Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 01:51 am BST

PDB ID	:	3JZT
Title	:	Structure of a cubic crystal form of X (ADRP) domain from FCoV with ADP-ribose
Authors	:	Wojdyla, J.A.; Manolaridis, I.; Tucker, P.A.
Deposited on	:	2009-09-24
Resolution	:	3.91 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
https://www.wwpdb.org/validation/2017/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:

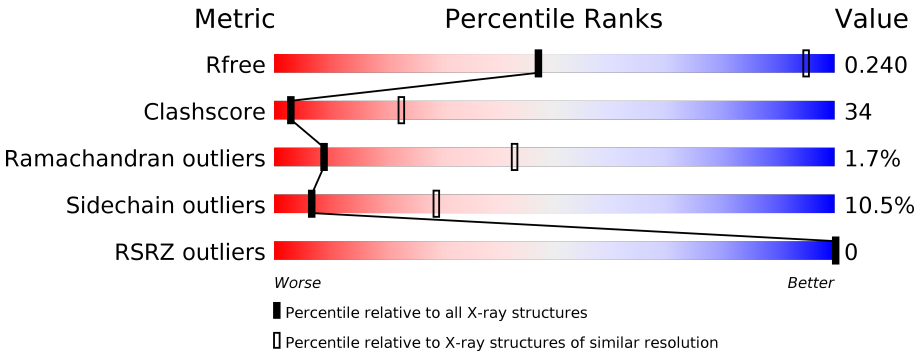
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.91 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}	130704	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

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 respectively. 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 <=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	168	45% 47% 8%
1	B	168	48% 44% 7%
1	C	168	42% 51% 7%
1	D	168	41% 54% 5%
1	E	168	42% 48% 10%
1	F	168	33% 49% 17%

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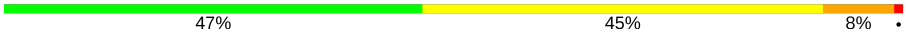
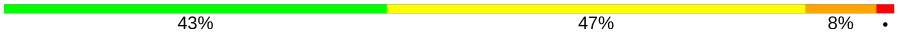
Mol	Chain	Length	Quality of chain
1	G	168	
1	H	168	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10495 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.

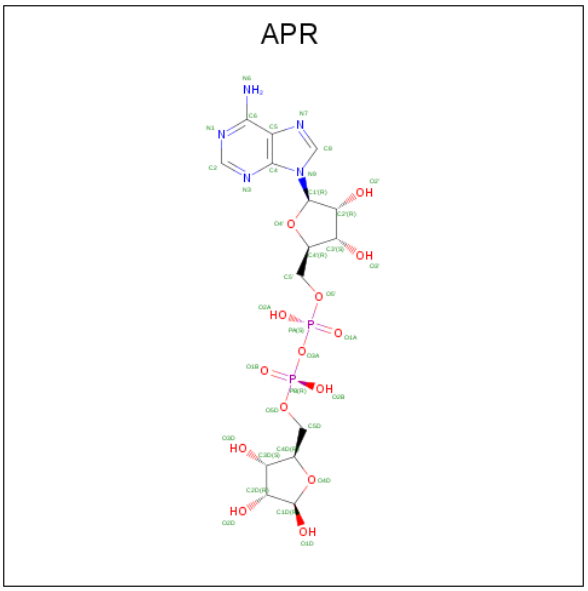
- Molecule 1 is a protein called macro domain of Non-structural protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1298	834	221	240	3			
1	B	168	Total	C	N	O	S	0	0	0
			1298	834	221	240	3			
1	C	168	Total	C	N	O	S	0	0	0
			1298	834	221	240	3			
1	D	168	Total	C	N	O	S	0	0	0
			1298	834	221	240	3			
1	E	168	Total	C	N	O	S	0	0	0
			1298	834	221	240	3			
1	F	168	Total	C	N	O	S	0	0	0
			1298	834	221	240	3			
1	G	168	Total	C	N	O	S	0	0	0
			1298	834	221	240	3			
1	H	168	Total	C	N	O	S	0	0	0
			1298	834	221	240	3			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula: $C_{15}H_{23}N_5O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
3	C	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
3	D	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		

3 Residue-property plots (i)

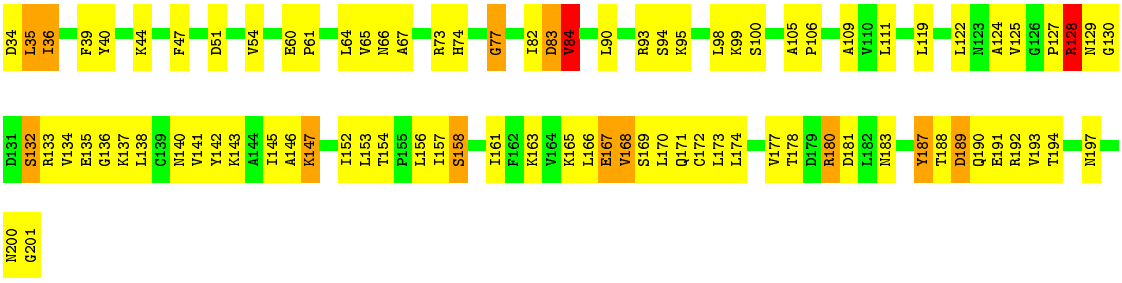
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: macro domain of Non-structural protein 3

Chain A:

- Molecule 1: macro domain of Non-structural protein 3

Chain B:



- Molecule 1: macro domain of Non-structural protein 3

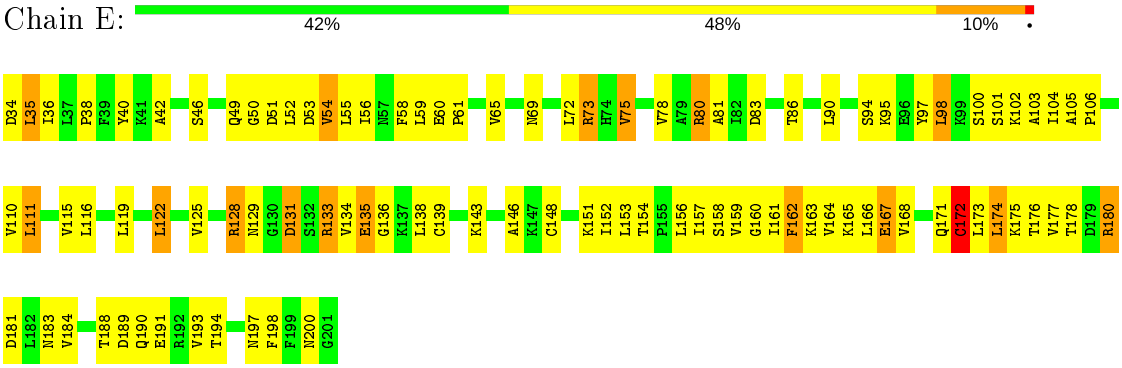
Chain C:

• Molecule 1: macro domain of Non-structural protein 3

Chain D:

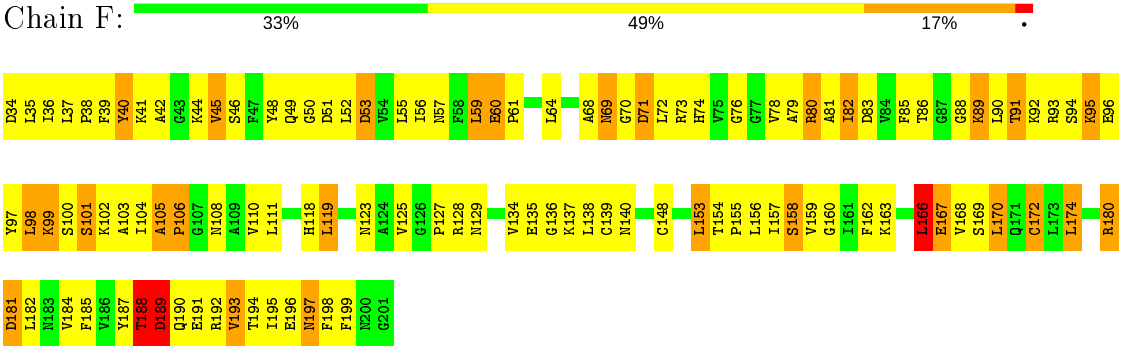
• Molecule 1: macro domain of Non-structural protein 3

Chain E:



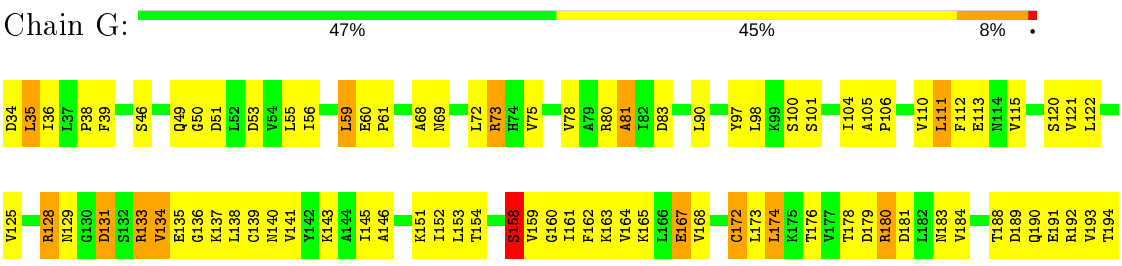
• Molecule 1: macro domain of Non-structural protein 3

Chain F:



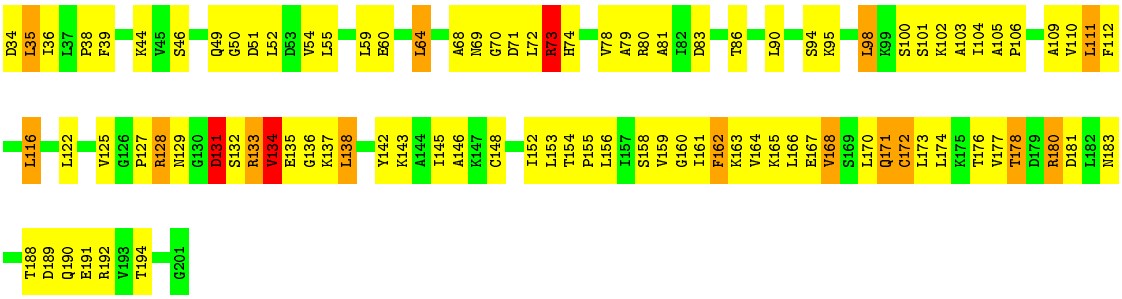
• Molecule 1: macro domain of Non-structural protein 3

Chain G:



• Molecule 1: macro domain of Non-structural protein 3

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	220.24Å 220.24Å 220.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 3.91 19.94 – 3.91	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.94-3.91) 99.8 (19.94-3.91)	Depositor EDS
R_{merge}	0.46	Depositor
R_{sym}	0.56	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 3.94Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.239 0.199 , 0.240	Depositor DCC
R_{free} test set	465 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å^2)	53.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.043 for l,-k,h	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10495	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: APR, NA, CL

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	1.34	4/1318 (0.3%)	1.23	8/1782 (0.4%)
1	B	1.32	2/1318 (0.2%)	1.18	6/1782 (0.3%)
1	C	1.33	7/1318 (0.5%)	1.30	7/1782 (0.4%)
1	D	1.32	5/1318 (0.4%)	1.19	5/1782 (0.3%)
1	E	1.37	6/1318 (0.5%)	1.27	8/1782 (0.4%)
1	F	1.36	7/1318 (0.5%)	1.37	10/1782 (0.6%)
1	G	1.36	5/1318 (0.4%)	1.26	4/1782 (0.2%)
1	H	1.39	4/1318 (0.3%)	1.30	13/1782 (0.7%)
All	All	1.35	40/10544 (0.4%)	1.26	61/14256 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	F	0	2
1	H	0	1
All	All	0	5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	134	VAL	CB-CG1	-9.38	1.33	1.52
1	C	128	ARG	CZ-NH1	-9.02	1.21	1.33
1	E	135	GLU	CB-CG	-8.98	1.35	1.52
1	G	172	CYS	CB-SG	8.40	1.96	1.82
1	C	167	GLU	CG-CD	7.90	1.63	1.51
1	A	148	CYS	CB-SG	-7.72	1.69	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	172	CYS	CB-SG	7.67	1.95	1.82
1	G	158	SER	CB-OG	-7.57	1.32	1.42
1	H	138	LEU	CG-CD1	-7.54	1.24	1.51
1	A	134	VAL	CB-CG1	-7.29	1.37	1.52
1	F	123	ASN	CB-CG	-7.17	1.34	1.51
1	D	197	ASN	CG-ND2	-6.44	1.16	1.32
1	D	148	CYS	CB-SG	-6.39	1.71	1.82
1	E	148	CYS	CB-SG	-6.27	1.71	1.82
1	D	197	ASN	CG-OD1	-6.24	1.10	1.24
1	H	148	CYS	CB-SG	-6.20	1.71	1.82
1	F	148	CYS	CB-SG	-6.17	1.71	1.82
1	G	60	GLU	CG-CD	6.06	1.61	1.51
1	D	78	VAL	CA-CB	-5.86	1.42	1.54
1	E	75	VAL	CB-CG2	-5.82	1.40	1.52
1	F	105	ALA	CA-CB	5.79	1.64	1.52
1	F	172	CYS	CB-SG	5.74	1.92	1.82
1	C	60	GLU	CB-CG	5.71	1.62	1.52
1	F	78	VAL	CB-CG1	5.66	1.64	1.52
1	G	81	ALA	CA-CB	-5.66	1.40	1.52
1	E	60	GLU	CG-CD	5.57	1.60	1.51
1	F	60	GLU	CD-OE2	5.47	1.31	1.25
1	E	167	GLU	CG-CD	-5.44	1.43	1.51
1	D	60	GLU	CG-CD	5.38	1.60	1.51
1	B	167	GLU	CG-CD	5.31	1.59	1.51
1	A	115	VAL	CA-CB	-5.26	1.43	1.54
1	C	148	CYS	CB-SG	-5.19	1.73	1.81
1	C	60	GLU	CG-CD	5.12	1.59	1.51
1	C	58	PHE	CE1-CZ	5.11	1.47	1.37
1	G	167	GLU	CG-CD	5.10	1.59	1.51
1	C	131	ASP	CG-OD2	-5.09	1.13	1.25
1	B	60	GLU	CD-OE2	5.03	1.31	1.25
1	A	60	GLU	CG-CD	5.02	1.59	1.51
1	F	102	LYS	CD-CE	5.01	1.63	1.51
1	H	168	VAL	CA-CB	-5.01	1.44	1.54

