR:O	1:E:161:ASP:HB3	2.17	0.43
1:F:125:ALA:O	1:F:127:ASP:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:MET:CE	1:G:68:LEU:HD11	2.47	0.43
1:D:33:GLN:HA	1:D:36:ILE:HD12	2.01	0.43
1:F:78:LEU:O	1:F:82:VAL:HG23	2.18	0.43
1:H:33:GLN:O	1:H:37:VAL:HG13	2.18	0.43
1:B:158:TYR:CE2	1:B:162:LEU:HG	2.53	0.43
1:D:82:VAL:O	1:D:85:ILE:HG22	2.18	0.43
1:H:128:ARG:O	2:H:1:ZCT:H32A	2.18	0.43
1:F:76:ASP:HA	1:F:79:LEU:HD12	2.00	0.43
1:F:158:TYR:O	1:F:159:GLY:C	2.56	0.43
1:H:79:LEU:HB2	1:H:128:ARG:NH1	2.34	0.43
1:H:224:ARG:HD2	1:H:224:ARG:O	2.19	0.43
1:E:105:LYS:HD3	1:E:109:ARG:NH1	2.32	0.43
1:G:243:GLU:O	1:G:245:ALA:N	2.51	0.43
1:A:168:THR:O	1:A:169:ALA:C	2.56	0.43
1:C:94:GLU:HG3	1:C:95:PRO:HD2	2.01	0.43
1:E:229:GLY:O	1:E:233:ILE:HG12	2.19	0.43
1:B:158:TYR:O	1:B:159:GLY:C	2.57	0.42
1:A:158:TYR:O	1:A:161:ASP:HB3	2.18	0.42
1:E:131:LEU:HA	1:E:131:LEU:HD12	1.86	0.42
1:E:165:THR:O	1:E:168:THR:OG1	2.32	0.42
1:E:90:VAL:O	2:E:1:ZCT:H2	2.19	0.42
1:A:33:GLN:HG2	1:A:33:GLN:O	2.19	0.42
1:A:50:ASP:N	1:A:50:ASP:OD2	2.51	0.42
1:G:214:ALA:O	1:G:218:THR:OG1	2.31	0.42
1:C:44:LEU:CD2	1:C:49:LEU:HA	2.49	0.42
1:C:54:MET:HE2	1:C:73:GLY:O	2.19	0.42
1:E:29:ALA:HB3	1:E:35:ARG:NH1	2.33	0.42
1:A:84:ASP:O	1:A:134:ASN:ND2	2.49	0.42
1:C:142:THR:CB	2:C:1:ZCT:O4	2.67	0.42
1:E:183:GLN:HE21	1:E:186:GLU:HB2	1.83	0.42
1:G:87:LEU:HD23	1:G:87:LEU:HA	1.70	0.42
1:H:76:ASP:HA	1:H:79:LEU:HD12	2.02	0.42
1:E:63:THR:OG1	1:E:64:GLY:N	2.53	0.42
1:E:87:LEU:HD23	1:E:87:LEU:HA	1.76	0.42
1:F:33:GLN:O	1:F:37:VAL:HG13	2.19	0.42
1:G:229:GLY:O	1:G:233:ILE:HG12	2.20	0.42
1:H:43:ILE:HD11	1:H:52:LEU:HD13	2.02	0.42
1:A:132:GLY:O	1:A:133:PRO:C	2.58	0.42
2:C:1:ZCT:O13	2:C:1:ZCT:O14	2.38	0.42
1:A:127:ASP:O	1:A:128:ARG:HG2	2.20	0.42
1:A:183:GLN:HE21	1:A:186:GLU:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:LYS:HE2	1:H:234:ILE:CD1	2.49	0.42
1:B:128:ARG:O	2:B:1:ZCT:H32B	2.20	0.42
1:C:168:THR:O	1:C:169:ALA:C	2.58	0.42
1:C:90:VAL:HG11	2:C:1:ZCT:C16	2.50	0.42
1:D:224:ARG:HD2	1:D:224:ARG:O	2.19	0.42
1:D:78:LEU:O	1:D:82:VAL:HG23	2.20	0.42
