



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:35 PM GMT

PDB ID : 3ZWY
Title : Crystal structure of ADP-ribosyl cyclase complexed with 8-bromo-ADP- ribose and cyclic 8-bromo-cyclic-ADP-ribose
Authors : Kotaka, M.; Graeff, R.; Zhang, L.H.; Lee, H.C.; Hao, Q.
Deposited on : 2011-08-03
Resolution : 2.40 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

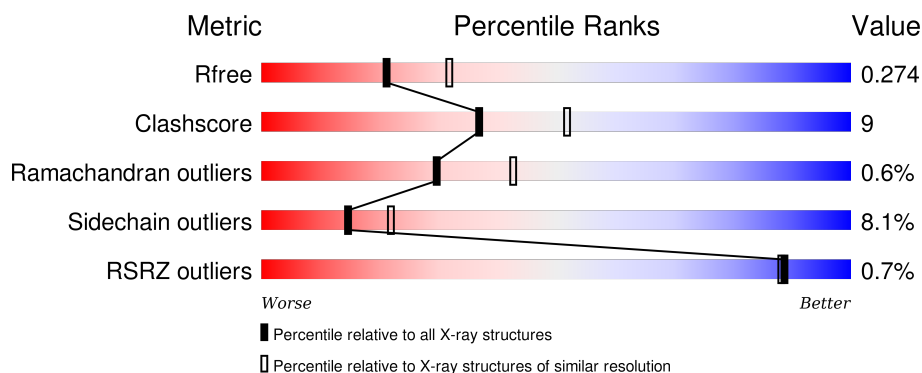
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



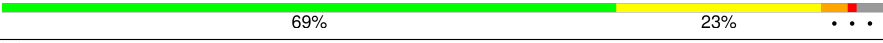


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	260	<div> <div>73%</div> <div>20%</div> <div>• •</div> </div>
1	B	260	<div> <div>77%</div> <div>18%</div> <div>• •</div> </div>
1	C	260	<div> <div>70%</div> <div>25%</div> <div>• •</div> </div>
1	D	260	<div> <div>75%</div> <div>20%</div> <div>• •</div> </div>
1	E	260	<div> <div>73%</div> <div>20%</div> <div>• •</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	260	
1	G	260	
1	H	260	

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	AV1	A	1682	-	-	-	X
2	AV1	C	1682	-	-	-	X
2	AV1	F	1682	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16759 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 ADP-RIBOSYL CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			2012	1288	342	368	14			
1	B	252	Total	C	N	O	S	0	0	0
			2017	1291	343	369	14			
1	C	252	Total	C	N	O	S	0	0	0
			2017	1291	343	369	14			
1	D	252	Total	C	N	O	S	0	0	0
			2017	1291	343	369	14			
1	E	251	Total	C	N	O	S	0	0	0
			2012	1288	342	368	14			
1	F	251	Total	C	N	O	S	0	0	0
			2012	1288	342	368	14			
1	G	251	Total	C	N	O	S	0	0	0
			2012	1288	342	368	14			
1	H	251	Total	C	N	O	S	0	0	0
			2012	1288	342	368	14			

There are 16 discrepancies between the modelled and reference sequences:

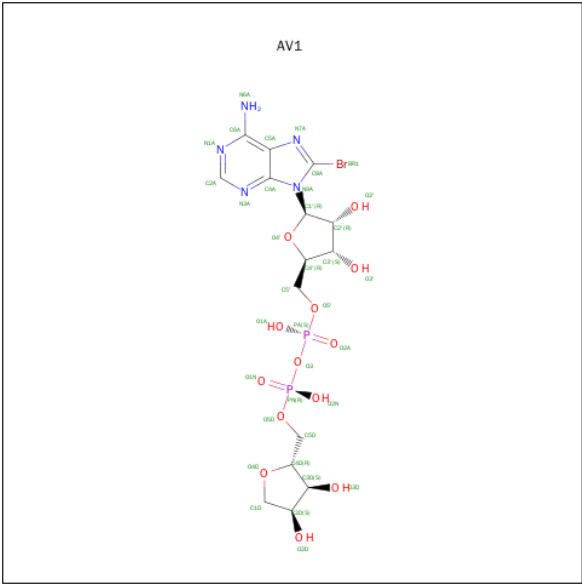
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	EXPRESSION TAG	UNP P29241
A	0	ALA	-	EXPRESSION TAG	UNP P29241
B	-1	ALA	-	EXPRESSION TAG	UNP P29241
B	0	ALA	-	EXPRESSION TAG	UNP P29241
C	-1	ALA	-	EXPRESSION TAG	UNP P29241
C	0	ALA	-	EXPRESSION TAG	UNP P29241
D	-1	ALA	-	EXPRESSION TAG	UNP P29241
D	0	ALA	-	EXPRESSION TAG	UNP P29241
E	-1	ALA	-	EXPRESSION TAG	UNP P29241
E	0	ALA	-	EXPRESSION TAG	UNP P29241
F	-1	ALA	-	EXPRESSION TAG	UNP P29241
F	0	ALA	-	EXPRESSION TAG	UNP P29241
G	-1	ALA	-	EXPRESSION TAG	UNP P29241

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	ALA	-	EXPRESSION TAG	UNP P29241
H	-1	ALA	-	EXPRESSION TAG	UNP P29241
H	0	ALA	-	EXPRESSION TAG	UNP P29241

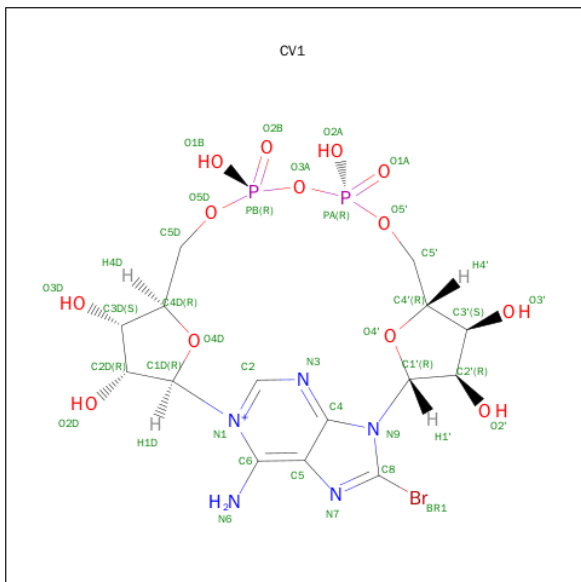
- Molecule 2 is [(2R,3S,4R,5R)-5-(6-AMINO-8-BROMO-9H-PURIN-9-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHYL [(2R,3S,4S)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHYL DIHYDROGEN DIPHOSPHATE (three-letter code: AV1) (formula: C₁₅H₂₂BrN₅O₁₃P₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	Br	C	N	O	P			
2	A	1	Total 36	Br 1	C 15	N 5	O 13	P 2		0	0
2	B	1	Total 36	Br 1	C 15	N 5	O 13	P 2		0	0
2	C	1	Total 36	Br 1	C 15	N 5	O 13	P 2		0	0
2	E	1	Total 36	Br 1	C 15	N 5	O 13	P 2		0	0
2	F	1	Total 36	Br 1	C 15	N 5	O 13	P 2		0	0
2	G	1	Total 36	Br 1	C 15	N 5	O 13	P 2		0	0
2	H	1	Total 36	Br 1	C 15	N 5	O 13	P 2		0	0

- Molecule 3 is (2R,3R,4S,5R,13R,14S,15R,16R)-24-AMINO-18-BROMO-3,4,14,15-TETRAHYDROXY-7,9,11,25,26-PENTAOXA-17,19,22-TRIAZA-1-AZONIA-8,10-DIPHOSPHAPEN

TACYCLO[18.3.1.1^{2,5}.1^{13,16}.0^{17,21}]HEXACOSA-1(24),18,20,22-TETRAENE-8,10-DIOLATE 8,10-DIOXIDE (three-letter code: CV1) (formula: C₁₅H₂₁BrN₅O₁₃P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	Br	C	N	O	P	
			36	1	15	5	13	2	