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	128	ARG	NE-CZ-NH2	20.58	130.59	120.30
1	F	98	LEU	CA-CB-CG	-10.59	90.94	115.30
1	E	35	LEU	CA-CB-CG	-10.51	91.13	115.30
1	H	35	LEU	CA-CB-CG	-10.31	91.59	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	128	ARG	NH1-CZ-NH2	-8.82	109.70	119.40
1	C	131	ASP	CB-CG-OD1	8.46	125.91	118.30
1	C	111	LEU	CA-CB-CG	-7.34	98.43	115.30
1	A	134	VAL	CB-CA-C	-7.31	97.51	111.40
1	H	138	LEU	CA-CB-CG	-7.05	99.08	115.30
1	A	35	LEU	CA-CB-CG	-6.83	99.58	115.30
1	G	111	LEU	CA-CB-CG	-6.79	99.68	115.30
1	G	35	LEU	CA-CB-CG	-6.71	99.86	115.30
1	H	131	ASP	N-CA-C	-6.59	93.20	111.00
1	B	128	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	F	174	LEU	CA-CB-CG	-6.37	100.65	115.30
1	G	174	LEU	CA-CB-CG	-6.33	100.75	115.30
1	H	134	VAL	CB-CA-C	-6.31	99.41	111.40
1	E	111	LEU	CA-CB-CG	-6.30	100.81	115.30
1	D	111	LEU	CA-CB-CG	-6.18	101.08	115.30
1	A	188	THR	CB-CA-C	-6.16	94.96	111.60
1	F	172	CYS	CA-CB-SG	6.10	124.99	114.00
1	F	170	LEU	CA-CB-CG	-6.03	101.44	115.30
1	E	35	LEU	N-CA-C	6.01	127.22	111.00
1	F	153	LEU	CA-CB-CG	-5.96	101.59	115.30
1	G	59	LEU	CA-CB-CG	-5.92	101.70	115.30
1	H	35	LEU	N-CA-C	5.91	126.95	111.00
1	D	36	ILE	CB-CA-C	-5.89	99.81	111.60
1	H	168	VAL	CB-CA-C	-5.81	100.36	111.40
1	F	188	THR	CB-CA-C	-5.79	95.98	111.60
1	H	138	LEU	CB-CG-CD1	-5.74	101.24	111.00
1	C	36	ILE	CB-CA-C	-5.73	100.13	111.60
1	E	135	GLU	CB-CA-C	-5.64	99.12	110.40
1	D	200	ASN	N-CA-C	5.62	126.19	111.00
1	A	111	LEU	CA-CB-CG	-5.62	102.37	115.30
1	H	98	LEU	CB-CG-CD2	-5.61	101.46	111.00
1	F	119	LEU	CA-CB-CG	-5.54	102.55	115.30
1	A	139	CYS	CA-CB-SG	-5.48	104.13	114.00
1	H	111	LEU	CA-CB-CG	-5.45	102.77	115.30
1	C	131	ASP	OD1-CG-OD2	-5.37	113.11	123.30
1	E	98	LEU	CA-CB-CG	-5.36	102.96	115.30
1	F	189	ASP	CB-CG-OD1	-5.36	113.47	118.30
1	B	36	ILE	CB-CA-C	-5.35	100.90	111.60
1	A	134	VAL	CA-CB-CG1	-5.32	102.92	110.90
1	A	54	VAL	CB-CA-C	-5.31	101.30	111.40
1	D	56	ILE	CB-CA-C	-5.31	100.98	111.60
1	H	116	LEU	CB-CG-CD1	5.28	119.97	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	168	VAL	CB-CA-C	-5.27	101.38	111.40
1	B	35	LEU	CA-CB-CG	-5.26	103.20	115.30
1	H	64	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	A	35	LEU	N-CA-C	5.25	125.17	111.00
1	D	189	ASP	CB-CA-C	-5.25	99.91	110.40
1	E	65	VAL	CB-CA-C	-5.21	101.50	111.40
1	E	174	LEU	CA-CB-CG	-5.21	103.32	115.30
1	B	174	LEU	CA-CB-CG	-5.20	103.35	115.30
1	B	84	VAL	CB-CA-C	-5.18	101.55	111.40
1	C	43	GLY	N-CA-C	-5.15	100.23	113.10
1	F	59	LEU	CA-CB-CG	-5.08	103.61	115.30
1	H	98	LEU	CA-CB-CG	-5.05	103.69	115.30
1	F	166	LEU	CA-CB-CG	5.03	126.87	115.30
1	H	73	ARG	NE-CZ-NH1	-5.01	117.79	120.30
1	E	54	VAL	CB-CA-C	-5.01	101.88	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	GLY	Peptide
1	B	130	GLY	Peptide
1	F	101	SER	Peptide
1	F	71	ASP	Peptide
1	H	71	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1298	0	1338	85	1
1	B	1298	0	1338	73	0
1	C	1298	0	1338	92	0
1	D	1298	0	1338	80	0
1	E	1298	0	1338	109	0
1	F	1298	0	1338	136	1
1	G	1298	0	1338	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1298	0	1338	98	0
2	A	1	0	0	0	0
2	G	1	0	0	0	0
3	B	36	0	21	7	0
3	C	36	0	21	1	0
3	D	36	0	21	1	0
4	B	1	0	0	0	0
All	All	10495	0	10767	733	2

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 34.