1:G:195:LEU:HD23	1:G:218:THR:HG22	2.02	0.42
1:H:104:VAL:O	1:H:107:MET:HB3	2.19	0.42
1:E:138:GLY:HA3	2:E:1:ZCT:C15	2.50	0.42
1:E:44:LEU:CD2	1:E:49:LEU:HA	2.50	0.42
1:E:56:ARG:O	1:E:59:GLN:HB3	2.20	0.42
1:H:158:TYR:HE2	1:H:162:LEU:HG	1.84	0.42
1:H:172:LEU:HA	1:H:172:LEU:HD12	1.90	0.42
1:D:228:LEU:O	1:D:232:ILE:HD12	2.19	0.41
1:C:105:LYS:HD3	1:C:109:ARG:NH1	2.31	0.41
2:C:1:ZCT:C4	2:C:1:ZCT:H16B	2.49	0.41
1:C:99:ARG:HD3	1:G:117:ALA:HA	2.01	0.41
1:E:90:VAL:CB	2:E:1:ZCT:H4	2.48	0.41
1:G:213:LEU:O	1:G:217:ILE:HD12	2.20	0.41
1:A:243:GLU:O	1:A:245:ALA:N	2.53	0.41
1:B:43:ILE:HD11	1:B:52:LEU:HD13	2.02	0.41
1:D:92:VAL:CG2	2:D:1:ZCT:H4A	2.44	0.41
1:F:107:MET:SD	1:F:142:THR:HG23	2.61	0.41
1:F:177:ARG:NH1	1:F:220:LEU:O	2.54	0.41
1:H:94:GLU:HA	1:H:95:PRO:HD3	1.92	0.41
1:B:124:ILE:HG23	1:B:128:ARG:HD2	2.03	0.41
1:F:138:GLY:HA3	2:F:1:ZCT:C14	2.50	0.41
1:D:87:LEU:HB3	2:D:1:ZCT:C16	2.51	0.41
1:G:113:ARG:HB2	1:G:113:ARG:NH2	2.34	0.41
1:B:82:VAL:O	1:B:85:ILE:HG22	2.20	0.41
1:D:158:TYR:O	1:D:159:GLY:C	2.56	0.41
1:F:82:VAL:O	1:F:85:ILE:HG22	2.21	0.41
1:A:170:GLU:O	1:A:173:GLU:HB2	2.21	0.41
1:F:119:ARG:O	1:F:121:LEU:N	2.54	0.41
1:G:168:THR:O	1:G:169:ALA:C	2.59	0.41
1:G:32:THR:C	1:G:34:ASP:N	2.75	0.41
1:G:54:MET:HE3	1:G:68:LEU:HD21	2.03	0.41
1:B:177:ARG:NH1	1:B:220:LEU:O	2.54	0.41
1:C:183:GLN:HE21	1:C:186:GLU:HB2	1.85	0.41
1:C:90:VAL:HG12	1:C:91:GLU:N	2.35	0.41
1:C:158:TYR:HE1	1:D:225:ARG:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:THR:O	1:G:34:ASP:N	2.53	0.41
1:C:172:LEU:O	1:C:175:SER:HB3	2.21	0.41
1:D:87:LEU:HB3	2:D:1:ZCT:H16B	2.03	0.41
1:B:125:ALA:O	1:B:127:ASP:N	2.50	0.41
1:D:125:ALA:O	1:D:127:ASP:N	2.53	0.41
1:E:243:GLU:O	1:E:245:ALA:N	2.54	0.41
1:C:243:GLU:O	1:C:245:ALA:N	2.54	0.40
1:C:50:ASP:N	1:C:50:ASP:OD2	2.55	0.40
1:D:188:ALA:C	1:D:190:VAL:N	2.75	0.40
1:E:132:GLY:O	1:E:133:PRO:C	2.59	0.40
1:E:99:ARG:HB3	1:E:99:ARG:HH21	1.86	0.40
1:A:134:ASN:O	2:A:1:ZCT:H15	2.20	0.40
1:B:137:VAL:O	1:B:141:ARG:HG3	2.22	0.40
1:C:127:ASP:O	1:C:128:ARG:HG2	2.21	0.40
1:D:188:ALA:C	1:D:190:VAL:H	2.24	0.40