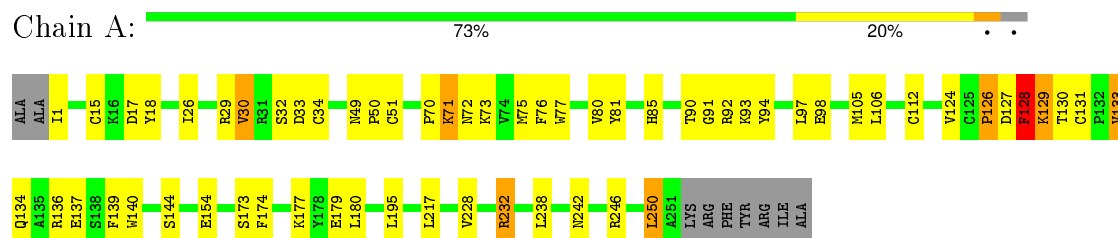
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O		
			41	41	0	0
4	B	61	Total	O		
			61	61	0	0
4	C	60	Total	O		
			60	60	0	0
4	D	52	Total	O		
			52	52	0	0
4	E	50	Total	O		
			50	50	0	0
4	F	34	Total	O		
			34	34	0	0
4	G	41	Total	O		
			41	41	0	0
4	H	21	Total	O		
			21	21	0	0

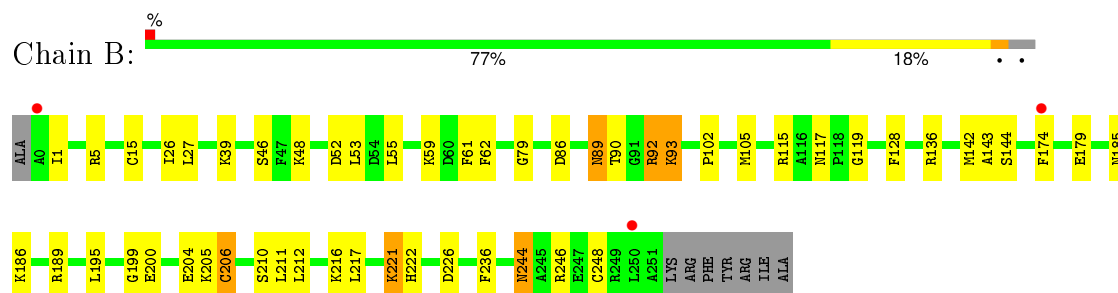
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

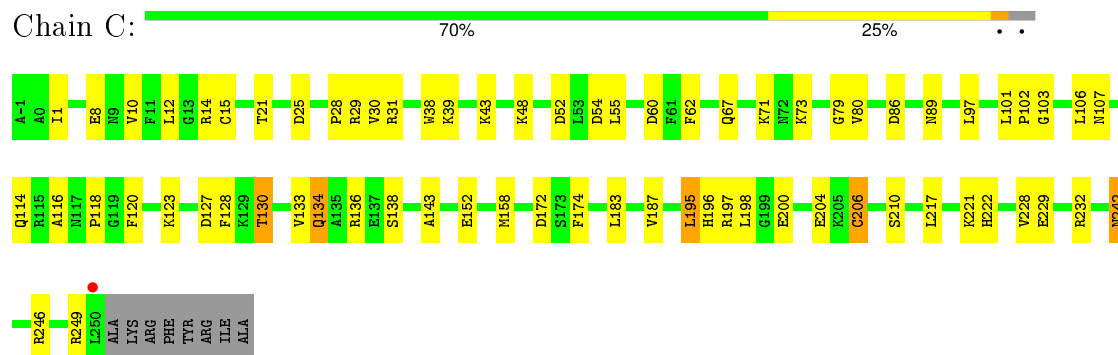
• Molecule 1: ADP-RIBOSYL CYCLASE



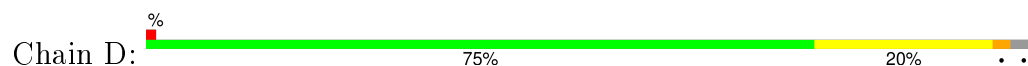
• Molecule 1: ADP-RIBOSYL CYCLASE

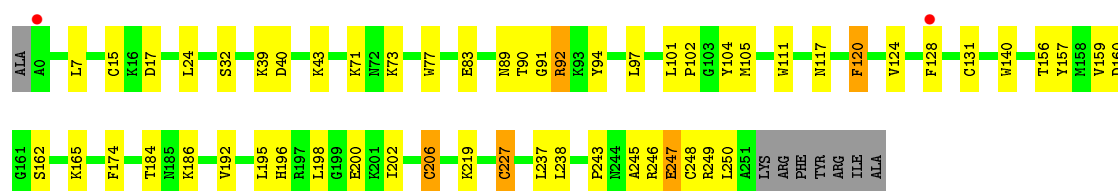


• Molecule 1: ADP-RIBOSYL CYCLASE

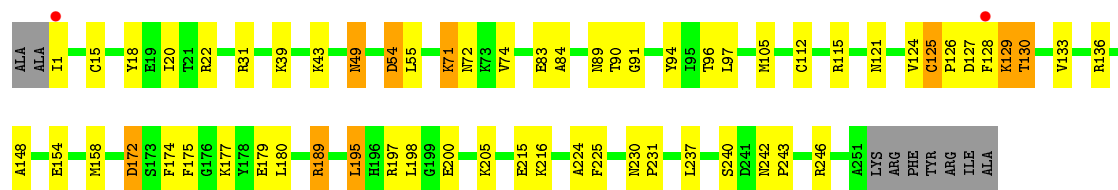
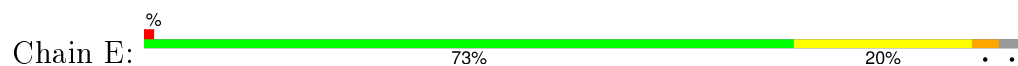


• Molecule 1: ADP-RIBOSYL CYCLASE

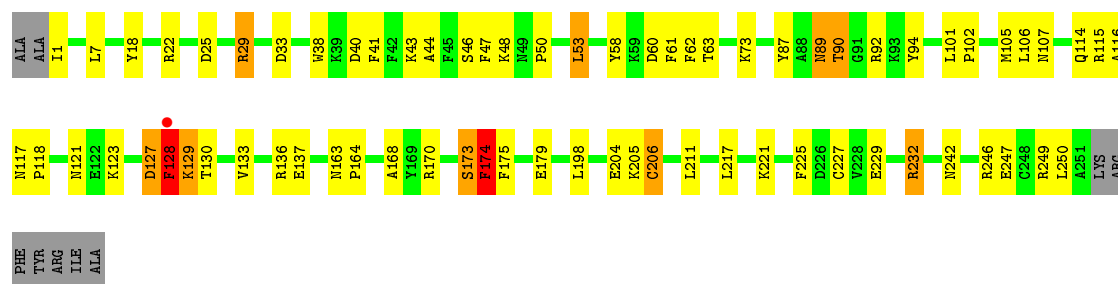




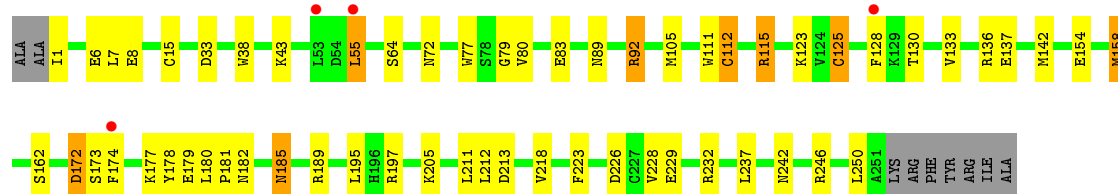
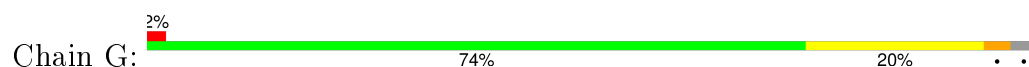
• Molecule 1: ADP-RIBOSYL CYCLASE