All (733) 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:H:35:LEU:HD23	1:H:36:ILE:CD1	1.58	1.30
1:H:35:LEU:HD23	1:H:36:ILE:HD13	1.18	1.15
1:H:35:LEU:CD2	1:H:36:ILE:CD1	2.27	1.12
1:F:34:ASP:OD2	1:F:35:LEU:N	1.86	1.08
1:D:177:VAL:O	1:D:177:VAL:HG12	1.55	1.05
1:H:35:LEU:CD2	1:H:36:ILE:HD13	1.85	1.02
1:A:188:THR:HG22	1:A:189:ASP:N	1.70	1.00
1:H:171:GLN:OE1	1:H:171:GLN:C	1.98	1.00
1:H:171:GLN:OE1	1:H:171:GLN:O	1.77	1.00
1:F:180:ARG:HH11	1:F:180:ARG:HG2	1.27	0.99
1:E:180:ARG:HH11	1:E:180:ARG:HG2	1.27	0.99
1:E:180:ARG:CG	1:E:180:ARG:HH11	1.74	0.98
1:D:180:ARG:HH11	1:D:180:ARG:CG	1.78	0.97
1:H:35:LEU:CD2	1:H:36:ILE:HD11	1.93	0.97
1:A:180:ARG:HH11	1:A:180:ARG:HG2	1.25	0.96
1:G:180:ARG:HH11	1:G:180:ARG:CG	1.77	0.96
1:A:69:ASN:O	1:A:69:ASN:OD1	1.83	0.96
1:C:190:GLN:HB2	1:E:198:PHE:O	1.66	0.96
1:G:69:ASN:O	1:G:69:ASN:OD1	1.83	0.95
1:A:180:ARG:CG	1:A:180:ARG:HH11	1.80	0.94
1:E:73:ARG:HG3	1:E:73:ARG:HH21	1.30	0.93
1:C:177:VAL:O	1:C:177:VAL:HG12	1.69	0.92
1:H:180:ARG:HH11	1:H:180:ARG:HG2	1.36	0.91
1:G:180:ARG:HH11	1:G:180:ARG:HG2	1.34	0.90
1:F:69:ASN:OD1	1:F:69:ASN:N	2.02	0.90
1:A:73:ARG:HG3	1:A:73:ARG:HH21	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ARG:HH11	1:B:180:ARG:CG	1.84	0.89
1:C:194:THR:HG23	1:E:171:GLN:NE2	1.86	0.88
1:D:143:LYS:O	1:D:146:ALA:HB3	1.74	0.88
1:C:197:ASN:HB3	1:E:175:LYS:NZ	1.88	0.87
1:F:100:SER:O	1:F:101:SER:OG	1.92	0.86
1:F:35:LEU:HG	1:F:36:ILE:N	1.91	0.85
1:G:73:ARG:HG3	1:G:73:ARG:HH21	1.40	0.85
1:H:180:ARG:CG	1:H:180:ARG:HH11	1.90	0.85
1:F:51:ASP:O	1:F:55:LEU:HG	1.77	0.84
1:D:180:ARG:HH11	1:D:180:ARG:HG2	1.41	0.84
1:C:143:LYS:O	1:C:146:ALA:HB3	1.78	0.84
1:H:35:LEU:O	1:H:35:LEU:HG	1.67	0.84
1:B:180:ARG:HH11	1:B:180:ARG:HG2	1.41	0.83
1:A:129:ASN:HB2	1:A:163:LYS:O	1.78	0.82
1:A:154:THR:HG23	1:A:154:THR:O	1.80	0.81
1:F:159:VAL:HG12	1:F:160:GLY:N	1.94	0.81
1:F:159:VAL:HG12	1:F:160:GLY:H	1.45	0.80
1:A:188:THR:CG2	1:A:189:ASP:N	2.41	0.80
1:F:128:ARG:HH11	1:F:128:ARG:HB2	1.44	0.80
1:F:188:THR:HG22	1:F:189:ASP:N	1.95	0.80
1:C:180:ARG:CG	1:C:180:ARG:HH11	1.93	0.80
1:F:53:ASP:HB2	1:G:75:VAL:HG12	1.64	0.80
1:D:132:SER:O	1:D:137:LYS:HE3	1.82	0.79
1:A:35:LEU:O	1:A:35:LEU:HG	1.82	0.79
1:D:80:ARG:HB3	1:D:80:ARG:CZ	2.13	0.79
1:G:152:ILE:O	1:G:183:ASN:HB2	1.83	0.79
1:D:73:ARG:HG3	1:D:73:ARG:HH21	1.47	0.79
1:B:143:LYS:O	1:B:146:ALA:HB3	1.82	0.79
1:E:106:PRO:HA	1:E:125:VAL:HG12	1.65	0.79
1:F:180:ARG:HH11	1:F:180:ARG:CG	1.95	0.78
1:E:73:ARG:CG	1:E:73:ARG:HH21	1.97	0.78
1:A:111:LEU:HD13	1:A:122:LEU:HD12	1.64	0.78
1:C:180:ARG:HH11	1:C:180:ARG:HG2	1.47	0.78
1:C:194:THR:HG23	1:E:171:GLN:HE21	1.45	0.77
1:F:56:ILE:HD12	1:F:85:PHE:CD2	2.20	0.77
1:E:188:THR:HG22	1:E:189:ASP:N	1.99	0.77
1:H:158:SER:HB3	1:H:164:VAL:HG21	1.66	0.76
1:E:69:ASN:OD1	1:E:69:ASN:O	2.02	0.76
1:H:73:ARG:HH21	1:H:73:ARG:HG3	1.50	0.76
1:F:76:GLY:O	1:F:80:ARG:HB3	1.85	0.76
1:G:111:LEU:HD23	1:G:113:GLU:HG2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:LYS:HB3	1:C:168:VAL:HG23	1.66	0.75
1:A:158:SER:O	1:A:164:VAL:HG23	1.87	0.75
1:G:106:PRO:HA	1:G:125:VAL:HG12	1.67	0.75
1:A:78:VAL:O	1:A:81:ALA:HB3	1.86	0.75
1:B:73:ARG:HG3	1:B:73:ARG:HH21	1.51	0.75
1:D:44:LYS:HD2	1:D:181:ASP:OD1	1.86	0.75
1:E:129:ASN:HB2	1:E:163:LYS:O	1.87	0.75
1:H:159:VAL:HG12	1:H:160:GLY:N	2.01	0.74
1:H:158:SER:O	1:H:164:VAL:HG23	1.87	0.74
1:E:73:ARG:NH2	1:E:73:ARG:HG3	2.01	0.74
1:H:134:VAL:HG23	1:H:135:GLU:N	2.03	0.74
1:A:158:SER:HB3	1:A:164:VAL:HG21	1.69	0.74
1:G:128:ARG:HB3	1:G:131:ASP:OD2	1.88	0.73
1:B:165:LYS:HB3	1:B:168:VAL:HG23	1.70	0.73
1:E:159:VAL:HG12	1:E:160:GLY:N	2.03	0.73
1:E:188:THR:HG22	1:E:190:GLN:N	2.04	0.73
1:A:171:GLN:OE1	1:A:171:GLN:HA	1.87	0.73
1:F:82:ILE:HG22	1:F:83:ASP:N	2.04	0.73
1:C:189:ASP:O	1:C:193:VAL:HG23	1.89	0.73
1:D:177:VAL:CG1	1:D:177:VAL:O	2.29	0.73
1:E:35:LEU:O	1:E:35:LEU:HG	1.64	0.72
1:C:132:SER:O	1:C:137:LYS:HE3	1.90	0.72
1:E:171:GLN:HA	1:E:171:GLN:OE1	1.88	0.72
1:A:106:PRO:HA	1:A:125:VAL:HG12	1.72	0.72
1:D:94:SER:O	1:D:95:LYS:C	2.26	0.71
1:F:110:VAL:HG12	1:F:111:LEU:N	2.05	0.71
1:F:104:ILE:HG22	1:F:125:VAL:CG2	2.21	0.71
1:C:188:THR:HB	1:C:190:GLN:HB3	1.73	0.71
1:E:75:VAL:HG12	1:G:53:ASP:HB2	1.70	0.71
1:F:159:VAL:CG1	1:F:160:GLY:H	2.03	0.71
1:F:188:THR:HG22	1:F:189:ASP:H	1.54	0.70
1:G:129:ASN:HB2	1:G:163:LYS:O	1.90	0.70
1:F:155:PRO:HD3	1:F:185:PHE:CE2	2.26	0.70
1:F:188:THR:HB	1:F:191:GLU:H	1.57	0.70
1:G:154:THR:O	1:G:154:THR:HG23	1.90	0.70
1:F:52:LEU:O	1:F:56:ILE:HG13	1.92	0.70
1:H:68:ALA:O	1:H:125:VAL:HG22	1.90	0.70
1:D:106:PRO:HA	1:D:125:VAL:HG12	1.73	0.70
1:E:158:SER:HB3	1:E:164:VAL:HG21	1.74	0.70
1:F:39:PHE:CE2	1:F:192:ARG:HG3	2.26	0.70
1:B:189:ASP:O	1:B:193:VAL:HG23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LEU:HD11	1:B:158:SER:HB2	1.72	0.69
1:H:154:THR:O	1:H:154:THR:HG23	1.92	0.69
1:F:110:VAL:CG1	1:F:111:LEU:N	2.55	0.69
1:F:69:ASN:C	1:F:71:ASP:H	1.93	0.69
1:B:36:ILE:O	1:B:36:ILE:HG22	1.92	0.69
1:D:133:ARG:O	1:D:135:GLU:N	2.26	0.69
1:F:45:VAL:HG13	1:F:182:LEU:HD23	1.74	0.69
1:B:54:VAL:O	1:B:54:VAL:HG12	1.92	0.69
1:E:152:ILE:O	1:E:183:ASN:HB2	1.92	0.69
1:F:104:ILE:CG2	1:F:125:VAL:CG2	2.71	0.69
1:E:111:LEU:CD1	1:E:122:LEU:HD12	2.22	0.69
1:F:34:ASP:CG	1:F:35:LEU:H	1.96	0.68
1:F:97:TYR:HD2	1:F:98:LEU:HG	1.56	0.68
1:A:73:ARG:CG	1:A:73:ARG:HH21	2.05	0.68
1:B:127:PRO:HD2	1:B:138:LEU:CD1	2.23	0.68
1:A:152:ILE:O	1:A:183:ASN:HB2	1.94	0.68
1:A:188:THR:HG22	1:A:189:ASP:H	1.53	0.68
1:H:129:ASN:HB2	1:H:163:LYS:O	1.93	0.68
1:A:76:GLY:HA2	1:A:80:ARG:HH12	1.59	0.68
1:F:104:ILE:HG22	1:F:125:VAL:HG21	1.75	0.68
1:H:159:VAL:CG1	1:H:160:GLY:N	2.57	0.68
1:H:171:GLN:CA	1:H:171:GLN:OE1	2.40	0.68
1:G:188:THR:HG22	1:G:189:ASP:N	2.09	0.68
1:A:83:ASP:OD2	1:A:90:LEU:HB3	1.94	0.67
1:F:180:ARG:NH1	1:F:180:ARG:HG2	2.03	0.67
1:G:111:LEU:HG	1:G:112:PHE:N	2.09	0.67
1:C:188:THR:HG22	1:E:200:ASN:O	1.94	0.67
1:H:100:SER:O	1:H:101:SER:OG	2.11	0.67
1:H:134:VAL:HG23	1:H:135:GLU:H	1.59	0.67
1:C:138:LEU:HD11	1:C:158:SER:HB2	1.75	0.67
1:E:111:LEU:HD13	1:E:122:LEU:HD12	1.75	0.67
1:C:44:LYS:HD2	1:C:181:ASP:OD1	1.94	0.66
1:D:165:LYS:HB3	1:D:168:VAL:HG23	1.75	0.66
1:H:35:LEU:HD21	1:H:36:ILE:CD1	2.24	0.66
1:C:190:GLN:CB	1:E:198:PHE:O	2.42	0.66
1:C:197:ASN:HB3	1:E:175:LYS:HZ1	1.60	0.66
1:F:56:ILE:HG21	1:F:85:PHE:HE2	1.60	0.66
1:H:159:VAL:CG1	1:H:160:GLY:H	2.09	0.66
1:C:165:LYS:HB3	1:C:168:VAL:CG2	2.26	0.66
1:C:177:VAL:O	1:C:177:VAL:CG1	2.43	0.66
1:E:102:LYS:HG2	1:E:103:ALA:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:PRO:HA	1:F:125:VAL:HG12	1.78	0.65
1:A:80:ARG:HG2	1:A:80:ARG:O	1.95	0.65
1:E:159:VAL:CG1	1:E:160:GLY:N	2.60	0.65
1:F:188:THR:HB	1:F:191:GLU:HB2	1.79	0.65
1:C:133:ARG:O	1:C:135:GLU:N	2.30	0.64
1:F:94:SER:O	1:F:95:LYS:C	2.34	0.64
1:H:35:LEU:HD23	1:H:36:ILE:HD11	1.58	0.64
1:H:73:ARG:HH21	1:H:73:ARG:CG	2.09	0.64
1:F:94:SER:C	1:F:96:GLU:N	2.48	0.64
1:F:71:ASP:O	1:F:72:LEU:HB2	1.96	0.64
1:D:133:ARG:C	1:D:135:GLU:N	2.47	0.64
1:A:76:GLY:HA2	1:A:80:ARG:NH1	2.13	0.64
1:F:34:ASP:CG	1:F:35:LEU:N	2.51	0.64
1:F:52:LEU:HG	1:F:56:ILE:HD11	1.80	0.64
1:H:102:LYS:HG2	1:H:103:ALA:N	2.12	0.63
1:F:94:SER:O	1:F:96:GLU:N	2.31	0.63
1:C:197:ASN:OD1	1:E:171:GLN:HG3	1.97	0.63
1:C:64:LEU:HB2	1:C:119:LEU:HD11	1.79	0.63
1:E:83:ASP:OD2	1:E:90:LEU:HB3	1.98	0.63
1:H:152:ILE:O	1:H:183:ASN:HB2	1.98	0.63
1:D:36:ILE:O	1:D:36:ILE:HG22	1.97	0.63
1:B:111:LEU:HD12	1:B:122:LEU:HA	1.80	0.62
1:D:180:ARG:CG	1:D:180:ARG:NH1	2.49	0.62
1:A:133:ARG:HG2	1:A:136:GLY:H	1.65	0.62
1:D:109:ALA:HB2	1:D:124:ALA:HA	1.82	0.62
1:A:102:LYS:HG2	1:A:103:ALA:N	2.15	0.62
1:F:40:TYR:CD2	1:F:41:LYS:N	2.67	0.62
1:B:127:PRO:HD2	1:B:138:LEU:HD12	1.80	0.62
1:D:94:SER:O	1:D:96:GLU:N	2.33	0.62
1:E:128:ARG:HB3	1:E:131:ASP:OD2	2.00	0.62
1:E:188:THR:CG2	1:E:189:ASP:N	2.62	0.62
1:D:189:ASP:O	1:D:193:VAL:HG23	2.00	0.62
1:E:159:VAL:CG1	1:E:160:GLY:H	2.13	0.62
1:E:75:VAL:CG1	1:G:53:ASP:HB2	2.28	0.62
1:E:188:THR:HG22	1:E:190:GLN:H	1.65	0.62
1:F:53:ASP:HB2	1:G:75:VAL:CG1	2.30	0.61
1:B:177:VAL:O	1:B:177:VAL:HG12	2.00	0.61
1:G:35:LEU:O	1:G:35:LEU:HG	1.95	0.61
1:F:80:ARG:CG	1:F:81:ALA:N	2.58	0.61
1:C:133:ARG:C	1:C:135:GLU:N	2.53	0.61
1:H:83:ASP:OD2	1:H:90:LEU:HB3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:188:THR:HG22	1:H:189:ASP:N	2.16	0.61
1:A:154:THR:CG2	1:A:154:THR:O	2.49	0.61
1:C:111:LEU:HD12	1:C:122:LEU:HA	1.82	0.61
1:A:180:ARG:NH1	1:A:180:ARG:CG	2.50	0.61
1:B:73:ARG:NH2	1:B:73:ARG:HG3	2.15	0.61
1:F:159:VAL:CG1	1:F:160:GLY:N	2.59	0.61
1:A:100:SER:O	1:A:101:SER:OG	2.20	0.60
1:F:44:LYS:HB3	1:F:181:ASP:HB3	1.83	0.60
1:A:105:ALA:O	1:A:106:PRO:C	2.40	0.60
1:E:180:ARG:CG	1:E:180:ARG:NH1	2.46	0.60
1:F:53:ASP:N	1:F:53:ASP:OD1	2.34	0.60
1:H:167:GLU:OE2	1:H:167:GLU:N	2.32	0.60
1:H:73:ARG:HG3	1:H:73:ARG:NH2	2.16	0.60
1:D:133:ARG:O	1:D:134:VAL:C	2.36	0.60
1:F:69:ASN:C	1:F:71:ASP:N	2.55	0.60
1:H:106:PRO:HA	1:H:125:VAL:HG12	1.83	0.60
1:C:127:PRO:HD2	1:C:138:LEU:CD1	2.32	0.60
1:F:69:ASN:O	1:F:71:ASP:N	2.34	0.59
1:C:153:LEU:HD12	1:C:183:ASN:O	2.01	0.59
1:F:97:TYR:CD2	1:F:98:LEU:HG	2.37	0.59
1:H:190:GLN:O	1:H:194:THR:OG1	2.19	0.59
1:B:106:PRO:HA	1:B:125:VAL:HG12	1.83	0.59
1:D:73:ARG:HG3	1:D:73:ARG:NH2	2.13	0.59
1:D:143:LYS:O	1:D:146:ALA:CB	2.48	0.59
1:F:155:PRO:HD3	1:F:185:PHE:HE2	1.66	0.59
1:F:138:LEU:HD11	1:F:158:SER:HB2	1.85	0.59
1:F:193:VAL:HG12	1:F:194:THR:N	2.16	0.59
1:D:65:VAL:CG2	1:D:154:THR:HB	2.32	0.59
1:F:91:THR:O	1:F:94:SER:N	2.32	0.58
1:B:39:PHE:O	1:B:40:TYR:HB2	2.03	0.58
1:G:159:VAL:HG12	1:G:160:GLY:N	2.18	0.58
1:H:133:ARG:C	1:H:135:GLU:N	2.52	0.58
1:C:133:ARG:O	1:C:134:VAL:C	2.41	0.58
1:E:100:SER:O	1:E:101:SER:OG	2.20	0.58
1:E:188:THR:HG21	1:E:190:GLN:HB2	1.86	0.58
1:F:82:ILE:CG2	1:F:90:LEU:HD22	2.33	0.58
1:C:143:LYS:O	1:C:146:ALA:CB	2.51	0.58
1:C:154:THR:OG1	1:C:155:PRO:HD2	2.04	0.58
1:D:109:ALA:CB	1:D:124:ALA:HA	2.34	0.58
1:C:188:THR:HG22	1:E:200:ASN:C	2.23	0.58
1:G:105:ALA:O	1:G:106:PRO:C	2.40	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ASP:HB2	1:E:40:TYR:CE1	2.38	0.58
1:H:35:LEU:HD23	1:H:36:ILE:CG1	2.28	0.58
1:A:73:ARG:NH2	1:A:73:ARG:HG3	2.08	0.58
1:A:159:VAL:HG12	1:A:160:GLY:N	2.16	0.58
1:F:110:VAL:CG1	1:F:111:LEU:H	2.17	0.58
1:H:111:LEU:HD12	1:H:122:LEU:HA	1.85	0.58
1:C:127:PRO:HD2	1:C:138:LEU:HD12	1.85	0.58
1:E:171:GLN:CA	1:E:171:GLN:OE1	2.52	0.58
1:C:39:PHE:O	1:C:40:TYR:HB2	2.04	0.57
1:D:165:LYS:HB3	1:D:168:VAL:CG2	2.34	0.57
1:G:133:ARG:C	1:G:135:GLU:N	2.54	0.57
1:G:100:SER:O	1:G:101:SER:OG	2.21	0.57