1:G:44:LEU:CD2	1:G:49:LEU:HA	2.51	0.40
1:H:177:ARG:NH1	1:H:220:LEU:O	2.53	0.40
1:E:69:TYR:CD1	1:E:73:GLY:HA2	2.54	0.40
1:G:81:LEU:HA	1:G:81:LEU:HD23	1.93	0.40
1:G:158:TYR:HE1	1:H:225:ARG:HB2	1.86	0.40
1:A:220:LEU:H	1:A:220:LEU:HD23	1.86	0.40
1:B:135:GLY:HA2	2:B:1:ZCT:O7	2.21	0.40
1:F:158:TYR:CE2	1:F:162:LEU:HG	2.56	0.40
1:H:152:HIS:O	1:H:153:ASP:C	2.59	0.40
1:A:172:LEU:O	1:A:175:SER:HB3	2.21	0.40
1:A:90:VAL:CB	2:A:1:ZCT:H4	2.50	0.40
1:B:33:GLN:O	1:B:37:VAL:HG13	2.21	0.40
1:C:237:LEU:HA	1:C:237:LEU:HD23	1.93	0.40
1:C:31:LEU:HD22	1:C:67:SER:HB3	2.04	0.40
1:D:139:MET:HB2	1:D:139:MET:HE3	1.99	0.40
1:G:172:LEU:O	1:G:175:SER:HB3	2.22	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	209/234 (89%)	176 (84%)	26 (12%)	7 (3%)	4	21
1	B	205/234 (88%)	173 (84%)	22 (11%)	10 (5%)	2	14
1	C	209/234 (89%)	173 (83%)	28 (13%)	8 (4%)	4	19
1	D	205/234 (88%)	173 (84%)	23 (11%)	9 (4%)	3	15
1	E	209/234 (89%)	169 (81%)	34 (16%)	6 (3%)	5	25
1	F	205/234 (88%)	176 (86%)	20 (10%)	9 (4%)	3	15
1	G	209/234 (89%)	172 (82%)	30 (14%)	7 (3%)	4	21
1	H	205/234 (88%)	177 (86%)	17 (8%)	11 (5%)	2	12
All	All	1656/1872 (88%)	1389 (84%)	200 (12%)	67 (4%)	3	17

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	ALA
1	B	72	VAL
1	B	126	ILE
1	C	241	ALA
1	D	72	VAL
1	D	126	ILE
1	E	241	ALA
1	F	126	ILE
1	G	241	ALA
1	H	72	VAL
1	H	126	ILE
1	A	244	ALA
1	B	178	ASN
1	C	244	ALA
1	D	178	ASN
1	E	244	ALA
1	F	72	VAL
1	F	120	ASP
1	F	178	ASN
1	G	244	ALA
1	H	178	ASN
1	A	97	PRO
1	C	30	PRO
1	C	33	GLN

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Mol	Chain	Res	Type
1	C	97	PRO
1	E	30	PRO
1	E	97	PRO
1	G	30	PRO
1	G	33	GLN
1	G	97	PRO
1	H	120	ASP
1	H	155	LEU
1	H	189	GLY
1	A	30	PRO
1	B	120	ASP
1	B	189	GLY
1	D	120	ASP
1	D	189	GLY
1	E	216	PRO
1	F	155	LEU
1	F	189	GLY
1	A	153	ASP
1	A	216	PRO
1	B	66	ALA
1	B	100	TRP
1	C	157	ALA
1	D	97	PRO
1	D	155	LEU
1	E	133	PRO
1	F	66	ALA
1	G	216	PRO
1	H	66	ALA
1	H	97	PRO
1	H	154	GLU
1	A	133	PRO
1	C	216	PRO
1	D	66	ALA
1	F	97	PRO
1	G	133	PRO
1	H	87	LEU
1	B	97	PRO
1	C	133	PRO
1	B	124	ILE
1	H	179	PRO
1	B	179	PRO