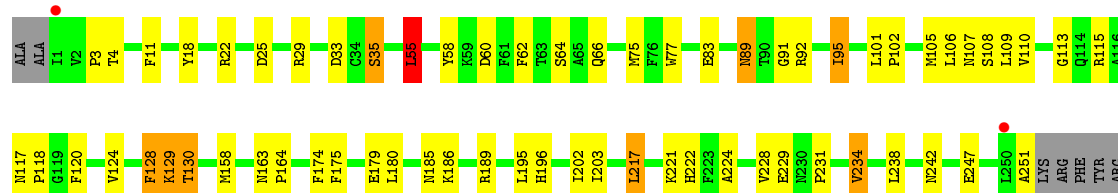
• Molecule 1: ADP-RIBOSYL CYCLASE



• Molecule 1: ADP-RIBOSYL CYCLASE



• Molecule 1: ADP-RIBOSYL CYCLASE



TLE
ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.29Å 77.01Å 140.34Å 87.50° 89.27° 88.99°	Depositor
Resolution (Å)	30.00 – 2.40 26.25 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.4 (30.00-2.40) 91.2 (26.25-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.215 , 0.283 0.209 , 0.274	Depositor DCC
R_{free} test set	4730 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.099 for h,-k,-l 0.014 for -h,k,-l 0.011 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 94865 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16759	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: AV1, CV1

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	0.92	0/2064	0.88	1/2793 (0.0%)
1	B	1.02	2/2069 (0.1%)	0.94	2/2800 (0.1%)
1	C	0.98	1/2069 (0.0%)	0.94	3/2800 (0.1%)
1	D	0.95	1/2069 (0.0%)	0.91	3/2800 (0.1%)
1	E	0.97	2/2064 (0.1%)	0.94	3/2793 (0.1%)
1	F	0.74	1/2064 (0.0%)	0.82	1/2793 (0.0%)
1	G	0.90	0/2064	0.87	3/2793 (0.1%)
1	H	0.74	0/2064	0.77	0/2793
All	All	0.91	7/16527 (0.0%)	0.88	16/22365 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	125	CYS	CB-SG	-8.17	1.68	1.82
1	D	104	TYR	CE1-CZ	5.70	1.46	1.38
1	F	48	LYS	CD-CE	5.59	1.65	1.51
1	B	248	CYS	CB-SG	5.49	1.91	1.82
1	B	206	CYS	CB-SG	5.22	1.91	1.82
1	C	15	CYS	CB-SG	-5.17	1.73	1.81
1	E	174	PHE	CE1-CZ	5.05	1.47	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	125	CYS	CA-CB-SG	-15.08	86.85	114.00
1	G	125	CYS	CA-CB-SG	-8.87	98.04	114.00
1	D	17	ASP	CB-CG-OD1	7.99	125.49	118.30
1	C	29	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	E	195	LEU	CB-CG-CD2	-7.00	99.10	111.00
1	D	160	ASP	CB-CG-OD1	6.23	123.91	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	206	CYS	CA-CB-SG	-6.03	103.15	114.00
1	C	86	ASP	CB-CG-OD1	5.77	123.49	118.30
1	C	206	CYS	CA-CB-SG	5.76	124.36	114.00
1	B	53	LEU	CA-CB-CG	5.75	128.51	115.30
1	G	55	LEU	CB-CG-CD1	5.69	120.67	111.00
1	G	172	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	E	54	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	86	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	206	CYS	N-CA-CB	-5.18	101.28	110.60
1	A	17	ASP	CB-CG-OD1	5.08	122.87	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	2012	0	1968	36	0
1	B	2017	0	1973	28	0
1	C	2017	0	1973	47	0
1	D	2017	0	1973	34	0
1	E	2012	0	1968	41	0
1	F	2012	0	1968	43	0
1	G	2012	0	1968	43	0
1	H	2012	0	1968	41	0
2	A	36	0	20	3	0
2	B	36	0	20	4	0
2	C	36	0	20	1	0
2	E	36	0	20	1	0
2	F	36	0	20	3	0
2	G	36	0	20	3	0
2	H	36	0	20	2	0
3	D	36	0	19	4	0
4	A	41	0	0	2	0
4	B	61	0	0	2	0
4	C	60	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	52	0	0	3	0
4	E	50	0	0	6	0
4	F	34	0	0	7	0
4	G	41	0	0	4	0
4	H	21	0	0	1	0
All	All	16759	0	15918	304	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 9.