1:A:111:LEU:HD12	1:A:122:LEU:HA	1.87	0.57
1:A:133:ARG:C	1:A:135:GLU:N	2.56	0.57
1:B:173:LEU:C	1:B:173:LEU:HD23	2.23	0.57
1:D:173:LEU:C	1:D:173:LEU:HD23	2.25	0.57
1:B:132:SER:O	1:B:137:LYS:HE3	2.04	0.57
1:C:93:ARG:NE	1:C:93:ARG:HA	2.20	0.57
1:G:55:LEU:O	1:G:56:ILE:C	2.40	0.57
1:A:173:LEU:C	1:A:173:LEU:HD23	2.24	0.57
1:E:190:GLN:O	1:E:194:THR:OG1	2.22	0.57
1:D:75:VAL:O	3:D:477:APR:HR'1	2.05	0.56
1:G:68:ALA:O	1:G:125:VAL:HG22	2.05	0.56
1:H:128:ARG:HB3	1:H:131:ASP:OD2	2.04	0.56
1:A:66:ASN:HB2	1:A:82:ILE:HD12	1.87	0.56
1:F:197:ASN:C	1:F:199:PHE:N	2.55	0.56
1:G:49:GLN:HG2	1:G:50:GLY:N	2.20	0.56
1:D:180:ARG:HH11	1:D:180:ARG:HG3	1.65	0.56
1:D:47:PHE:CD2	1:D:47:PHE:N	2.73	0.56
1:G:159:VAL:CG1	1:G:160:GLY:N	2.68	0.56
1:C:74:HIS:CE1	1:C:90:LEU:HD21	2.41	0.56
1:G:180:ARG:NH1	1:G:180:ARG:HG2	2.15	0.56
1:H:133:ARG:HG2	1:H:136:GLY:H	1.70	0.56
1:B:105:ALA:O	1:B:106:PRO:C	2.43	0.56
1:F:80:ARG:HG3	1:F:81:ALA:N	2.01	0.56
1:B:128:ARG:HB2	1:B:128:ARG:HH11	1.70	0.56
1:B:129:ASN:HB2	1:B:163:LYS:O	2.06	0.56
1:F:100:SER:C	1:F:101:SER:HG	2.03	0.56
1:F:39:PHE:CZ	1:F:192:ARG:HG3	2.41	0.56
1:H:166:LEU:O	1:H:167:GLU:C	2.42	0.56
1:C:184:VAL:HG12	1:C:185:PHE:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:ILE:HG21	1:F:125:VAL:HG23	1.88	0.56
1:F:155:PRO:CD	1:F:185:PHE:CE2	2.89	0.56
1:H:158:SER:HB3	1:H:164:VAL:CG2	2.33	0.56
1:E:154:THR:O	1:E:154:THR:HG23	2.05	0.56
1:C:197:ASN:HB3	1:E:175:LYS:HZ2	1.70	0.55
1:F:56:ILE:HD12	1:F:85:PHE:CE2	2.40	0.55
1:E:158:SER:O	1:E:164:VAL:HG23	2.06	0.55
1:G:145:ILE:O	1:G:146:ALA:C	2.44	0.55
1:A:128:ARG:HB3	1:A:131:ASP:OD2	2.06	0.55
1:G:180:ARG:CG	1:G:180:ARG:NH1	2.50	0.55
1:A:159:VAL:CG1	1:A:160:GLY:N	2.69	0.55
1:B:65:VAL:HG12	1:B:66:ASN:N	2.22	0.55
1:E:180:ARG:HG2	1:E:180:ARG:NH1	2.08	0.55
1:D:190:GLN:HA	1:E:193:VAL:HG11	1.87	0.55
1:E:111:LEU:HD12	1:E:122:LEU:HA	1.88	0.55
1:G:80:ARG:HH11	1:G:80:ARG:HB3	1.72	0.55
1:C:74:HIS:CD2	1:C:90:LEU:HD23	2.42	0.54
1:D:188:THR:HB	1:D:190:GLN:HB3	1.87	0.54
1:D:94:SER:C	1:D:96:GLU:N	2.60	0.54
1:A:49:GLN:HG2	1:A:50:GLY:N	2.22	0.54
1:E:105:ALA:O	1:E:106:PRO:C	2.45	0.54
1:D:65:VAL:HG21	1:D:154:THR:HB	1.89	0.54
1:F:170:LEU:HD23	1:F:198:PHE:CD1	2.42	0.54
1:G:80:ARG:NH1	1:G:80:ARG:HB3	2.23	0.54
1:D:111:LEU:HD12	1:D:122:LEU:HA	1.90	0.54
1:F:40:TYR:HE2	1:F:42:ALA:HB2	1.73	0.54
1:G:133:ARG:HG2	1:G:136:GLY:H	1.72	0.54
1:H:49:GLN:HG2	1:H:50:GLY:N	2.23	0.54
1:F:180:ARG:NH1	1:F:180:ARG:CG	2.64	0.54
1:G:83:ASP:OD2	1:G:90:LEU:HB3	2.08	0.53
1:D:138:LEU:CD2	1:D:169:SER:HA	2.38	0.53
1:D:138:LEU:HD21	1:D:169:SER:HA	1.91	0.53
1:D:79:ALA:O	1:D:80:ARG:C	2.41	0.53
1:F:154:THR:HG23	1:F:154:THR:O	2.08	0.53
1:B:44:LYS:HD2	1:B:181:ASP:OD1	2.09	0.53
1:E:159:VAL:HG12	1:E:160:GLY:H	1.70	0.53
1:G:73:ARG:HH21	1:G:73:ARG:CG	2.16	0.53
1:H:159:VAL:HG12	1:H:160:GLY:H	1.69	0.53
1:H:128:ARG:NH1	1:H:162:PHE:HE1	2.06	0.53
1:B:157:ILE:O	1:B:158:SER:HB2	2.07	0.53
1:B:167:GLU:OE1	1:B:194:THR:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:ILE:HG22	1:F:125:VAL:CB	2.39	0.53
1:C:65:VAL:HG21	1:C:154:THR:HB	1.91	0.53
1:D:145:ILE:O	1:D:146:ALA:C	2.46	0.53
1:E:173:LEU:HD23	1:E:173:LEU:C	2.28	0.53
1:G:143:LYS:O	1:G:146:ALA:HB3	2.09	0.53
1:H:127:PRO:HD2	1:H:138:LEU:HD12	1.91	0.53
1:C:157:ILE:O	1:C:158:SER:HB2	2.08	0.53
1:B:94:SER:O	1:B:95:LYS:C	2.46	0.52
1:C:47:PHE:N	1:C:47:PHE:CD2	2.75	0.52
1:C:81:ALA:O	1:C:84:VAL:HB	2.09	0.52
1:C:188:THR:CB	1:C:190:GLN:HB3	2.38	0.52
1:F:35:LEU:O	1:F:37:LEU:HG	2.10	0.52
1:F:40:TYR:C	1:F:40:TYR:CD2	2.82	0.52
1:A:116:LEU:HB2	1:A:119:LEU:HB3	1.91	0.52
1:E:166:LEU:O	1:E:167:GLU:C	2.45	0.52
1:F:104:ILE:HG22	1:F:125:VAL:HB	1.91	0.52
1:F:155:PRO:HB3	1:F:185:PHE:CZ	2.45	0.52
1:F:71:ASP:O	1:F:72:LEU:CB	2.58	0.52
1:A:188:THR:HG22	1:A:190:GLN:N	2.24	0.52
1:D:39:PHE:O	1:D:40:TYR:HB2	2.07	0.52
1:D:100:SER:O	1:D:100:SER:OG	2.28	0.52
1:E:35:LEU:HD23	1:E:36:ILE:HD11	1.90	0.52
1:F:158:SER:HA	1:F:162:PHE:CD2	2.44	0.52
1:F:39:PHE:CG	1:F:192:ARG:HD2	2.45	0.52
1:B:143:LYS:O	1:B:147:LYS:HE3	2.10	0.52
1:D:116:LEU:HB2	1:D:119:LEU:HB3	1.92	0.52
1:D:200:ASN:O	1:G:190:GLN:OE1	2.28	0.52
1:H:44:LYS:HB2	1:H:180:ARG:O	2.10	0.52
1:D:191:GLU:O	1:D:192:ARG:C	2.49	0.51
1:C:52:LEU:HD13	1:C:185:PHE:CE1	2.45	0.51
1:F:181:ASP:OD1	1:F:181:ASP:N	2.43	0.51
1:G:190:GLN:O	1:G:194:THR:OG1	2.22	0.51
1:H:173:LEU:HD23	1:H:173:LEU:C	2.31	0.51
1:H:94:SER:O	1:H:95:LYS:C	2.48	0.51
1:H:154:THR:O	1:H:154:THR:CG2	2.57	0.51
1:C:173:LEU:HD23	1:C:173:LEU:C	2.31	0.51
1:C:53:ASP:N	1:C:53:ASP:OD1	2.44	0.51
1:E:51:ASP:O	1:E:55:LEU:HG	2.10	0.51
1:B:54:VAL:HG22	1:C:75:VAL:HB	1.93	0.51
1:G:154:THR:CG2	1:G:154:THR:O	2.58	0.51
1:B:77:GLY:HA2	3:B:477:APR:N7	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:GLU:OE1	1:C:194:THR:HG22	2.11	0.51
1:B:93:ARG:HA	1:B:93:ARG:NE	2.26	0.51
1:C:133:ARG:C	1:C:135:GLU:H	2.14	0.51
1:G:165:LYS:HB2	1:G:168:VAL:HG23	1.93	0.51
1:A:190:GLN:O	1:A:194:THR:OG1	2.27	0.51
1:C:106:PRO:HA	1:C:125:VAL:HG12	1.93	0.51
1:E:133:ARG:C	1:E:135:GLU:N	2.56	0.51
1:A:153:LEU:HD12	1:A:183:ASN:O	2.11	0.50
1:F:38:PRO:HD3	1:F:48:TYR:CZ	2.47	0.50
1:A:66:ASN:HB2	1:A:82:ILE:CD1	2.41	0.50
1:D:157:ILE:CG2	1:D:158:SER:N	2.75	0.50
1:G:51:ASP:O	1:G:55:LEU:HG	2.11	0.50
1:D:133:ARG:C	1:D:135:GLU:H	2.12	0.50
1:E:80:ARG:HH21	1:G:53:ASP:CG	2.14	0.50
1:G:104:ILE:CD1	1:G:110:VAL:HB	2.41	0.50
1:A:176:THR:C	1:A:178:THR:H	2.14	0.50
1:B:189:ASP:HB2	1:E:40:TYR:HE1	1.75	0.50
1:H:180:ARG:CG	1:H:180:ARG:NH1	2.60	0.50
1:F:88:GLY:O	1:F:92:LYS:HG2	2.12	0.50
1:H:170:LEU:O	1:H:171:GLN:C	2.50	0.50
1:C:52:LEU:O	1:C:54:VAL:N	2.45	0.50
1:F:96:GLU:HA	1:F:99:LYS:HE3	1.93	0.50
1:A:111:LEU:CD1	1:A:122:LEU:HD12	2.38	0.49
1:B:109:ALA:CB	1:B:124:ALA:HA	2.42	0.49
1:C:63:VAL:HB	1:C:152:ILE:HG23	1.94	0.49
1:F:104:ILE:HG21	1:F:125:VAL:CG2	2.41	0.49
1:B:109:ALA:HB2	1:B:124:ALA:HA	1.93	0.49
1:C:109:ALA:HB2	1:C:124:ALA:HA	1.93	0.49
1:E:153:LEU:HD12	1:E:183:ASN:O	2.12	0.49
1:F:128:ARG:NH1	1:F:128:ARG:HB2	2.20	0.49
1:A:158:SER:HB3	1:A:164:VAL:CG2	2.41	0.49
1:B:111:LEU:HD12	1:B:122:LEU:CA	2.42	0.49
1:E:111:LEU:HD12	1:E:122:LEU:HD12	1.94	0.49
1:E:172:CYS:O	1:E:173:LEU:C	2.49	0.49
1:G:188:THR:CG2	1:G:189:ASP:N	2.76	0.49
1:H:39:PHE:CE2	1:H:192:ARG:HG2	2.48	0.49
1:A:76:GLY:CA	1:A:80:ARG:NH1	2.76	0.49
1:F:192:ARG:O	1:F:195:ILE:HB	2.12	0.49
1:G:73:ARG:NH2	1:G:73:ARG:HG3	2.13	0.49
1:B:138:LEU:CD2	1:B:169:SER:HA	2.42	0.49
1:B:169:SER:O	1:B:170:LEU:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:THR:HB	1:B:190:GLN:HB3	1.95	0.49
1:G:136:GLY:O	1:G:137:LYS:C	2.50	0.49
1:H:105:ALA:O	1:H:106:PRO:C	2.49	0.49
1:B:138:LEU:HD23	1:B:169:SER:HA	1.95	0.48
1:B:191:GLU:OE1	3:B:477:APR:O3'	2.25	0.48
1:D:154:THR:OG1	1:D:155:PRO:HD2	2.13	0.48
1:G:112:PHE:CD1	1:G:112:PHE:N	2.79	0.48
1:H:134:VAL:CG2	1:H:135:GLU:N	2.73	0.48
1:B:143:LYS:O	1:B:146:ALA:CB	2.58	0.48
1:C:145:ILE:O	1:C:146:ALA:C	2.52	0.48
1:D:129:ASN:HB2	1:D:163:LYS:O	2.13	0.48
1:F:174:LEU:HD23	1:F:174:LEU:HA	1.28	0.48
1:B:180:ARG:NH1	1:B:180:ARG:CG	2.56	0.48
1:C:52:LEU:O	1:C:53:ASP:C	2.52	0.48
1:E:133:ARG:HG2	1:E:136:GLY:H	1.78	0.48
1:E:158:SER:HB3	1:E:164:VAL:CG2	2.41	0.48
1:F:35:LEU:HG	1:F:36:ILE:HG13	1.94	0.48
1:G:104:ILE:HD11	1:G:110:VAL:HB	1.96	0.48
1:B:153:LEU:HD12	1:B:183:ASN:O	2.13	0.48
1:B:65:VAL:HG21	1:B:154:THR:HB	1.95	0.48
1:C:160:GLY:O	1:C:162:PHE:N	2.47	0.48
1:C:197:ASN:OD1	1:E:171:GLN:CG	2.61	0.48
1:G:176:THR:C	1:G:178:THR:H	2.17	0.48
1:H:128:ARG:NH1	1:H:162:PHE:CE1	2.82	0.48
1:H:172:CYS:O	1:H:173:LEU:C	2.50	0.48
1:G:38:PRO:HB3	1:G:46:SER:HB3	1.95	0.48
1:H:35:LEU:HD21	1:H:36:ILE:HD11	1.86	0.48
1:C:138:LEU:CD2	1:C:169:SER:HA	2.44	0.48
1:C:80:ARG:HE	1:C:84:VAL:HG23	1.77	0.48
1:F:157:ILE:HG22	1:F:158:SER:N	2.27	0.48
1:C:180:ARG:CG	1:C:180:ARG:NH1	2.63	0.48
1:A:188:THR:HB	1:A:191:GLU:H	1.79	0.47
1:B:127:PRO:HD2	1:B:138:LEU:HD13	1.94	0.47
1:F:104:ILE:CG2	1:F:125:VAL:HG21	2.38	0.47
1:G:159:VAL:CG1	1:G:160:GLY:H	2.27	0.47
1:B:77:GLY:CA	3:B:477:APR:N7	2.77	0.47
1:C:105:ALA:O	1:C:108:ASN:N	2.48	0.47
1:D:112:PHE:CD1	1:D:112:PHE:N	2.80	0.47
1:F:138:LEU:CD2	1:F:169:SER:HA	2.44	0.47
1:F:155:PRO:N	1:F:185:PHE:CE2	2.82	0.47
1:G:154:THR:O	1:G:184:VAL:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:173:LEU:C	1:G:173:LEU:HD23	2.35	0.47
1:E:80:ARG:NH2	1:G:53:ASP:OD1	2.41	0.47
1:B:133:ARG:C	1:B:135:GLU:N	2.66	0.47
1:F:135:GLU:O	1:F:136:GLY:C	2.52	0.47
1:A:176:THR:O	1:A:178:THR:HG23	2.15	0.47
1:E:104:ILE:HD11	1:E:110:VAL:HB	1.96	0.47
1:F:39:PHE:O	1:F:40:TYR:HB2	2.15	0.47
1:F:59:LEU:HD23	1:F:59:LEU:HA	1.61	0.47
1:G:136:GLY:O	1:G:139:CYS:N	2.48	0.47
1:C:65:VAL:CG2	1:C:154:THR:HB	2.45	0.47
1:F:94:SER:C	1:F:96:GLU:H	2.17	0.47
1:D:157:ILE:HG22	1:D:158:SER:N	2.29	0.47
1:F:104:ILE:CG2	1:F:125:VAL:HB	2.45	0.47
1:F:129:ASN:HB2	1:F:163:LYS:O	2.15	0.47
1:G:111:LEU:CD2	1:G:113:GLU:HG2	2.42	0.47
1:B:133:ARG:O	1:B:134:VAL:C	2.52	0.47
1:E:78:VAL:O	1:E:81:ALA:HB3	2.15	0.47
1:F:100:SER:OG	1:F:100:SER:O	2.24	0.47
1:F:70:GLY:O	1:F:103:ALA:HB1	2.15	0.47
1:H:78:VAL:O	1:H:81:ALA:HB3	2.14	0.47
1:D:98:LEU:HD23	1:D:98:LEU:HA	1.67	0.47
1:F:93:ARG:NH2	1:F:96:GLU:OE2	2.37	0.47
1:G:78:VAL:O	1:G:81:ALA:HB3	2.15	0.47
1:B:66:ASN:HB2	1:B:82:ILE:HD13	1.97	0.47
1:C:142:TYR:CZ	1:C:173:LEU:HB2	2.50	0.47
1:C:184:VAL:CG1	1:C:185:PHE:N	2.78	0.47
1:E:180:ARG:HG3	1:E:180:ARG:HH11	1.72	0.47
1:F:40:TYR:HD2	1:F:41:LYS:N	2.11	0.47
1:H:109:ALA:HB1	1:H:122:LEU:HD21	1.97	0.47
1:D:195:ILE:O	1:D:198:PHE:HB3	2.15	0.46
1:F:157:ILE:O	1:F:158:SER:HB2	2.15	0.46
1:F:40:TYR:CE2	1:F:42:ALA:HB2	2.50	0.46
1:B:65:VAL:CG2	1:B:154:THR:HB	2.45	0.46
1:G:158:SER:HB2	1:G:164:VAL:HG21	1.97	0.46
1:F:74:HIS:HB3	1:F:79:ALA:HB1	1.96	0.46
1:H:36:ILE:HD13	1:H:36:ILE:N	2.28	0.46
1:H:38:PRO:HB3	1:H:46:SER:HB3	1.97	0.46
1:B:74:HIS:CD2	1:B:90:LEU:HD23	2.50	0.46
1:D:81:ALA:O	1:D:84:VAL:HB	2.15	0.46
1:E:106:PRO:HA	1:E:125:VAL:CG1	2.41	0.46
1:E:35:LEU:HD23	1:E:36:ILE:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:ILE:HG22	1:F:90:LEU:HD22	1.96	0.46
1:G:180:ARG:HH11	1:G:180:ARG:HG3	1.68	0.46
1:C:188:THR:CG2	1:E:200:ASN:O	2.63	0.46
1:E:52:LEU:O	1:E:53:ASP:C	2.54	0.46
1:B:170:LEU:HA	1:B:170:LEU:HD12	1.65	0.46
1:B:35:LEU:HA	1:B:35:LEU:HD12	1.69	0.46
1:F:195:ILE:O	1:F:199:PHE:HD1	1.99	0.46
1:F:68:ALA:O	1:F:125:VAL:HG22	2.15	0.46
1:G:98:LEU:HD23	1:G:98:LEU:HA	1.44	0.46
1:A:188:THR:CG2	1:A:189:ASP:H	2.17	0.46
1:E:115:VAL:O	1:E:116:LEU:HD23	2.15	0.46
1:E:49:GLN:HG2	1:E:50:GLY:N	2.30	0.46
1:H:170:LEU:HD12	1:H:170:LEU:C	2.37	0.46