1	D	179	PRO

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Mol	Chain	Res	Type
1	F	179	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/184 (91%)	148 (89%)	19 (11%)	7	24
1	B	165/184 (90%)	138 (84%)	27 (16%)	2	10
1	C	167/184 (91%)	149 (89%)	18 (11%)	7	27
1	D	165/184 (90%)	138 (84%)	27 (16%)	2	10
1	E	167/184 (91%)	148 (89%)	19 (11%)	7	24
1	F	165/184 (90%)	139 (84%)	26 (16%)	3	11
1	G	167/184 (91%)	150 (90%)	17 (10%)	8	29
1	H	165/184 (90%)	136 (82%)	29 (18%)	2	9
All	All	1328/1472 (90%)	1146 (86%)	182 (14%)	4	17

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	49	LEU
1	A	50	ASP
1	A	68	LEU
1	A	78	LEU
1	A	85	ILE
1	A	86	VAL
1	A	111	LEU
1	A	114	MET
1	A	136	MET
1	A	173	GLU
1	A	174	GLN
1	A	183	GLN
1	A	193	ASP

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Mol	Chain	Res	Type
1	A	220	LEU
1	A	223	ASP
1	A	224	ARG
1	A	225	ARG
1	A	231	GLU
1	B	32	THR
1	B	33	GLN
1	B	41	LEU
1	B	44	LEU
1	B	50	ASP
1	B	60	GLU
1	B	63	THR
1	B	71	HIS
1	B	72	VAL
1	B	76	ASP
1	B	85	ILE
1	B	102	GLU
1	B	111	LEU
1	B	126	ILE
1	B	128	ARG
1	B	129	VAL
1	B	134	ASN
1	B	136	MET
1	B	162	LEU
1	B	177	ARG
1	B	193	ASP
1	B	205	THR
1	B	210	LEU
1	B	220	LEU
1	B	222	SER
1	B	224	ARG
1	B	230	LEU
1	C	44	LEU
1	C	49	LEU
1	C	50	ASP
1	C	68	LEU
1	C	78	LEU
1	C	85	ILE
1	C	86	VAL
1	C	91	GLU
1	C	111	LEU
1	C	114	MET

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Mol	Chain	Res	Type
1	C	136	MET
1	C	173	GLU
1	C	174	GLN
1	C	183	GLN
1	C	193	ASP
1	C	223	ASP
1	C	224	ARG
1	C	231	GLU
1	D	32	THR
1	D	33	GLN
1	D	41	LEU
1	D	44	LEU
1	D	50	ASP
1	D	60	GLU
1	D	63	THR
1	D	71	HIS
1	D	72	VAL
1	D	76	ASP
1	D	85	ILE
1	D	102	GLU
1	D	111	LEU
1	D	126	ILE
1	D	128	ARG
1	D	129	VAL
1	D	134	ASN
1	D	139	MET
1	D	162	LEU
1	D	177	ARG
1	D	193	ASP
1	D	205	THR
1	D	210	LEU
1	D	220	LEU
1	D	222	SER
1	D	224	ARG
1	D	230	LEU
1	E	44	LEU
1	E	49	LEU
1	E	50	ASP
1	E	68	LEU
1	E	78	LEU
1	E	85	ILE
1	E	86	VAL

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Mol	Chain	Res	Type
1	E	91	GLU
1	E	111	LEU
1	E	114	MET
1	E	136	MET
1	E	173	GLU
1	E	174	GLN
1	E	183	GLN
1	E	193	ASP