All (304) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:128:PHE:O	1:G:136:ARG:HD3	1.52	1.09
1:C:127:ASP:O	1:C:130:THR:HG22	1.56	1.06
1:E:121:ASN:OD1	1:E:124:VAL:O	1.77	1.02
1:F:33:ASP:HB3	4:F:2009:HOH:O	1.58	1.02
1:D:198:LEU:HD22	1:D:247:GLU:HG3	1.39	1.02
1:C:128:PHE:O	1:C:136:ARG:HD3	1.64	0.96
1:A:129:LYS:H	1:A:129:LYS:HZ1	1.18	0.90
1:G:128:PHE:O	1:G:136:ARG:CD	2.18	0.90
1:C:127:ASP:O	1:C:130:THR:CG2	2.19	0.89
1:G:1:ILE:HG22	1:G:125:CYS:O	1.74	0.87
1:G:80:VAL:HG21	1:G:158:MET:HG2	1.56	0.87
1:C:128:PHE:O	1:C:136:ARG:CD	2.23	0.86
1:A:127:ASP:O	1:A:130:THR:HG22	1.77	0.85
1:C:133:VAL:HB	1:G:177:LYS:HB2	1.61	0.81
1:A:129:LYS:NZ	1:A:129:LYS:H	1.78	0.81
1:D:97:LEU:HD23	3:D:303:CV1:N6	1.97	0.79
1:G:115:ARG:HH11	1:G:115:ARG:HG2	1.47	0.79
1:D:198:LEU:CD2	1:D:247:GLU:HG3	2.13	0.78
1:F:174:PHE:CD1	2:F:1682:AV1:O1N	2.35	0.78
1:G:115:ARG:CG	1:G:115:ARG:HH11	1.96	0.78
1:D:97:LEU:HD23	3:D:303:CV1:HN6	1.51	0.73
1:H:89:ASN:OD1	1:H:92:ARG:HD3	1.90	0.71
1:H:107:ASN:OD1	2:H:1682:AV1:H2A	1.93	0.69
1:F:43:LYS:N	4:F:2010:HOH:O	2.22	0.68
1:C:80:VAL:HG21	1:C:158:MET:HG2	1.76	0.68
1:G:83:GLU:HG2	1:G:195:LEU:HD21	1.76	0.68
1:A:195:LEU:HD11	1:A:238:LEU:HD21	1.77	0.66
1:D:246:ARG:O	1:D:249:ARG:HD3	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:180:LEU:HD21	1:H:217:LEU:HD22	1.77	0.66
1:G:133:VAL:HA	1:G:136:ARG:HG3	1.79	0.64
1:F:40:ASP:O	4:F:2011:HOH:O	2.15	0.64
1:C:134:GLN:HG2	1:G:55:LEU:HD23	1.80	0.64
1:F:41:PHE:C	4:F:2010:HOH:O	2.36	0.63
1:E:49:ASN:HB2	4:E:2012:HOH:O	1.97	0.63
1:B:92:ARG:HH22	1:B:93:LYS:NZ	1.96	0.63
1:F:43:LYS:HA	1:F:46:SER:HG	1.64	0.63
1:E:128:PHE:O	1:E:136:ARG:CD	2.48	0.62
2:E:1682:AV1:BR1	2:E:1682:AV1:O4'	2.72	0.62
1:E:125:CYS:SG	1:E:126:PRO:HD2	2.39	0.62
1:H:107:ASN:O	1:H:108:SER:HB2	1.98	0.62
1:C:134:GLN:HG2	1:G:55:LEU:CD2	2.30	0.62
1:E:128:PHE:O	1:E:136:ARG:HD2	1.98	0.62
1:A:85:HIS:NE2	1:A:98:GLU:OE1	2.32	0.62
1:B:204:GLU:OE2	1:B:210:SER:OG	2.11	0.61
1:D:117:ASN:ND2	4:D:2029:HOH:O	2.31	0.61
1:D:174:PHE:HB2	3:D:303:CV1:O5D	2.00	0.61
1:D:198:LEU:HD22	1:D:247:GLU:CG	2.22	0.61
1:H:77:TRP:O	2:H:1682:AV1:H5DA	1.99	0.61
1:F:1:ILE:N	4:F:2001:HOH:O	2.12	0.61
1:H:33:ASP:OD2	1:H:35:SER:HB2	2.01	0.61
1:D:157:TYR:CE2	1:D:159:VAL:HG11	2.36	0.60
1:A:30:VAL:HG13	4:A:2012:HOH:O	2.00	0.60
1:B:128:PHE:HD2	1:B:136:ARG:HA	1.66	0.60
1:C:174:PHE:HZ	4:C:2050:HOH:O	1.84	0.60
1:H:117:ASN:OD1	1:H:118:PRO:HA	2.01	0.60
1:C:118:PRO:HB2	1:C:120:PHE:CE1	2.35	0.59
1:C:79:GLY:N	2:C:1682:AV1:O1A	2.33	0.59
1:F:127:ASP:O	1:F:129:LYS:HE2	2.02	0.59
1:E:133:VAL:HA	1:E:136:ARG:HG3	1.83	0.59
1:F:107:ASN:OD1	2:F:1682:AV1:H2A	2.02	0.59
1:A:34:CYS:HB2	4:A:2013:HOH:O	2.03	0.59
1:G:8:GLU:HG3	1:G:38:TRP:CE2	2.38	0.58
1:E:90:THR:O	1:E:90:THR:HG22	2.03	0.58
1:D:15:CYS:HB2	1:D:105:MET:SD	2.43	0.58
1:E:49:ASN:ND2	4:E:2012:HOH:O	2.37	0.57
1:E:124:VAL:O	1:E:125:CYS:SG	2.62	0.57
1:C:80:VAL:HG11	1:C:195:LEU:CD1	2.34	0.57
1:B:174:PHE:HB2	2:B:1682:AV1:PN	2.45	0.57
1:E:127:ASP:OD1	1:E:129:LYS:HG3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:ASN:HA	1:G:154:GLU:O	2.05	0.56
1:A:128:PHE:CD2	1:A:129:LYS:HE3	2.40	0.56
1:G:1:ILE:N	4:G:2001:HOH:O	2.37	0.56
1:C:62:PHE:CZ	1:C:143:ALA:HB2	2.40	0.56
1:C:48:LYS:HB3	1:C:52:ASP:HB3	1.87	0.56
1:C:114:GLN:HG2	1:C:120:PHE:C	2.26	0.56
1:A:91:GLY:HA2	1:A:94:TYR:O	2.06	0.55
1:G:55:LEU:HD12	1:G:142:MET:HB2	1.88	0.55
1:E:127:ASP:O	1:E:130:THR:HG23	2.06	0.55
1:D:245:ALA:HB3	1:D:248:CYS:SG	2.47	0.55
1:E:1:ILE:N	4:E:2001:HOH:O	2.38	0.55
1:A:174:PHE:HB2	2:A:1682:AV1:PN	2.47	0.55
1:C:80:VAL:HG11	1:C:195:LEU:HD12	1.88	0.55
1:D:140:TRP:HB3	1:D:174:PHE:HE2	1.73	0.54
1:C:196:HIS:CE1	1:C:229:GLU:HB3	2.43	0.54
1:F:47:PHE:HA	1:F:114:GLN:O	2.08	0.54
1:D:140:TRP:CB	1:D:174:PHE:HE2	2.21	0.54
1:F:43:LYS:HA	1:F:46:SER:OG	2.07	0.54
1:A:15:CYS:HB2	1:A:105:MET:SD	2.48	0.53
1:G:7:LEU:HD22	4:G:2002:HOH:O	2.08	0.53
1:H:128:PHE:C	1:H:130:THR:N	2.62	0.53
4:G:2041:HOH:O	1:H:251:ALA:N	2.41	0.53
1:H:4:THR:HG21	1:H:109:LEU:HD22	1.89	0.53
1:C:246:ARG:O	1:C:249:ARG:HG3	2.08	0.53
1:A:144:SER:HB3	1:A:179:GLU:HG2	1.90	0.53
1:H:128:PHE:C	1:H:130:THR:H	2.12	0.53
1:A:232:ARG:HH22	1:B:244:ASN:HD22	1.55	0.53
1:G:179:GLU:OE2	2:G:1682:AV1:O2D	2.24	0.53
4:B:2027:HOH:O	1:D:165:LYS:NZ	2.41	0.52
1:B:48:LYS:CE	1:B:52:ASP:O	2.57	0.52
1:B:92:ARG:HH22	1:B:93:LYS:HZ2	1.55	0.52
1:C:206:CYS:HB2	1:C:229:GLU:OE2	2.10	0.52
1:F:168:ALA:H	1:F:204:GLU:HG3	1.74	0.52
1:B:48:LYS:HE2	1:B:52:ASP:O	2.09	0.52
1:G:115:ARG:CG	1:G:115:ARG:NH1	2.63	0.52