1:D:180:ARG:NH1	1:D:180:ARG:HG3	2.26	0.46
1:H:74:HIS:HB3	1:H:79:ALA:HB1	1.97	0.46
1:A:136:GLY:O	1:A:137:LYS:C	2.55	0.45
1:C:143:LYS:HB2	1:C:143:LYS:NZ	2.31	0.45
1:F:197:ASN:C	1:F:199:PHE:H	2.19	0.45
1:G:53:ASP:OD1	1:G:53:ASP:N	2.50	0.45
1:A:157:ILE:HD13	1:A:157:ILE:HA	1.74	0.45
1:A:79:ALA:C	1:A:81:ALA:N	2.69	0.45
1:F:196:GLU:O	1:F:199:PHE:HB2	2.16	0.45
1:H:104:ILE:HD11	1:H:110:VAL:HB	1.97	0.45
1:A:39:PHE:CD2	1:A:39:PHE:C	2.90	0.45
1:B:191:GLU:O	1:B:194:THR:N	2.48	0.45
1:B:98:LEU:HA	1:B:98:LEU:HD23	1.68	0.45
1:D:170:LEU:HA	1:D:170:LEU:HD12	1.47	0.45
1:F:188:THR:CG2	1:F:189:ASP:N	2.64	0.45
1:H:136:GLY:O	1:H:137:LYS:C	2.54	0.45
1:H:165:LYS:HB2	1:H:168:VAL:HG23	1.98	0.45
1:H:180:ARG:NH1	1:H:180:ARG:HG2	2.17	0.45
1:C:197:ASN:HB3	1:E:175:LYS:CE	2.47	0.45
1:G:69:ASN:CG	1:G:69:ASN:O	2.50	0.45
1:H:51:ASP:O	1:H:55:LEU:HG	2.15	0.45
1:D:160:GLY:O	1:D:161:ILE:C	2.55	0.45
1:G:188:THR:HB	1:G:191:GLU:H	1.81	0.45
1:G:191:GLU:O	1:G:192:ARG:C	2.55	0.45
1:E:181:ASP:OD2	1:E:181:ASP:N	2.50	0.45
1:A:79:ALA:C	1:A:81:ALA:H	2.20	0.45
1:C:86:THR:O	1:C:87:GLY:C	2.54	0.45
1:D:131:ASP:O	1:D:134:VAL:CG2	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:156:LEU:HA	1:H:156:LEU:HD23	1.64	0.45
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.56	0.45
1:A:35:LEU:HD23	1:A:36:ILE:HD11	1.99	0.45
1:C:76:GLY:O	1:C:77:GLY:C	2.52	0.45
1:F:106:PRO:HA	1:F:125:VAL:CG1	2.47	0.45
1:F:119:LEU:HA	1:F:119:LEU:HD12	1.30	0.45
1:G:115:VAL:HG21	1:G:121:VAL:HB	1.99	0.45
1:H:59:LEU:HA	1:H:59:LEU:HD23	1.46	0.45
1:A:154:THR:O	1:A:184:VAL:HA	2.17	0.45
1:C:76:GLY:N	1:C:80:ARG:HB2	2.32	0.45
1:D:105:ALA:O	1:D:106:PRO:C	2.55	0.45
1:A:110:VAL:CG1	1:A:111:LEU:N	2.78	0.44
1:A:145:ILE:O	1:A:146:ALA:C	2.54	0.44
1:B:100:SER:OG	1:B:100:SER:O	2.34	0.44
1:C:130:GLY:C	1:C:131:ASP:O	2.55	0.44
1:F:156:LEU:HD23	1:F:156:LEU:HA	1.84	0.44
1:F:92:LYS:O	1:F:96:GLU:HB2	2.16	0.44
1:G:61:PRO:HA	1:G:151:LYS:HB3	1.99	0.44
1:G:36:ILE:HD12	1:G:36:ILE:HG23	1.64	0.44
1:A:145:ILE:HD13	1:A:145:ILE:HG21	1.76	0.44
1:A:143:LYS:O	1:A:146:ALA:HB3	2.17	0.44
1:B:39:PHE:CE1	1:B:192:ARG:HG3	2.51	0.44
1:D:160:GLY:O	1:D:162:PHE:N	2.51	0.44
1:D:74:HIS:NE2	1:D:90:LEU:HD21	2.32	0.44
1:A:54:VAL:O	1:A:54:VAL:HG12	2.16	0.44
1:A:89:LYS:HD3	1:A:93:ARG:HH12	1.83	0.44
1:C:66:ASN:HB2	1:C:82:ILE:HD13	1.99	0.44
1:D:74:HIS:CE1	1:D:90:LEU:HD21	2.53	0.44
1:G:113:GLU:HA	1:G:120:SER:OG	2.17	0.44
1:C:65:VAL:HG11	1:C:145:ILE:HD11	2.00	0.44
1:E:102:LYS:HG2	1:E:103:ALA:O	2.17	0.44
1:F:127:PRO:HD2	1:F:138:LEU:CD1	2.48	0.44
1:G:110:VAL:CG1	1:G:111:LEU:N	2.80	0.44
1:B:74:HIS:NE2	1:B:90:LEU:HD21	2.33	0.44
1:F:89:LYS:HD3	1:F:93:ARG:NH1	2.32	0.44
1:G:188:THR:HG22	1:G:190:GLN:N	2.33	0.44
1:B:67:ALA:HB1	3:B:477:APR:O1B	2.17	0.44
1:C:69:ASN:OD1	1:C:69:ASN:N	2.51	0.44
1:E:98:LEU:HD23	1:E:98:LEU:HA	1.38	0.44
1:H:176:THR:C	1:H:178:THR:H	2.20	0.44
1:E:156:LEU:HD23	1:E:156:LEU:HA	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:VAL:O	1:G:196:GLU:N	2.51	0.44
1:H:70:GLY:HA2	1:H:125:VAL:HG21	1.99	0.44
1:A:59:LEU:HA	1:A:59:LEU:HD23	1.60	0.44
1:B:47:PHE:CD2	1:B:47:PHE:N	2.86	0.44
1:B:65:VAL:HG12	1:B:66:ASN:H	1.81	0.44
1:A:174:LEU:HA	1:A:174:LEU:HD23	1.75	0.44
1:E:180:ARG:HG3	1:E:180:ARG:NH1	2.32	0.44
1:F:64:LEU:HD13	1:F:153:LEU:HB3	2.00	0.44
1:C:190:GLN:HA	1:E:198:PHE:CE1	2.53	0.43
1:C:74:HIS:NE2	1:C:90:LEU:HD21	2.33	0.43
1:D:63:VAL:HA	1:D:120:SER:O	2.18	0.43
1:F:127:PRO:HD2	1:F:138:LEU:HD12	2.00	0.43
1:F:50:GLY:O	1:F:187:TYR:HD1	2.01	0.43
1:G:174:LEU:HD23	1:G:174:LEU:HA	1.62	0.43
1:G:188:THR:HG22	1:G:190:GLN:H	1.83	0.43
1:H:133:ARG:O	1:H:134:VAL:C	2.55	0.43
1:B:141:VAL:O	1:B:145:ILE:HG13	2.18	0.43
1:B:200:ASN:HB3	1:B:201:GLY:H	1.54	0.43
1:D:74:HIS:CD2	1:D:90:LEU:HD23	2.53	0.43
1:G:179:ASP:O	1:G:180:ARG:HB2	2.18	0.43
1:H:98:LEU:HA	1:H:98:LEU:HD23	1.24	0.43
1:B:166:LEU:O	1:B:166:LEU:HD23	2.19	0.43
1:B:54:VAL:CG1	1:B:54:VAL:O	2.63	0.43
1:E:86:THR:HG22	1:E:116:LEU:HG	2.01	0.43
1:H:188:THR:HB	1:H:191:GLU:H	1.83	0.43
1:A:104:ILE:CD1	1:A:110:VAL:HB	2.48	0.43
1:D:131:ASP:O	1:D:134:VAL:HG23	2.19	0.43
1:F:86:THR:HB	1:F:89:LYS:HB2	2.01	0.43
1:G:112:PHE:HD1	1:G:112:PHE:N	2.17	0.43
1:G:158:SER:HB2	1:G:164:VAL:CG2	2.49	0.43
1:H:102:LYS:HB3	1:H:102:LYS:HE2	1.75	0.43
1:H:112:PHE:N	1:H:112:PHE:CD1	2.83	0.43
1:C:54:VAL:O	1:C:54:VAL:HG12	2.19	0.43
1:D:156:LEU:CD1	1:D:166:LEU:HD21	2.49	0.43
1:D:167:GLU:OE1	1:D:194:THR:HG22	2.18	0.43
1:E:154:THR:O	1:E:184:VAL:HA	2.19	0.43
1:H:142:TYR:O	1:H:145:ILE:HB	2.19	0.43
1:A:80:ARG:O	1:A:84:VAL:HG23	2.18	0.43
1:E:157:ILE:O	1:E:158:SER:HB2	2.19	0.43
1:F:154:THR:O	1:F:184:VAL:HA	2.19	0.43
1:H:153:LEU:HD12	1:H:153:LEU:HA	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:86:THR:HG22	1:H:116:LEU:HG	2.01	0.43
1:A:166:LEU:C	1:A:166:LEU:HD23	2.39	0.43
1:A:55:LEU:HA	1:A:55:LEU:HD23	1.70	0.43
1:C:165:LYS:O	1:C:168:VAL:HG23	2.19	0.43
1:C:52:LEU:C	1:C:54:VAL:N	2.71	0.43
1:D:52:LEU:O	1:D:53:ASP:C	2.57	0.43
1:E:165:LYS:HB2	1:E:168:VAL:HG23	2.01	0.43
1:H:145:ILE:O	1:H:146:ALA:C	2.57	0.43
1:A:188:THR:HG22	1:A:189:ASP:CA	2.45	0.43
1:B:83:ASP:HB3	1:B:84:VAL:H	1.72	0.43
1:E:54:VAL:O	1:E:58:PHE:HD2	2.02	0.43
1:F:157:ILE:O	1:F:158:SER:CB	2.66	0.43
1:G:167:GLU:N	1:G:167:GLU:OE2	2.50	0.43
1:H:170:LEU:O	1:H:170:LEU:HD12	2.18	0.43
1:E:104:ILE:CD1	1:E:110:VAL:HB	2.49	0.42
1:F:127:PRO:O	1:F:158:SER:OG	2.37	0.42
1:F:188:THR:CG2	1:F:189:ASP:H	2.26	0.42
1:F:76:GLY:O	1:F:80:ARG:CZ	2.67	0.42
1:G:158:SER:O	1:G:164:VAL:HG23	2.19	0.42
1:C:114:ASN:O	1:C:115:VAL:C	2.55	0.42
1:E:97:TYR:O	1:E:101:SER:HB2	2.19	0.42
1:H:59:LEU:O	1:H:60:GLU:C	2.57	0.42
1:E:94:SER:O	1:E:95:LYS:C	2.56	0.42
1:H:79:ALA:O	1:H:80:ARG:C	2.55	0.42
1:E:153:LEU:HD12	1:E:153:LEU:HA	1.59	0.42
1:E:35:LEU:O	1:E:35:LEU:CG	2.50	0.42
1:E:55:LEU:O	1:E:56:ILE:C	2.58	0.42
1:H:143:LYS:O	1:H:146:ALA:HB3	2.20	0.42
1:H:64:LEU:HD12	1:H:64:LEU:HA	1.70	0.42
1:A:131:ASP:N	1:A:131:ASP:OD2	2.52	0.42
1:A:158:SER:O	1:A:164:VAL:CG2	2.61	0.42
1:C:171:GLN:HB3	1:C:172:CYS:H	1.65	0.42
1:C:98:LEU:HD23	1:C:98:LEU:HA	1.68	0.42
1:D:200:ASN:HB3	1:D:201:GLY:H	1.52	0.42
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.50	0.42
1:B:64:LEU:HB2	1:B:119:LEU:HD11	2.02	0.42
1:D:169:SER:O	1:D:170:LEU:C	2.58	0.42
1:F:154:THR:HG21	1:F:182:LEU:HD11	2.00	0.42
1:G:133:ARG:C	1:G:135:GLU:H	2.20	0.42
1:G:153:LEU:HA	1:G:153:LEU:HD12	1.67	0.42
1:A:112:PHE:N	1:A:112:PHE:CD1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ASP:O	1:A:55:LEU:HG	2.19	0.42
1:E:174:LEU:HD23	1:E:174:LEU:HA	1.62	0.42
1:H:154:THR:OG1	1:H:155:PRO:HD2	2.19	0.42
1:H:174:LEU:HA	1:H:174:LEU:HD23	1.63	0.42
1:B:156:LEU:HD23	1:B:156:LEU:HA	1.88	0.42
3:B:477:APR:HO'2	3:B:477:APR:HO'3	1.57	0.42
1:C:104:ILE:HD11	1:C:110:VAL:CG2	2.50	0.42
1:D:65:VAL:HG12	1:D:66:ASN:N	2.35	0.42
1:D:69:ASN:HB2	1:D:70:GLY:H	1.74	0.42
1:E:176:THR:C	1:E:178:THR:H	2.22	0.42
1:G:59:LEU:HD23	1:G:59:LEU:HA	1.58	0.42
1:A:193:VAL:O	1:A:194:THR:C	2.55	0.42
1:C:94:SER:O	1:C:95:LYS:C	2.57	0.42
1:D:132:SER:O	1:D:133:ARG:CB	2.68	0.42
1:E:111:LEU:HD12	1:E:111:LEU:HA	1.80	0.42
1:E:38:PRO:HB3	1:E:46:SER:HB3	2.00	0.42
1:F:110:VAL:HG13	1:F:111:LEU:H	1.83	0.42
1:D:80:ARG:HB3	1:D:80:ARG:NH1	2.35	0.42
1:E:59:LEU:HD23	1:E:59:LEU:HA	1.59	0.42
1:G:140:ASN:O	1:G:141:VAL:C	2.57	0.41
1:A:188:THR:HG21	1:A:190:GLN:HB2	2.01	0.41
1:A:188:THR:HG22	1:A:190:GLN:H	1.85	0.41
1:C:170:LEU:HD12	1:C:170:LEU:HA	1.56	0.41
1:C:67:ALA:HB1	3:C:477:APR:O1B	2.20	0.41
1:E:110:VAL:CG1	1:E:111:LEU:N	2.84	0.41
1:F:166:LEU:O	1:F:167:GLU:C	2.58	0.41
1:H:52:LEU:HD12	1:H:52:LEU:HA	1.83	0.41
1:A:105:ALA:O	1:A:108:ASN:N	2.51	0.41
1:C:105:ALA:O	1:C:108:ASN:HB2	2.21	0.41
1:D:64:LEU:HB2	1:D:119:LEU:HD11	2.00	0.41
1:D:153:LEU:HD12	1:D:183:ASN:O	2.20	0.41
1:E:61:PRO:HA	1:E:151:LYS:HB3	2.01	0.41
1:F:91:THR:O	1:F:92:LYS:C	2.59	0.41
1:G:39:PHE:CD2	1:G:39:PHE:C	2.93	0.41
1:G:55:LEU:HD23	1:G:55:LEU:HA	1.79	0.41
1:B:136:GLY:O	1:B:140:ASN:HB2	2.19	0.41
1:H:100:SER:C	1:H:101:SER:OG	2.58	0.41
1:E:143:LYS:O	1:E:146:ALA:HB3	2.20	0.41
1:A:64:LEU:HA	1:A:64:LEU:HD12	1.68	0.41
1:B:191:GLU:OE1	3:B:477:APR:O2'	2.26	0.41
1:C:192:ARG:HD3	1:C:192:ARG:HH11	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:138:LEU:HG	1:H:138:LEU:O	2.21	0.41
1:H:54:VAL:H	1:H:54:VAL:HG23	1.58	0.41
1:A:55:LEU:O	1:A:56:ILE:C	2.58	0.41
1:D:86:THR:O	1:D:87:GLY:C	2.59	0.41
1:E:168:VAL:O	1:E:172:CYS:HB2	2.20	0.41
1:F:52:LEU:CG	1:F:56:ILE:HD11	2.47	0.41
1:H:159:VAL:HG13	1:H:160:GLY:H	1.84	0.41
1:F:82:ILE:HG21	1:F:90:LEU:HD22	2.01	0.41
1:C:156:LEU:HD23	1:C:156:LEU:HA	1.87	0.41
1:H:112:PHE:N	1:H:112:PHE:HD1	2.19	0.41
1:C:157:ILE:HD13	1:C:157:ILE:HA	1.72	0.41
1:F:170:LEU:HD11	1:F:174:LEU:HG	2.03	0.41
1:A:153:LEU:HD12	1:A:153:LEU:HA	1.65	0.41
1:B:187:TYR:HB2	3:B:477:APR:C4	2.51	0.41
1:E:188:THR:HB	1:E:191:GLU:H	1.86	0.41
1:E:40:TYR:HE2	1:E:42:ALA:HB2	1.86	0.41
1:E:55:LEU:HD23	1:E:55:LEU:HA	1.79	0.41
1:E:73:ARG:NH2	1:E:73:ARG:CG	2.66	0.41
1:F:55:LEU:C	1:F:57:ASN:N	2.72	0.41
1:H:110:VAL:CG1	1:H:111:LEU:N	2.83	0.41
1:H:69:ASN:OD1	1:H:73:ARG:O	2.39	0.41
1:A:109:ALA:HB1	1:A:122:LEU:HD21	2.03	0.40
1:A:61:PRO:HA	1:A:151:LYS:HB3	2.02	0.40
1:B:133:ARG:O	1:B:137:LYS:HG3	2.21	0.40
1:E:116:LEU:HB2	1:E:119:LEU:HB3	2.03	0.40
1:F:105:ALA:HB3	1:F:108:ASN:HB2	2.03	0.40
1:F:158:SER:HA	1:F:162:PHE:HD2	1.86	0.40
1:G:153:LEU:HD12	1:G:183:ASN:O	2.21	0.40
1:B:142:TYR:CE1	1:B:173:LEU:HB2	2.56	0.40
1:E:188:THR:HG22	1:E:189:ASP:CA	2.50	0.40
1:F:111:LEU:HA	1:F:111:LEU:HD12	1.78	0.40
1:F:89:LYS:HG3	1:F:89:LYS:HZ3	1.54	0.40
1:H:173:LEU:HD23	1:H:173:LEU:O	2.21	0.40
1:C:111:LEU:HG	1:C:112:PHE:N	2.32	0.40
1:C:56:ILE:HG21	1:C:56:ILE:HD13	1.86	0.40
1:D:137:LYS:O	1:D:141:VAL:HG23	2.21	0.40
1:D:171:GLN:HB3	1:D:172:CYS:H	1.72	0.40
1:D:93:ARG:NE	1:D:93:ARG:HA	2.36	0.40
1:E:100:SER:C	1:E:101:SER:OG	2.59	0.40
1:E:162:PHE:HD1	1:E:162:PHE:HA	1.81	0.40
1:F:38:PRO:HD3	1:F:48:TYR:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:TYR:O	1:G:101:SER:HB2	2.22	0.40
1:H:116:LEU:HD23	1:H:116:LEU:HA	1.73	0.40
1:F:192:ARG:HA	1:F:195:ILE:HD12	2.04	0.40
1:A:69:ASN:C	1:A:69:ASN:OD1	2.47	0.40
1:C:100:SER:OG	1:C:100:SER:O	2.39	0.40
1:D:155:PRO:N	1:D:185:PHE:CE2	2.90	0.40
1:D:48:TYR:CD2	1:D:48:TYR:N	2.89	0.40
1:E:36:ILE:HD13	1:E:36:ILE:HA	1.75	0.40
1:E:53:ASP:N	1:E:53:ASP:OD1	2.55	0.40
1:F:60:GLU:N	1:F:61:PRO:CD	2.85	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:SER:OG	1:F:118:HIS:O[8_544]	2.08	0.12
1:A:35:LEU:O	1:A:163:LYS:NZ[6_445]	2.11	0.09