1	E	220	LEU
1	E	223	ASP
1	E	224	ARG
1	E	231	GLU
1	F	32	THR
1	F	33	GLN
1	F	41	LEU
1	F	44	LEU
1	F	50	ASP
1	F	60	GLU
1	F	63	THR
1	F	71	HIS
1	F	72	VAL
1	F	76	ASP
1	F	85	ILE
1	F	102	GLU
1	F	111	LEU
1	F	126	ILE
1	F	128	ARG
1	F	129	VAL
1	F	134	ASN
1	F	162	LEU
1	F	177	ARG
1	F	193	ASP
1	F	205	THR
1	F	210	LEU
1	F	220	LEU
1	F	222	SER
1	F	224	ARG
1	F	230	LEU
1	G	44	LEU
1	G	49	LEU
1	G	50	ASP
1	G	68	LEU

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Mol	Chain	Res	Type
1	G	78	LEU
1	G	85	ILE
1	G	86	VAL
1	G	111	LEU
1	G	114	MET
1	G	136	MET
1	G	173	GLU
1	G	174	GLN
1	G	183	GLN
1	G	193	ASP
1	G	223	ASP
1	G	224	ARG
1	G	231	GLU
1	H	32	THR
1	H	33	GLN
1	H	41	LEU
1	H	44	LEU
1	H	50	ASP
1	H	60	GLU
1	H	63	THR
1	H	71	HIS
1	H	72	VAL
1	H	76	ASP
1	H	85	ILE
1	H	102	GLU
1	H	111	LEU
1	H	123	ARG
1	H	126	ILE
1	H	128	ARG
1	H	129	VAL
1	H	134	ASN
1	H	136	MET
1	H	139	MET
1	H	162	LEU
1	H	177	ARG
1	H	193	ASP
1	H	205	THR
1	H	210	LEU
1	H	220	LEU
1	H	222	SER
1	H	224	ARG
1	H	230	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	183	GLN
1	B	71	HIS
1	B	134	ASN
1	C	118	HIS
1	C	183	GLN
1	D	71	HIS
1	D	134	ASN
1	E	118	HIS
1	E	183	GLN
1	F	71	HIS
1	F	134	ASN
1	G	118	HIS
1	G	183	GLN
1	H	71	HIS
1	H	134	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ZCT	A	1	-	45,51,51	3.00	2 (4%)	60,80,80	1.31	8 (13%)
2	ZCT	B	1	-	45,51,51	3.23	5 (11%)	60,80,80	1.26	10 (16%)
2	ZCT	C	1	-	45,51,51	2.94	5 (11%)	60,80,80	1.78	12 (20%)
2	ZCT	D	1	-	45,51,51	3.17	4 (8%)	60,80,80	1.47	8 (13%)
2	ZCT	E	1	-	45,51,51	2.92	4 (8%)	60,80,80	1.50	13 (21%)
2	ZCT	F	1	-	45,51,51	3.17	5 (11%)	60,80,80	1.21	7 (11%)
2	ZCT	G	1	-	45,51,51	3.06	6 (13%)	60,80,80	1.33	7 (11%)
2	ZCT	H	1	-	45,51,51	3.14	5 (11%)	60,80,80	1.54	11 (18%)

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	ZCT	A	1	-	-	0/8/76/76	0/6/6/6
2	ZCT	B	1	-	-	0/8/76/76	0/6/6/6
2	ZCT	C	1	-	-	0/8/76/76	0/6/6/6
2	ZCT	D	1	-	-	0/8/76/76	0/6/6/6
2	ZCT	E	1	-	-	0/8/76/76	0/6/6/6
2	ZCT	F	1	-	-	0/8/76/76	0/6/6/6
2	ZCT	G	1	-	-	0/8/76/76	0/6/6/6
2	ZCT	H	1	-	-	0/8/76/76	0/6/6/6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	ZCT	C15-C14	-3.08	1.46	1.51