1:H:55:LEU:O	1:H:55:LEU:HG	2.09	0.52
1:G:15:CYS:HB2	1:G:105:MET:SD	2.50	0.52
1:C:114:GLN:NE2	1:C:116:ALA:O	2.27	0.51
1:C:204:GLU:OE2	1:C:210:SER:OG	2.23	0.51
1:C:10:VAL:O	1:C:14:ARG:HG3	2.10	0.51
1:A:133:VAL:HA	1:A:136:ARG:HE	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:THR:O	1:G:181:PRO:HB3	2.11	0.51
1:B:199:GLY:HA2	1:B:246:ARG:HH21	1.75	0.51
1:H:18:TYR:HA	1:H:22:ARG:HB2	1.93	0.51
1:F:174:PHE:N	1:F:174:PHE:CD1	2.71	0.51
1:E:18:TYR:HA	1:E:22:ARG:CG	2.41	0.51
1:A:71:LYS:O	1:A:72:ASN:HB2	2.11	0.51
1:H:174:PHE:O	1:H:179:GLU:HG3	2.11	0.50
1:D:89:ASN:OD1	1:D:92:ARG:HD3	2.11	0.50
1:B:117:ASN:ND2	4:B:2044:HOH:O	2.44	0.50
1:G:79:GLY:N	2:G:1682:AV1:O1A	2.44	0.50
1:G:179:GLU:O	1:G:180:LEU:C	2.49	0.50
1:G:137:GLU:HG2	1:G:174:PHE:CZ	2.47	0.50
1:D:157:TYR:CE2	1:D:159:VAL:CG1	2.95	0.50
1:E:198:LEU:HD12	1:E:242:ASN:HB3	1.93	0.50
1:A:75:MET:HG2	1:A:76:PHE:N	2.27	0.50
1:E:84:ALA:HA	1:E:158:MET:CE	2.42	0.50
1:D:184:THR:OG1	1:D:186:LYS:HE2	2.12	0.50
1:G:250:LEU:C	4:G:2041:HOH:O	2.50	0.49
1:C:8:GLU:HG3	1:C:38:TRP:CE2	2.47	0.49
1:B:205:LYS:O	1:B:211:LEU:HD12	2.12	0.49
1:B:217:LEU:HD11	1:E:129:LYS:HB2	1.94	0.49
1:D:90:THR:O	1:D:90:THR:HG22	2.13	0.49
1:D:219:LYS:HG2	4:D:2048:HOH:O	2.11	0.49
1:E:15:CYS:HB2	1:E:105:MET:SD	2.53	0.49
1:F:217:LEU:O	1:F:221:LYS:HG3	2.12	0.49
1:F:44:ALA:HB2	4:F:2011:HOH:O	2.13	0.48
1:D:243:PRO:HD2	4:D:2050:HOH:O	2.13	0.48
1:A:70:PRO:HG2	1:A:73:LYS:HB2	1.94	0.48
1:F:87:TYR:CE2	1:F:94:TYR:HE2	2.31	0.48
1:G:89:ASN:O	1:G:92:ARG:HB2	2.13	0.48
1:C:232:ARG:NH1	1:D:250:LEU:HD12	2.28	0.48
1:F:205:LYS:NZ	1:F:229:GLU:OE1	2.46	0.48
1:F:18:TYR:O	1:F:29:ARG:NH1	2.47	0.48
1:E:189:ARG:HB2	1:E:224:ALA:HB3	1.94	0.48
1:E:54:ASP:HB2	4:E:2013:HOH:O	2.13	0.48
1:C:54:ASP:HB2	4:C:2021:HOH:O	2.12	0.48
1:F:198:LEU:HD22	1:F:247:GLU:HB2	1.96	0.48
1:E:55:LEU:O	1:E:55:LEU:HG	2.12	0.48
1:E:18:TYR:HA	1:E:22:ARG:HB2	1.96	0.48
1:C:54:ASP:O	1:C:138:SER:OG	2.28	0.48
1:C:217:LEU:HD23	4:C:2054:HOH:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:TYR:O	1:F:62:PHE:HD2	1.97	0.47
1:B:221:LYS:O	1:B:222:HIS:HB2	2.14	0.47
1:A:250:LEU:HD21	1:B:236:PHE:CE1	2.49	0.47
1:D:192:VAL:HB	1:D:227:CYS:HB2	1.96	0.47
1:B:189:ARG:HD3	1:B:226:ASP:OD2	2.14	0.47
1:B:179:GLU:OE2	2:B:1682:AV1:H1D	2.13	0.47
1:A:140:TRP:HB3	1:A:174:PHE:HE2	1.80	0.47
1:H:58:TYR:O	1:H:62:PHE:HD2	1.97	0.47
1:H:185:ASN:OD1	1:H:186:LYS:HE2	2.14	0.47
1:G:137:GLU:OE1	1:G:178:TYR:OH	2.23	0.47
1:H:83:GLU:HG2	1:H:238:LEU:HD21	1.96	0.47
1:E:215:GLU:HG3	1:E:225:PHE:CD2	2.49	0.47
1:E:179:GLU:O	1:E:180:LEU:C	2.53	0.47
1:D:40:ASP:HA	1:D:43:LYS:HD3	1.97	0.47
1:H:89:ASN:O	1:H:92:ARG:HG2	2.15	0.47
1:G:211:LEU:HA	1:G:211:LEU:HD23	1.76	0.47
1:C:101:LEU:HB3	1:C:102:PRO:HD3	1.96	0.47
1:H:91:GLY:HA2	1:H:95:ILE:HD12	1.96	0.47
1:A:106:LEU:HG	1:A:139:PHE:CZ	2.49	0.47
1:F:101:LEU:N	1:F:102:PRO:HD2	2.30	0.47
1:C:197:ARG:HH11	1:C:197:ARG:HG2	1.80	0.47
1:F:50:PRO:O	1:F:53:LEU:HD21	2.15	0.46
1:A:50:PRO:HB2	1:A:126:PRO:HG2	1.97	0.46
1:G:173:SER:O	1:G:177:LYS:HG2	2.16	0.46
1:E:128:PHE:HD2	1:E:136:ARG:HA	1.80	0.46
1:E:74:VAL:HB	4:E:2019:HOH:O	2.15	0.46
1:B:79:GLY:N	2:B:1682:AV1:O1A	2.44	0.46
1:G:137:GLU:HG2	1:G:174:PHE:HZ	1.80	0.46
1:E:205:LYS:HB3	1:E:205:LYS:HE2	1.71	0.46
1:C:128:PHE:O	1:C:136:ARG:HD2	2.13	0.46
1:B:217:LEU:HA	1:B:217:LEU:HD23	1.65	0.46
1:D:7:LEU:HD22	1:D:111:TRP:HB3	1.98	0.46
1:E:115:ARG:HD2	4:E:2012:HOH:O	2.16	0.46
1:F:101:LEU:HD12	1:F:105:MET:HG3	1.98	0.46
1:E:243:PRO:O	1:F:232:ARG:NH2	2.48	0.46
1:C:71:LYS:HG3	1:C:152:GLU:HB2	1.98	0.46
1:D:195:LEU:HD11	1:D:238:LEU:HD21	1.97	0.46
1:A:140:TRP:CB	1:A:174:PHE:HE2	2.29	0.46
1:C:198:LEU:HD12	1:C:242:ASN:HB3	1.98	0.46
1:H:3:PRO:HA	1:H:110:VAL:HB	1.98	0.45
1:C:242:ASN:ND2	4:C:2058:HOH:O	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:HZ1	1:A:129:LYS:N	2.00	0.45
1:F:40:ASP:C	4:F:2010:HOH:O	2.53	0.45
1:B:174:PHE:HB2	2:B:1682:AV1:O5D	2.17	0.45
1:F:7:LEU:HD23	1:F:38:TRP:HH2	1.82	0.45
1:G:80:VAL:O	1:G:80:VAL:HG23	2.17	0.45
1:H:175:PHE:HA	1:H:179:GLU:HG3	1.98	0.45
1:D:91:GLY:HA2	1:D:94:TYR:O	2.16	0.45
1:A:49:ASN:C	1:A:51:CYS:H	2.19	0.45
1:G:128:PHE:HD2	1:G:136:ARG:HA	1.82	0.45
1:C:120:PHE:CD1	1:C:120:PHE:N	2.85	0.45
1:F:206:CYS:SG	1:F:211:LEU:HD13	2.57	0.44
1:G:77:TRP:O	2:G:1682:AV1:H5DA	2.17	0.44
1:B:89:ASN:HD22	1:B:89:ASN:C	2.19	0.44
1:E:91:GLY:HA2	1:E:94:TYR:O	2.18	0.44
1:E:20:ILE:O	1:E:20:ILE:HG22	2.16	0.44
1:H:11:PHE:C	1:H:11:PHE:CD1	2.90	0.44
1:F:117:ASN:OD1	1:F:118:PRO:HA	2.18	0.44