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	166/168 (99%)	138 (83%)	26 (16%)	2 (1%)	13 49
1	B	166/168 (99%)	130 (78%)	30 (18%)	6 (4%)	3 29
1	C	166/168 (99%)	130 (78%)	33 (20%)	3 (2%)	8 41
1	D	166/168 (99%)	127 (76%)	37 (22%)	2 (1%)	13 49
1	E	166/168 (99%)	139 (84%)	26 (16%)	1 (1%)	25 63
1	F	166/168 (99%)	132 (80%)	30 (18%)	4 (2%)	6 36
1	G	166/168 (99%)	137 (82%)	28 (17%)	1 (1%)	25 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	166/168 (99%)	138 (83%)	25 (15%)	3 (2%)	8 41
All	All	1328/1344 (99%)	1071 (81%)	235 (18%)	22 (2%)	9 43

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	161	ILE
1	D	161	ILE
1	C	134	VAL
1	D	134	VAL
1	G	134	VAL
1	F	95	LYS
1	H	178	THR
1	B	83	ASP
1	B	161	ILE
1	B	171	GLN
1	B	84	VAL
1	B	77	GLY
1	C	77	GLY
1	E	177	VAL
1	F	134	VAL
1	H	134	VAL
1	H	177	VAL
1	F	106	PRO
1	A	134	VAL
1	F	193	VAL
1	B	61	PRO
1	A	106	PRO