2	E	1	ZCT	C31-C30	-2.51	1.47	1.51
2	G	1	ZCT	C31-C30	-2.35	1.47	1.51
2	H	1	ZCT	C31-C30	-2.31	1.48	1.51
2	D	1	ZCT	C14-C13	2.01	1.51	1.47
2	G	1	ZCT	C23-C22	2.02	1.51	1.46
2	C	1	ZCT	C2-C3	2.03	1.55	1.52
2	H	1	ZCT	C14-C13	2.05	1.51	1.47
2	E	1	ZCT	C14-C13	2.09	1.51	1.47
2	G	1	ZCT	C18-C19	2.10	1.55	1.52
2	D	1	ZCT	C7-C6	2.14	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	ZCT	C14-C13	2.24	1.52	1.47
2	B	1	ZCT	C20-C21	2.24	1.54	1.51
2	H	1	ZCT	C12-C13	2.26	1.52	1.46
2	B	1	ZCT	C23-C22	2.29	1.52	1.46
2	F	1	ZCT	C7-C6	2.30	1.52	1.46
2	C	1	ZCT	C4-C5	2.36	1.54	1.51
2	B	1	ZCT	C7-C6	2.40	1.52	1.46
2	F	1	ZCT	C23-C22	2.45	1.52	1.46
2	F	1	ZCT	C12-C13	2.65	1.53	1.46
2	C	1	ZCT	C14-C5	11.90	1.47	1.34
2	E	1	ZCT	C14-C5	12.59	1.47	1.34
2	F	1	ZCT	C14-C5	12.81	1.48	1.34
2	A	1	ZCT	C14-C5	12.98	1.48	1.34
2	G	1	ZCT	C14-C5	13.41	1.48	1.34
2	E	1	ZCT	C30-C21	13.44	1.48	1.34
2	H	1	ZCT	C14-C5	13.46	1.48	1.34
2	G	1	ZCT	C30-C21	13.68	1.49	1.34
2	B	1	ZCT	C14-C5	13.84	1.49	1.34
2	A	1	ZCT	C30-C21	13.90	1.49	1.34
2	D	1	ZCT	C30-C21	13.93	1.49	1.34
2	C	1	ZCT	C30-C21	13.95	1.49	1.34
2	D	1	ZCT	C14-C5	14.28	1.49	1.34
2	H	1	ZCT	C30-C21	14.53	1.50	1.34
2	B	1	ZCT	C30-C21	14.60	1.50	1.34
2	F	1	ZCT	C30-C21	15.24	1.50	1.34

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	ZCT	C15-C14-C5	-6.75	114.33	121.70
2	D	1	ZCT	C31-C30-C21	-5.71	115.46	121.70
2	C	1	ZCT	C16-C15-C14	-4.95	106.10	112.55
2	G	1	ZCT	C15-C14-C5	-4.02	117.31	121.70
2	E	1	ZCT	C15-C14-C5	-3.79	117.56	121.70
2	G	1	ZCT	C32-C31-C30	-3.76	107.65	112.55
2	H	1	ZCT	C10-C26-C27	-3.67	115.56	121.93
2	E	1	ZCT	C10-C11-C12	-3.58	117.69	121.43
2	A	1	ZCT	C15-C14-C5	-3.50	117.88	121.70
2	B	1	ZCT	C31-C30-C21	-3.17	118.24	121.70
2	A	1	ZCT	C10-C26-C27	-3.12	116.51	121.93
2	H	1	ZCT	C31-C30-C21	-3.05	118.37	121.70
2	E	1	ZCT	C32-C31-C30	-3.01	108.62	112.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	ZCT	C10-C26-C27	-2.99	116.73	121.93
2	C	1	ZCT	C10-C26-C27	-2.97	116.78	121.93
2	D	1	ZCT	C26-C27-C28	-2.96	118.34	121.43