1:B:55:LEU:HD12	1:B:142:MET:HB2	2.00	0.44
1:F:33:ASP:OD1	1:F:33:ASP:C	2.56	0.44
1:D:83:GLU:H	1:D:83:GLU:CD	2.21	0.44
1:G:218:VAL:HG13	1:G:223:PHE:HB2	1.99	0.44
1:H:60:ASP:HB2	4:H:2007:HOH:O	2.18	0.44
1:H:231:PRO:HG2	1:H:234:VAL:HB	2.00	0.44
1:A:128:PHE:C	1:A:128:PHE:CD1	2.90	0.44
1:G:83:GLU:HG2	1:G:195:LEU:CD2	2.47	0.44
1:C:183:LEU:HD22	1:C:187:VAL:HG21	2.00	0.44
1:C:28:PRO:HG2	1:C:67:GLN:HB3	2.00	0.44
1:H:196:HIS:NE2	1:H:202:ILE:HG23	2.33	0.43
1:C:127:ASP:O	1:C:130:THR:HG23	2.10	0.43
1:E:125:CYS:SG	1:E:126:PRO:CD	3.06	0.43
1:E:175:PHE:HA	1:E:179:GLU:HB2	1.99	0.43
1:H:101:LEU:N	1:H:102:PRO:HD2	2.32	0.43
1:F:106:LEU:O	1:F:107:ASN:C	2.57	0.43
1:H:128:PHE:H	1:H:130:THR:CG2	2.31	0.43
1:A:136:ARG:HB3	1:A:137:GLU:HG3	1.99	0.43
1:H:195:LEU:HD11	1:H:238:LEU:HD11	2.01	0.43
1:B:62:PHE:CZ	1:B:143:ALA:HB2	2.52	0.43
1:D:73:LYS:O	1:D:94:TYR:HB3	2.18	0.43
1:E:172:ASP:O	1:E:177:LYS:HD2	2.18	0.43
1:F:22:ARG:O	1:F:29:ARG:NH2	2.46	0.43
1:E:230:ASN:O	1:E:231:PRO:C	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:LEU:HA	1:D:24:LEU:HD23	1.84	0.43
1:G:205:LYS:HA	1:G:229:GLU:OE2	2.18	0.43
1:F:89:ASN:O	1:F:90:THR:C	2.57	0.43
1:H:163:ASN:HA	1:H:164:PRO:HD3	1.83	0.43
1:E:128:PHE:O	1:E:136:ARG:HD3	2.18	0.43
1:C:174:PHE:CZ	4:C:2050:HOH:O	2.57	0.43
1:E:189:ARG:HA	1:E:224:ALA:O	2.19	0.43
1:B:61:PHE:CE2	1:B:102:PRO:HB3	2.53	0.43
1:A:80:VAL:O	1:A:81:TYR:C	2.57	0.43
1:C:43:LYS:NZ	1:C:60:ASP:OD2	2.42	0.43
1:E:124:VAL:HG22	1:E:125:CYS:N	2.33	0.43
1:A:85:HIS:CE1	1:A:98:GLU:OE1	2.72	0.43
1:G:128:PHE:O	1:G:136:ARG:HD2	2.10	0.42
1:H:101:LEU:O	1:H:105:MET:HG3	2.18	0.42
1:C:221:LYS:O	1:C:222:HIS:HB2	2.19	0.42
1:F:174:PHE:CD1	2:F:1682:AV1:PN	3.12	0.42
1:A:97:LEU:HD23	2:A:1682:AV1:H1D	2.02	0.42
1:F:47:PHE:HD1	1:F:115:ARG:O	2.02	0.42
1:F:232:ARG:HG2	1:F:232:ARG:H	1.33	0.42
1:A:180:LEU:HD12	1:A:180:LEU:O	2.20	0.42
1:C:106:LEU:O	1:C:107:ASN:C	2.58	0.42
1:H:228:VAL:HG22	1:H:229:GLU:N	2.35	0.42
1:H:228:VAL:CG2	1:H:229:GLU:N	2.83	0.42
1:A:77:TRP:O	2:A:1682:AV1:H5DA	2.20	0.42
1:D:77:TRP:O	3:D:303:CV1:H5DA	2.19	0.42
1:H:77:TRP:HA	1:H:158:MET:O	2.20	0.42
1:D:94:TYR:HE2	1:D:156:THR:HG1	1.67	0.42
1:H:128:PHE:H	1:H:130:THR:HG23	1.85	0.42
1:G:185:ASN:ND2	1:G:185:ASN:C	2.73	0.42
1:G:177:LYS:HG3	1:G:178:TYR:CE2	2.55	0.41
1:H:106:LEU:HD13	1:H:109:LEU:HD12	2.02	0.41
1:H:62:PHE:O	1:H:66:GLN:HB2	2.19	0.41
1:C:133:VAL:HA	1:C:136:ARG:HG3	2.01	0.41
1:H:106:LEU:HD13	1:H:106:LEU:HA	1.82	0.41
1:G:162:SER:HB2	1:G:197:ARG:HG3	2.02	0.41
1:E:96:THR:O	1:E:97:LEU:C	2.58	0.41
1:B:144:SER:HB3	1:B:179:GLU:CG	2.49	0.41
1:A:232:ARG:HH22	1:B:244:ASN:ND2	2.18	0.41
1:H:221:LYS:O	1:H:222:HIS:HB2	2.20	0.41
1:F:170:ARG:HB2	1:F:173:SER:HB3	2.02	0.41
1:B:26:ILE:HG22	1:B:27:LEU:HG	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:189:ARG:HA	1:H:224:ALA:O	2.21	0.41
1:D:120:PHE:H	1:D:120:PHE:HD1	1.69	0.41
1:C:12:LEU:HD23	1:C:12:LEU:HA	1.89	0.41
1:F:198:LEU:CD2	1:F:247:GLU:HB2	2.50	0.41
1:C:97:LEU:O	1:C:103:GLY:HA3	2.20	0.41
1:A:50:PRO:HB3	1:A:112:CYS:HB2	2.03	0.41
1:C:80:VAL:HG11	1:C:195:LEU:HD13	2.03	0.41
1:E:148:ALA:HB2	1:E:179:GLU:HG2	2.02	0.41
1:A:18:TYR:C	1:A:18:TYR:CD1	2.93	0.41
1:D:196:HIS:NE2	1:D:202:ILE:HG23	2.35	0.41
1:H:106:LEU:O	1:H:107:ASN:C	2.59	0.41
1:F:127:ASP:O	1:F:128:PHE:HB2	2.21	0.41
1:B:15:CYS:HB2	1:B:105:MET:SD	2.60	0.41
1:A:173:SER:O	1:A:177:LYS:HB2	2.21	0.41
1:A:72:ASN:HA	1:A:154:GLU:O	2.21	0.41
1:F:60:ASP:O	1:F:61:PHE:C	2.60	0.41
1:F:225:PHE:C	1:F:225:PHE:CD1	2.95	0.41
1:B:46:SER:HA	1:B:119:GLY:O	2.20	0.41
1:G:111:TRP:C	1:G:112:CYS:SG	2.98	0.40
1:D:101:LEU:HB3	1:D:102:PRO:CD	2.51	0.40
1:F:163:ASN:HA	1:F:164:PRO:HD2	1.82	0.40
1:G:212:LEU:O	1:G:213:ASP:C	2.58	0.40
1:C:101:LEU:N	1:C:102:PRO:HD2	2.36	0.40
1:G:178:TYR:O	1:G:182:ASN:HB2	2.22	0.40
1:F:116:ALA:O	1:F:117:ASN:C	2.60	0.40
1:E:83:GLU:OE2	1:E:197:ARG:NH1	2.54	0.40
1:F:175:PHE:HA	1:F:179:GLU:HB2	2.03	0.40
1:E:72:ASN:HA	1:E:154:GLU:O	2.22	0.40
1:G:189:ARG:HD3	1:G:226:ASP:OD2	2.21	0.40
1:H:113:GLY:HA2	1:H:120:PHE:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	249/260 (96%)	233 (94%)	14 (6%)	2 (1%)	24	35
1	B	250/260 (96%)	239 (96%)	10 (4%)	1 (0%)	39	56
1	C	250/260 (96%)	236 (94%)	13 (5%)	1 (0%)	39	56
1	D	250/260 (96%)	239 (96%)	11 (4%)	0	100	100
1	E	249/260 (96%)	238 (96%)	10 (4%)	1 (0%)	39	56
1	F	249/260 (96%)	226 (91%)	20 (8%)	3 (1%)	16	23
1	G	249/260 (96%)	237 (95%)	12 (5%)	0	100	100
1	H	249/260 (96%)	230 (92%)	15 (6%)	4 (2%)	12	16
All	All	1995/2080 (96%)	1878 (94%)	105 (5%)	12 (1%)	30	43