5.3.2 Protein sidechains (i)

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	143/143 (100%)	129 (90%)	14 (10%)	8 31
1	B	143/143 (100%)	129 (90%)	14 (10%)	8 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	143/143 (100%)	132 (92%)	11 (8%)	13 41
1	D	143/143 (100%)	134 (94%)	9 (6%)	18 47
1	E	143/143 (100%)	127 (89%)	16 (11%)	6 27
1	F	143/143 (100%)	117 (82%)	26 (18%)	1 11
1	G	143/143 (100%)	127 (89%)	16 (11%)	6 27
1	H	143/143 (100%)	129 (90%)	14 (10%)	8 31
All	All	1144/1144 (100%)	1024 (90%)	120 (10%)	7 29

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	72	LEU
1	A	73	ARG
1	A	128	ARG
1	A	131	ASP
1	A	133	ARG
1	A	138	LEU
1	A	139	CYS
1	A	161	ILE
1	A	162	PHE
1	A	168	VAL
1	A	171	GLN
1	A	172	CYS
1	A	180	ARG
1	B	34	ASP
1	B	51	ASP
1	B	99	LYS
1	B	128	ARG
1	B	132	SER
1	B	147	LYS
1	B	152	ILE
1	B	158	SER
1	B	172	CYS
1	B	178	THR
1	B	180	ARG
1	B	187	TYR
1	B	189	ASP
1	B	197	ASN
1	C	34	ASP

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Mol	Chain	Res	Type
1	C	51	ASP
1	C	91	THR
1	C	100	SER
1	C	128	ARG
1	C	152	ILE
1	C	158	SER
1	C	172	CYS
1	C	180	ARG
1	C	187	TYR
1	C	197	ASN
1	D	34	ASP
1	D	51	ASP
1	D	91	THR
1	D	128	ARG
1	D	152	ILE
1	D	158	SER
1	D	172	CYS
1	D	180	ARG
1	D	187	TYR
1	E	34	ASP
1	E	72	LEU
1	E	73	ARG
1	E	80	ARG
1	E	122	LEU
1	E	128	ARG
1	E	131	ASP
1	E	133	ARG
1	E	134	VAL
1	E	138	LEU
1	E	139	CYS
1	E	161	ILE
1	E	162	PHE
1	E	172	CYS
1	E	180	ARG
1	E	197	ASN
1	F	40	TYR
1	F	45	VAL
1	F	46	SER
1	F	49	GLN
1	F	53	ASP
1	F	69	ASN
1	F	73	ARG

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Mol	Chain	Res	Type
1	F	80	ARG
1	F	82	ILE
1	F	89	LYS
1	F	91	THR
1	F	99	LYS
1	F	137	LYS
1	F	139	CYS
1	F	140	ASN
1	F	158	SER
1	F	166	LEU
1	F	167	GLU
1	F	168	VAL
1	F	172	CYS
1	F	180	ARG
1	F	181	ASP
1	F	188	THR
1	F	189	ASP
1	F	190	GLN
1	F	197	ASN
1	G	34	ASP
1	G	72	LEU
1	G	73	ARG
1	G	122	LEU
1	G	128	ARG
1	G	131	ASP
1	G	133	ARG
1	G	134	VAL
1	G	138	LEU
1	G	158	SER
1	G	161	ILE
1	G	162	PHE
1	G	172	CYS
1	G	180	ARG
1	G	181	ASP
1	G	197	ASN
1	H	34	ASP
1	H	72	LEU
1	H	73	ARG
1	H	128	ARG
1	H	131	ASP
1	H	132	SER
1	H	133	ARG

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Mol	Chain	Res	Type
1	H	134	VAL
1	H	161	ILE
1	H	162	PHE
1	H	171	GLN
1	H	172	CYS
1	H	180	ARG
1	H	181	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	APR	B	477	-	34,39,39	1.60	8 (23%)	40,60,60	1.64	10 (25%)
3	APR	C	477	-	34,39,39	1.12	3 (8%)	40,60,60	1.95	10 (25%)
3	APR	D	477	-	34,39,39	1.02	2 (5%)	40,60,60	1.73	11 (27%)

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	APR	B	477	-	-	4/18/54/54	0/4/4/4
3	APR	C	477	-	-	5/18/54/54	0/4/4/4
3	APR	D	477	-	-	4/18/54/54	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	477	APR	C4-N3	4.25	1.41	1.35
3	B	477	APR	C2-N3	3.58	1.37	1.32
3	B	477	APR	C5-C4	3.52	1.50	1.40
3	C	477	APR	C5-N7	-2.63	1.30	1.39
3	C	477	APR	O4'-C1'	2.54	1.44	1.41
3	B	477	APR	O4'-C1'	2.53	1.44	1.41
3	B	477	APR	O1D-C1D	2.26	1.46	1.39
3	D	477	APR	O1D-C1D	2.24	1.46	1.39
3	D	477	APR	C5-N7	-2.23	1.31	1.39
3	B	477	APR	C8-N7	2.15	1.38	1.34
3	B	477	APR	C1D-C2D	2.10	1.55	1.52
3	B	477	APR	C2-N1	2.09	1.37	1.33
3	C	477	APR	C5D-C4D	2.01	1.57	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	477	APR	O4'-C1'-C2'	-5.91	98.29	106.93
3	C	477	APR	C3'-C2'-C1'	4.98	108.47	100.98
3	C	477	APR	N6-C6-N1	4.25	127.39	118.57
3	D	477	APR	C5-C6-N6	-3.94	114.37	120.35
3	D	477	APR	N6-C6-N1	3.83	126.53	118.57
3	D	477	APR	O3'-C3'-C4'	-3.74	100.22	111.05
3	D	477	APR	C1D-C2D-C3D	3.36	106.50	102.30
3	D	477	APR	N3-C2-N1	-3.34	123.45	128.68
3	B	477	APR	C3'-C2'-C1'	3.30	105.95	100.98
3	B	477	APR	O4'-C1'-C2'	-3.18	102.28	106.93
3	D	477	APR	O3D-C3D-C2D	-3.06	101.92	111.82
3	B	477	APR	O2A-PA-O1A	2.88	126.47	112.24
3	B	477	APR	C2D-C3D-C4D	2.86	108.20	102.64
3	C	477	APR	C5-C6-N6	-2.84	116.03	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	477	APR	C4-C5-N7	-2.83	106.45	109.40
3	C	477	APR	N3-C2-N1	-2.81	124.28	128.68
3	D	477	APR	O4'-C1'-C2'	-2.75	102.90	106.93
3	B	477	APR	O4D-C1D-C2D	2.75	107.85	104.46
3	B	477	APR	N3-C2-N1	-2.71	124.44	128.68
3	C	477	APR	O3'-C3'-C4'	-2.57	103.61	111.05
3	C	477	APR	O2A-PA-O1A	2.51	124.63	112.24
3	B	477	APR	O2'-C2'-C3'	-2.44	103.92	111.82
3	B	477	APR	O3D-C3D-C2D	-2.37	104.16	111.82
3	B	477	APR	N6-C6-N1	2.33	123.41	118.57
3	C	477	APR	C1'-N9-C4	2.31	130.71	126.64
3	D	477	APR	O2D-C2D-C3D	-2.30	104.39	111.82
3	D	477	APR	C1'-N9-C4	2.27	130.63	126.64
3	D	477	APR	O2A-PA-O1A	2.23	123.25	112.24
3	C	477	APR	O3D-C3D-C4D	-2.17	104.78	111.05
3	C	477	APR	O4D-C1D-C2D	2.07	107.01	104.46
3	D	477	APR	C3'-C2'-C1'	2.01	104.00	100.98

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	477	APR	C5'-O5'-PA-O1A
3	B	477	APR	C5'-O5'-PA-O3A
3	C	477	APR	C3D-C4D-C5D-O5D
3	C	477	APR	O4D-C4D-C5D-O5D
3	C	477	APR	PA-O3A-PB-O5D
3	B	477	APR	PA-O3A-PB-O5D
3	C	477	APR	O4'-C4'-C5'-O5'
3	D	477	APR	PA-O3A-PB-O1B
3	D	477	APR	C3D-C4D-C5D-O5D
3	C	477	APR	C3'-C4'-C5'-O5'
3	D	477	APR	PA-O3A-PB-O5D
3	B	477	APR	C5'-O5'-PA-O2A
3	D	477	APR	C5'-O5'-PA-O1A