2	H	1	ZCT	C26-C27-C28	-2.93	118.36	121.43
2	C	1	ZCT	C10-C11-C12	-2.93	118.37	121.43
2	G	1	ZCT	C10-C11-C12	-2.69	118.62	121.43
2	G	1	ZCT	C10-C26-C27	-2.59	117.43	121.93
2	B	1	ZCT	C10-C26-C27	-2.52	117.55	121.93
2	A	1	ZCT	C32-C31-C30	-2.51	109.27	112.55
2	E	1	ZCT	C9-C10-C26	-2.51	112.57	119.01
2	H	1	ZCT	O4-C6-C7	-2.41	117.28	121.94
2	A	1	ZCT	C8-C7-C6	-2.40	117.90	121.44
2	C	1	ZCT	C26-C25-C24	-2.39	117.77	121.06
2	B	1	ZCT	C26-C27-C28	-2.38	118.95	121.43
2	E	1	ZCT	O7-C13-C12	-2.34	117.43	121.94
2	F	1	ZCT	O7-C13-C14	-2.34	117.09	120.73
2	H	1	ZCT	C32-C31-C30	-2.23	109.64	112.55
2	E	1	ZCT	C8-C7-C6	-2.22	118.17	121.44
2	C	1	ZCT	O4-C6-C7	-2.21	117.67	121.94
2	A	1	ZCT	C10-C11-C12	-2.18	119.15	121.43
2	G	1	ZCT	C9-C8-C7	-2.14	118.45	120.99
2	E	1	ZCT	C26-C25-C24	-2.13	118.14	121.06
2	B	1	ZCT	O7-C13-C12	-2.10	117.88	121.94
2	F	1	ZCT	C15-C14-C5	-2.09	119.41	121.70
2	D	1	ZCT	O7-C13-C12	-2.08	117.93	121.94
2	E	1	ZCT	C31-C30-C21	-2.06	119.45	121.70
2	E	1	ZCT	C9-C8-C7	-2.06	118.56	120.99
2	C	1	ZCT	O7-C13-C12	-2.03	118.02	121.94
2	A	1	ZCT	C7-C6-C5	2.02	121.34	118.36
2	G	1	ZCT	C4-C5-C6	2.02	122.72	118.50
2	B	1	ZCT	O3-C3-C4	2.04	113.31	109.50
2	E	1	ZCT	C23-C22-C21	2.07	121.42	118.36
2	C	1	ZCT	C23-C28-C29	2.08	123.40	119.68
2	G	1	ZCT	C19-O10-C31	2.11	116.16	112.69
2	B	1	ZCT	C3-O3-C15	2.13	116.20	112.69
2	B	1	ZCT	C12-C13-C14	2.14	122.06	118.67
2	B	1	ZCT	C25-C26-C27	2.15	121.17	118.46
2	B	1	ZCT	C4-C5-C6	2.15	123.00	118.50
2	D	1	ZCT	C9-C10-C11	2.17	121.19	118.46
2	F	1	ZCT	C4-C5-C6	2.24	123.17	118.50
2	C	1	ZCT	C25-C26-C27	2.24	121.28	118.46
2	B	1	ZCT	C7-C6-C5	2.28	121.73	118.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	ZCT	C9-C10-C11	2.30	121.35	118.46
2	A	1	ZCT	C23-C22-C21	2.32	121.79	118.36
2	H	1	ZCT	C7-C6-C5	2.32	121.79	118.36
2	D	1	ZCT	O10-C19-C20	2.33	113.85	109.50
2	D	1	ZCT	C19-O10-C31	2.37	116.59	112.69
2	F	1	ZCT	C12-C13-C14	2.58	122.76	118.67
2	H	1	ZCT	C9-C10-C11	2.65	121.79	118.46
2	E	1	ZCT	O3-C3-C2	2.75	113.82	107.22
2	F	1	ZCT	C7-C6-C5	2.79	122.49	118.36
2	C	1	ZCT	C7-C6-C5	2.85	122.57	118.36