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	PHE
1	A	126	PRO
1	F	174	PHE
1	H	128	PHE
1	F	127	ASP
1	H	129	LYS
1	F	128	PHE
1	H	55	LEU
1	B	185	ASN
1	E	71	LYS
1	C	1	ILE
1	H	247	GLU

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	220/226 (97%)	198 (90%)	22 (10%)	9	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	220/226 (97%)	203 (92%)	17 (8%)	16	24
1	C	220/226 (97%)	204 (93%)	16 (7%)	17	27
1	D	220/226 (97%)	206 (94%)	14 (6%)	22	34
1	E	220/226 (97%)	203 (92%)	17 (8%)	16	24
1	F	220/226 (97%)	196 (89%)	24 (11%)	8	11
1	G	220/226 (97%)	203 (92%)	17 (8%)	16	24
1	H	220/226 (97%)	204 (93%)	16 (7%)	17	27
All	All	1760/1808 (97%)	1617 (92%)	143 (8%)	15	22

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	26	ILE
1	A	29	ARG
1	A	30	VAL
1	A	32	SER
1	A	33	ASP
1	A	71	LYS
1	A	90	THR
1	A	92	ARG
1	A	93	LYS
1	A	124	VAL
1	A	128	PHE
1	A	129	LYS
1	A	131	CYS
1	A	133	VAL
1	A	134	GLN
1	A	217	LEU
1	A	228	VAL
1	A	232	ARG
1	A	242	ASN
1	A	246	ARG
1	A	250	LEU
1	B	1	ILE
1	B	5	ARG
1	B	39	LYS
1	B	59	LYS
1	B	89	ASN
1	B	90	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	92	ARG
1	B	93	LYS
1	B	115	ARG
1	B	186	LYS
1	B	195	LEU
1	B	200	GLU
1	B	206	CYS
1	B	212	LEU
1	B	216	LYS
1	B	221	LYS
1	B	244	ASN
1	C	21	THR
1	C	25	ASP
1	C	30	VAL
1	C	31	ARG
1	C	39	LYS
1	C	55	LEU
1	C	73	LYS
1	C	89	ASN
1	C	123	LYS
1	C	130	THR
1	C	134	GLN
1	C	172	ASP
1	C	195	LEU
1	C	200	GLU
1	C	228	VAL
1	C	242	ASN
1	D	32	SER
1	D	39	LYS
1	D	71	LYS
1	D	92	ARG
1	D	120	PHE
1	D	124	VAL
1	D	128	PHE
1	D	131	CYS
1	D	162	SER
1	D	200	GLU
1	D	206	CYS
1	D	227	CYS
1	D	237	LEU
1	D	247	GLU
1	E	31	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	39	LYS
1	E	43	LYS
1	E	49	ASN
1	E	71	LYS
1	E	89	ASN
1	E	112	CYS
1	E	129	LYS
1	E	130	THR
1	E	172	ASP
1	E	189	ARG
1	E	195	LEU
1	E	200	GLU
1	E	216	LYS
1	E	237	LEU
1	E	240	SER
1	E	246	ARG
1	F	25	ASP
1	F	29	ARG
1	F	53	LEU
1	F	63	THR
1	F	73	LYS
1	F	89	ASN
1	F	90	THR
1	F	92	ARG
1	F	121	ASN
1	F	123	LYS
1	F	128	PHE
1	F	129	LYS
1	F	130	THR
1	F	133	VAL
1	F	136	ARG
1	F	137	GLU
1	F	173	SER
1	F	174	PHE
1	F	227	CYS
1	F	232	ARG
1	F	242	ASN
1	F	246	ARG
1	F	249	ARG
1	F	250	LEU
1	G	6	GLU
1	G	33	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	43	LYS
1	G	64	SER
1	G	92	ARG
1	G	112	CYS
1	G	115	ARG
1	G	123	LYS
1	G	130	THR
1	G	158	MET
1	G	172	ASP
1	G	185	ASN
1	G	228	VAL
1	G	232	ARG
1	G	237	LEU
1	G	242	ASN
1	G	246	ARG
1	H	25	ASP
1	H	29	ARG
1	H	35	SER
1	H	55	LEU
1	H	64	SER
1	H	75	MET
1	H	89	ASN
1	H	95	ILE
1	H	115	ARG
1	H	124	VAL
1	H	129	LYS
1	H	130	THR
1	H	203	ILE
1	H	217	LEU
1	H	234	VAL
1	H	242	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	117	ASN
1	A	242	ASN
1	B	89	ASN
1	B	242	ASN
1	B	244	ASN
1	C	49	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	89	ASN
1	C	196	HIS
1	C	242	ASN
1	D	117	ASN
1	D	242	ASN
1	D	244	ASN
1	E	242	ASN
1	F	89	ASN
1	F	242	ASN
1	G	107	ASN
1	G	185	ASN
1	G	242	ASN
1	H	242	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	AV1	A	1682	-	32,39,39	1.14	3 (9%)	38,60,60	2.15	7 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AV1	B	1682	-	32,39,39	1.69	4 (12%)	38,60,60	3.63	13 (34%)
2	AV1	C	1682	-	32,39,39	1.53	5 (15%)	38,60,60	3.05	8 (21%)
3	CV1	D	303	-	30,40,40	2.00	5 (16%)	36,64,64	1.31	4 (11%)
2	AV1	E	1682	-	32,39,39	1.38	3 (9%)	38,60,60	2.38	11 (28%)
2	AV1	F	1682	-	32,39,39	1.59	2 (6%)	38,60,60	2.08	6 (15%)
2	AV1	G	1682	-	32,39,39	1.31	4 (12%)	38,60,60	3.22	10 (26%)
2	AV1	H	1682	-	32,39,39	1.76	2 (6%)	38,60,60	2.73	7 (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	AV1	A	1682	-	-	0/18/51/51	0/4/4/4
2	AV1	B	1682	-	-	0/18/51/51	0/4/4/4
2	AV1	C	1682	-	-	0/18/51/51	0/4/4/4
3	CV1	D	303	-	-	0/18/58/58	0/1/5/5
2	AV1	E	1682	-	-	0/18/51/51	0/4/4/4
2	AV1	F	1682	-	-	0/18/51/51	0/4/4/4
2	AV1	G	1682	-	-	0/18/51/51	0/4/4/4
2	AV1	H	1682	-	-	0/18/51/51	0/4/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1682	AV1	C5A-N7A	-5.45	1.31	1.38
2	F	1682	AV1	C5A-N7A	-4.53	1.32	1.38
2	G	1682	AV1	C5A-N7A	-4.46	1.32	1.38
2	B	1682	AV1	C5A-N7A	-4.42	1.32	1.38
2	A	1682	AV1	C5A-N7A	-4.16	1.33	1.38
3	D	303	CV1	C5-N7	-4.09	1.33	1.38
2	C	1682	AV1	C5A-N7A	-3.90	1.33	1.38
2	E	1682	AV1	C5A-N7A	-2.90	1.34	1.38
3	D	303	CV1	C5'-C4'	2.00	1.58	1.51
2	B	1682	AV1	PA-O1A	2.07	1.63	1.54
2	C	1682	AV1	C1D-C2D	2.07	1.55	1.51
2	A	1682	AV1	PN-O2N	2.13	1.64	1.54
2	E	1682	AV1	C5D-C4D	2.17	1.58	1.51
2	G	1682	AV1	PN-O5D	2.20	1.69	1.59
2	G	1682	AV1	PN-O2N	2.20	1.64	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1682	AV1	PN-O2N	2.31	1.64	1.54
2	C	1682	AV1	PN-O2N	2.50	1.65	1.54
2	A	1682	AV1	O4'-C1'	2.78	1.44	1.41
3	D	303	CV1	C6-N1	3.05	1.41	1.36
2	G	1682	AV1	O4'-C1'	3.12	1.45	1.41
2	C	1682	AV1	O4D-C4D	3.29	1.50	1.44
3	D	303	CV1	O4D-C1D	3.72	1.45	1.41
2	C	1682	AV1	O4'-C1'	4.61	1.47	1.41
2	E	1682	AV1	O4'-C1'	5.57	1.48	1.41
2	F	1682	AV1	O4'-C1'	6.47	1.49	1.41
2	H	1682	AV1	O4'-C1'	6.61	1.49	1.41
2	B	1682	AV1	O4'-C1'	7.05	1.50	1.41
3	D	303	CV1	O4'-C1'	7.23	1.50	1.41