2	H	1	ZCT	C19-O10-C31	2.86	117.40	112.69
2	D	1	ZCT	O10-C19-C18	2.90	114.17	107.22
2	A	1	ZCT	C19-O10-C31	2.90	117.47	112.69
2	E	1	ZCT	C26-C10-C11	2.98	127.11	121.93
2	F	1	ZCT	C19-O10-C31	3.17	117.92	112.69
2	C	1	ZCT	C4-C5-C6	3.28	125.36	118.50
2	D	1	ZCT	C25-C26-C27	3.33	122.65	118.46
2	H	1	ZCT	C3-O3-C15	3.34	118.20	112.69
2	H	1	ZCT	C25-C26-C27	3.36	122.68	118.46
2	H	1	ZCT	O3-C3-C4	3.39	115.84	109.50
2	F	1	ZCT	C3-O3-C15	3.54	118.53	112.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	ZCT	13	0
2	B	1	ZCT	9	0
2	C	1	ZCT	14	0
2	D	1	ZCT	9	0
2	E	1	ZCT	12	0
2	F	1	ZCT	5	0
2	G	1	ZCT	12	0
2	H	1	ZCT	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	213/234 (91%)	-0.17	4 (1%)	67 44	41, 57, 80, 90	1 (0%)
1	B	209/234 (89%)	-0.17	2 (0%)	82 64	44, 57, 81, 95	0
1	C	213/234 (91%)	-0.23	1 (0%)	90 78	42, 55, 72, 83	1 (0%)
1	D	209/234 (89%)	-0.06	3 (1%)	75 54	44, 58, 84, 97	0
1	E	213/234 (91%)	-0.18	4 (1%)	67 44	42, 57, 78, 88	1 (0%)
1	F	209/234 (89%)	-0.13	2 (0%)	82 64	44, 58, 82, 94	0
1	G	213/234 (91%)	-0.16	1 (0%)	90 78	44, 57, 74, 82	1 (0%)
1	H	209/234 (89%)	-0.11	2 (0%)	82 64	43, 58, 82, 97	0
All	All	1688/1872 (90%)	-0.15	19 (1%)	80 61	41, 57, 80, 97	4 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	243	GLU	4.2
1	F	29	ALA	3.9
1	H	179	PRO	3.7
1	B	179	PRO	3.5
1	A	243	GLU	3.0
1	D	179	PRO	2.9
1	G	243	GLU	2.9
1	D	188	ALA	2.9
1	B	188	ALA	2.6
1	C	28	MET	2.6
1	A	242	GLY	2.6
1	F	179	PRO	2.5
1	E	244	ALA	2.5
1	E	245	ALA	2.3
1	E	242	GLY	2.3
1	H	188	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	192	ALA	2.2
1	A	245	ALA	2.1
1	A	244	ALA	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
2	ZCT	B	1	46/46	0.50	0.57	6.34	90,90,90,90	0
2	ZCT	F	1	46/46	0.62	0.54	6.03	90,90,90,90	0
2	ZCT	H	1	46/46	0.61	0.46	5.18	90,90,90,90	0
2	ZCT	E	1	46/46	0.65	0.41	4.64	90,90,90,90	0
2	ZCT	D	1	46/46	0.59	0.48	4.56	90,90,90,90	0
2	ZCT	G	1	46/46	0.61	0.42	3.68	90,90,90,90	0
2	ZCT	A	1	46/46	0.70	0.37	3.00	90,90,90,90	0
2	ZCT	C	1	46/46	0.73	0.36	2.79	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.