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1682	AV1	N3A-C2A-N1A	-10.15	121.12	128.89
2	C	1682	AV1	N3A-C2A-N1A	-9.56	121.57	128.89
2	A	1682	AV1	N3A-C2A-N1A	-9.53	121.60	128.89
2	G	1682	AV1	N3A-C2A-N1A	-9.41	121.69	128.89
2	B	1682	AV1	N3A-C2A-N1A	-9.35	121.73	128.89
2	B	1682	AV1	C4'-O4'-C1'	-8.50	100.38	109.72
2	F	1682	AV1	N3A-C2A-N1A	-8.48	122.40	128.89
2	H	1682	AV1	N3A-C2A-N1A	-8.30	122.54	128.89
2	G	1682	AV1	C4'-O4'-C1'	-7.42	101.57	109.72
2	C	1682	AV1	C4'-O4'-C1'	-6.17	102.94	109.72
2	A	1682	AV1	C4'-O4'-C1'	-5.76	103.39	109.72
2	H	1682	AV1	PN-O3-PA	-5.35	117.70	132.73
2	E	1682	AV1	C4'-O4'-C1'	-5.27	103.93	109.72
2	G	1682	AV1	PN-O3-PA	-5.12	118.36	132.73
2	F	1682	AV1	PN-O3-PA	-4.85	119.12	132.73
2	C	1682	AV1	C5D-C4D-C3D	-3.89	99.78	115.21
2	G	1682	AV1	C5'-C4'-C3'	-3.59	100.97	115.21
2	H	1682	AV1	C4'-O4'-C1'	-3.47	105.91	109.72
2	A	1682	AV1	PN-O3-PA	-2.99	124.34	132.73
2	G	1682	AV1	O4D-C1D-C2D	-2.85	100.33	106.16
2	B	1682	AV1	C4A-C5A-N7A	-2.80	107.09	109.55
2	B	1682	AV1	PN-O3-PA	-2.75	125.00	132.73
2	G	1682	AV1	C5D-C4D-C3D	-2.66	104.64	115.21
3	D	303	CV1	O4'-C1'-N9	-2.65	105.26	108.29
2	A	1682	AV1	C5D-C4D-C3D	-2.62	104.83	115.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	303	CV1	PB-O3A-PA	-2.59	125.46	132.73
2	C	1682	AV1	PN-O3-PA	-2.58	125.49	132.73
2	H	1682	AV1	C5D-C4D-C3D	-2.53	105.17	115.21
2	C	1682	AV1	C4A-C5A-N7A	-2.51	107.34	109.55
2	B	1682	AV1	C5D-C4D-C3D	-2.48	105.36	115.21
2	B	1682	AV1	O4'-C4'-C3'	-2.46	100.19	105.15
2	E	1682	AV1	C5'-C4'-C3'	-2.45	105.50	115.21
2	H	1682	AV1	C4A-C5A-N7A	-2.40	107.44	109.55
2	E	1682	AV1	O4D-C1D-C2D	-2.33	101.40	106.16
2	B	1682	AV1	C1'-N9A-C4A	-2.32	123.57	127.04
2	C	1682	AV1	C1'-N9A-C4A	-2.32	123.58	127.04
2	G	1682	AV1	O2D-C2D-C3D	-2.31	106.80	111.23
2	E	1682	AV1	PN-O3-PA	-2.30	126.28	132.73
2	E	1682	AV1	C4A-C5A-N7A	-2.28	107.54	109.55
2	A	1682	AV1	C5'-C4'-C3'	-2.22	106.41	115.21
2	B	1682	AV1	C5'-C4'-C3'	-2.06	107.05	115.21
2	F	1682	AV1	C4A-C5A-N7A	-2.04	107.76	109.55
3	D	303	CV1	C2'-C3'-C4'	2.15	107.04	102.61
2	H	1682	AV1	O3-PA-O5'	2.16	108.67	102.94
2	A	1682	AV1	O3-PN-O5D	2.21	108.79	102.94
2	F	1682	AV1	O3-PN-O5D	2.23	108.86	102.94
2	B	1682	AV1	C1D-C2D-C3D	2.24	105.24	101.64
2	E	1682	AV1	O5'-PA-O2A	2.26	118.40	109.62
2	B	1682	AV1	O4D-C4D-C3D	2.42	108.69	104.43
2	E	1682	AV1	O4'-C4'-C5'	2.44	118.04	109.32
2	G	1682	AV1	O4D-C4D-C5D	2.64	115.31	109.53
2	E	1682	AV1	O3-PA-O5'	2.68	110.04	102.94
2	F	1682	AV1	O3-PA-O5'	2.87	110.54	102.94
2	G	1682	AV1	O5'-PA-O2A	3.04	121.41	109.62
2	E	1682	AV1	O4D-C4D-C5D	3.10	116.31	109.53
2	B	1682	AV1	O4'-C4'-C5'	3.23	120.89	109.32
2	E	1682	AV1	O4'-C1'-N9A	3.45	112.23	108.29
2	A	1682	AV1	O4'-C1'-N9A	3.55	112.35	108.29
3	D	303	CV1	C2-N3-C4	3.76	122.22	116.40
2	C	1682	AV1	O3-PA-O5'	3.92	113.32	102.94
2	B	1682	AV1	O3-PA-O5'	4.47	114.81	102.94
2	F	1682	AV1	O4'-C1'-N9A	5.61	114.70	108.29
2	H	1682	AV1	O4'-C1'-N9A	11.30	121.20	108.29
2	C	1682	AV1	O4'-C1'-N9A	12.12	122.13	108.29
2	G	1682	AV1	O4'-C1'-N9A	12.41	122.47	108.29
2	B	1682	AV1	O4'-C1'-N9A	15.84	126.38	108.29

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	1682	AV1	3	0
2	B	1682	AV1	4	0
2	C	1682	AV1	1	0
3	D	303	CV1	4	0
2	E	1682	AV1	1	0
2	F	1682	AV1	3	0
2	G	1682	AV1	3	0
2	H	1682	AV1	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	251/260 (96%)	-0.45	0 100 100	34, 50, 73, 87	0
1	B	252/260 (96%)	-0.44	3 (1%) 81 81	32, 45, 66, 78	0
1	C	252/260 (96%)	-0.47	1 (0%) 93 93	32, 48, 67, 79	0
1	D	252/260 (96%)	-0.44	2 (0%) 87 87	34, 48, 73, 91	0
1	E	251/260 (96%)	-0.40	2 (0%) 87 87	34, 49, 70, 89	0
1	F	251/260 (96%)	-0.19	1 (0%) 93 93	49, 71, 91, 108	0
1	G	251/260 (96%)	-0.38	4 (1%) 74 74	38, 52, 72, 91	0
1	H	251/260 (96%)	-0.25	2 (0%) 87 87	50, 67, 89, 98	0
All	All	2011/2080 (96%)	-0.38	15 (0%) 89 88	32, 53, 82, 108	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	128	PHE	7.9
1	E	1	ILE	4.2
1	B	0	ALA	3.5
1	B	250	LEU	3.2
1	C	250	LEU	3.1
1	E	128	PHE	2.9
1	F	128	PHE	2.7
1	G	174	PHE	2.7
1	D	0	ALA	2.5
1	H	250	LEU	2.4
1	G	55	LEU	2.4
1	G	128	PHE	2.3
1	B	174	PHE	2.2
1	G	53	LEU	2.1
1	H	1	ILE	2.1

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(\AA^2)	Q<0.9
2	AV1	A	1682	36/36	0.73	0.21	3.18	119,140,150,153	0
2	AV1	C	1682	36/36	0.77	0.19	3.03	66,112,126,136	0
2	AV1	F	1682	36/36	0.72	0.21	2.12	110,132,141,146	0
2	AV1	B	1682	36/36	0.80	0.20	1.87	72,105,128,138	0
2	AV1	H	1682	36/36	0.82	0.15	0.82	96,122,130,134	0
3	CV1	D	303	36/36	0.68	0.23	0.71	147,153,159,160	0
2	AV1	E	1682	36/36	0.86	0.14	0.57	66,90,117,126	0
2	AV1	G	1682	36/36	0.89	0.13	0.08	54,78,99,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.