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	477	APR	7	0

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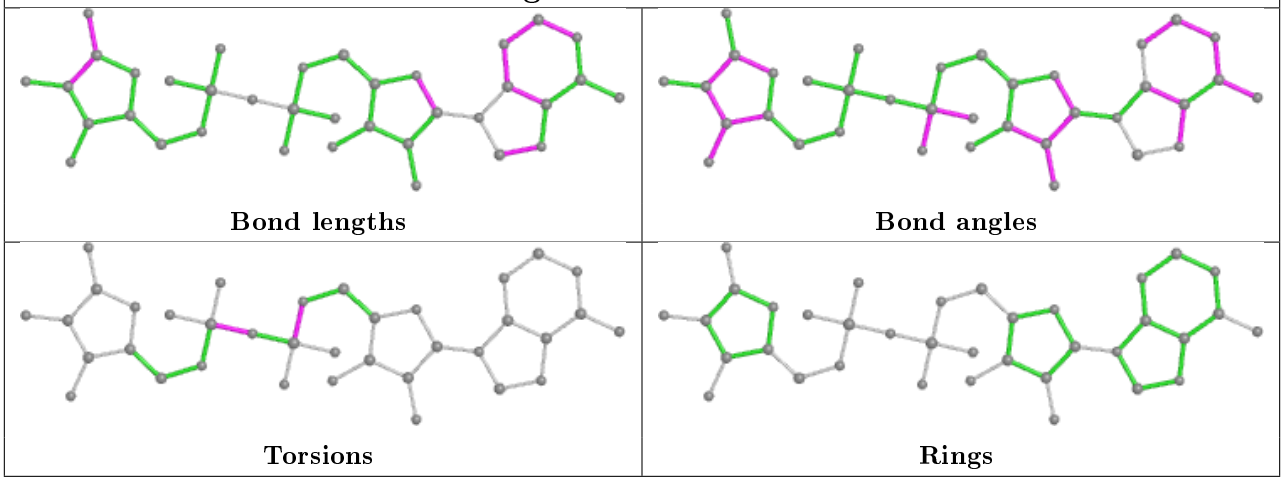
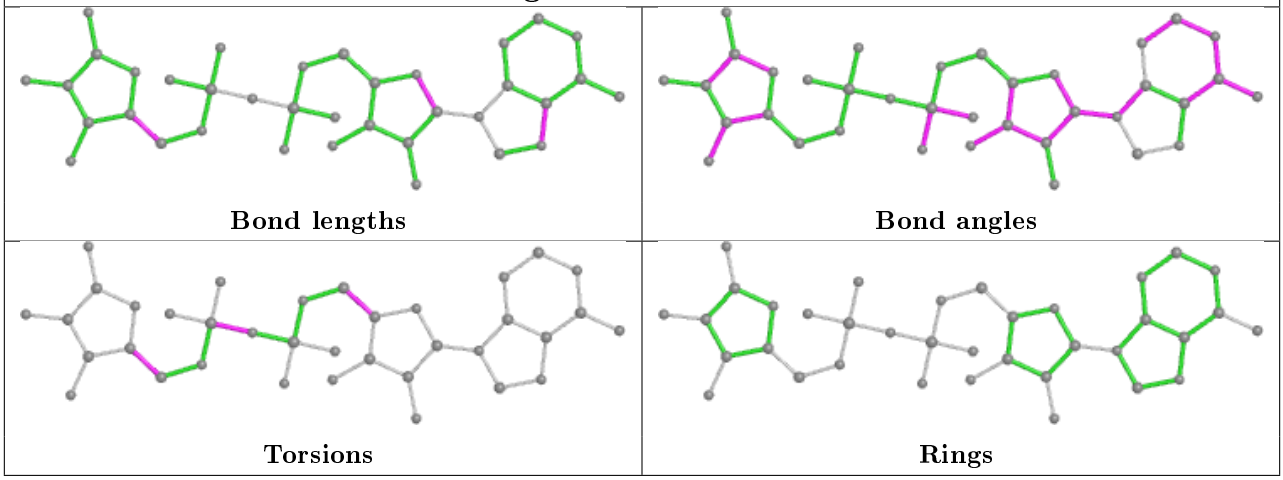
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	477	APR	1	0
3	D	477	APR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

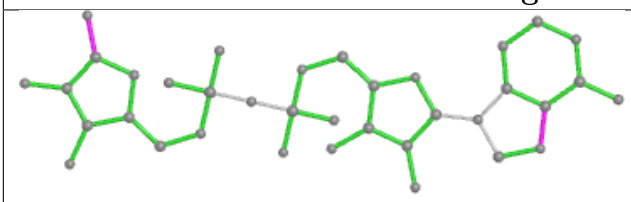
Ligand APR B 477



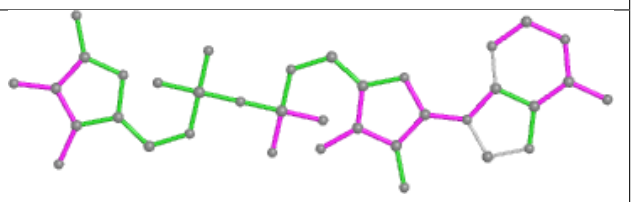
Ligand APR C 477



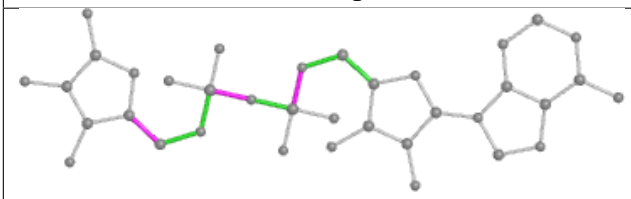
Ligand APR D 477



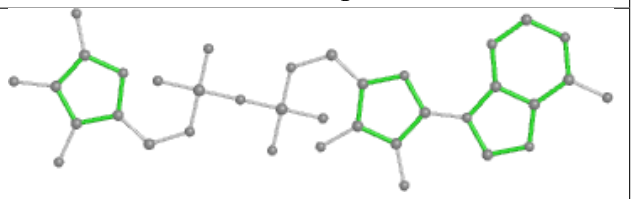
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	168/168 (100%)	-0.87	0	100	100	9, 26, 44, 51	8 (4%)
1	B	168/168 (100%)	-0.76	0	100	100	17, 32, 50, 58	5 (2%)
1	C	168/168 (100%)	-0.79	0	100	100	17, 32, 50, 58	4 (2%)
1	D	168/168 (100%)	-0.76	0	100	100	17, 32, 51, 58	6 (3%)
1	E	168/168 (100%)	-0.82	0	100	100	9, 26, 44, 53	5 (2%)
1	F	168/168 (100%)	-0.74	0	100	100	10, 31, 59, 65	6 (3%)
1	G	168/168 (100%)	-0.78	0	100	100	11, 26, 44, 56	6 (3%)
1	H	168/168 (100%)	-0.81	0	100	100	12, 26, 44, 52	7 (4%)
All	All	1344/1344 (100%)	-0.79	0	100	100	9, 29, 49, 65	47 (3%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

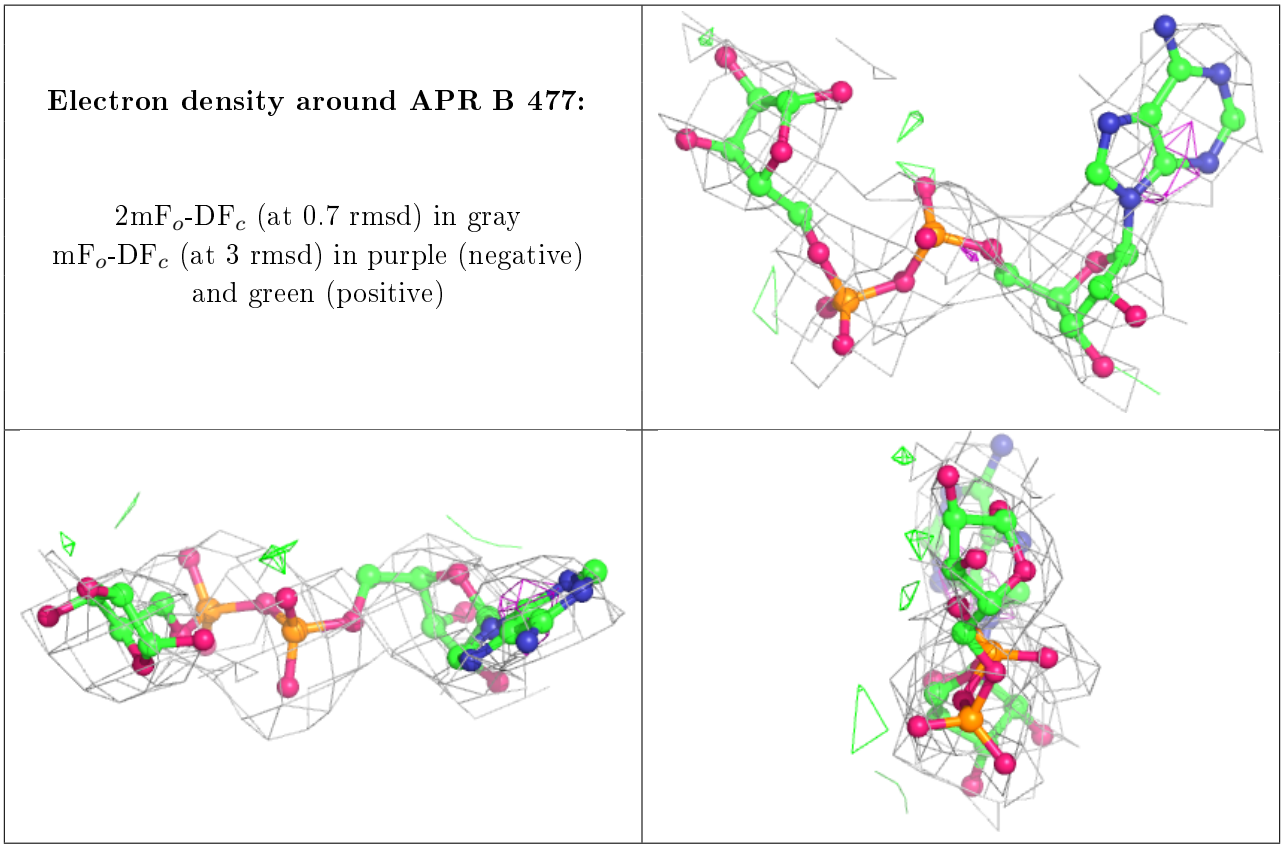
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	B	3	1/1	0.83	0.22	16,16,16,16	0
2	CL	G	2	1/1	0.89	0.18	41,41,41,41	0
2	CL	A	1	1/1	0.89	0.20	52,52,52,52	0
3	APR	B	477	36/36	0.94	0.20	55,59,64,64	0
3	APR	C	477	36/36	0.95	0.16	55,59,63,64	0
3	APR	D	477	36/36	0.96	0.14	55,59,63,64	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

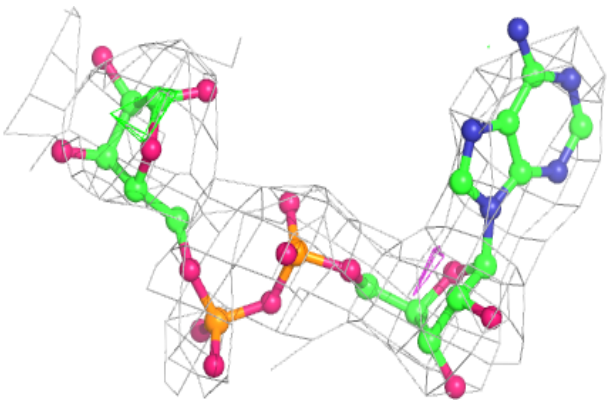
Electron density around APR B 477:

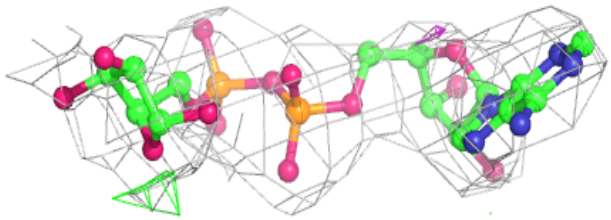
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

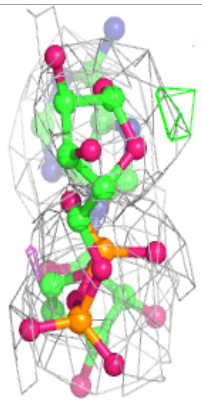


Electron density around APR C 477:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

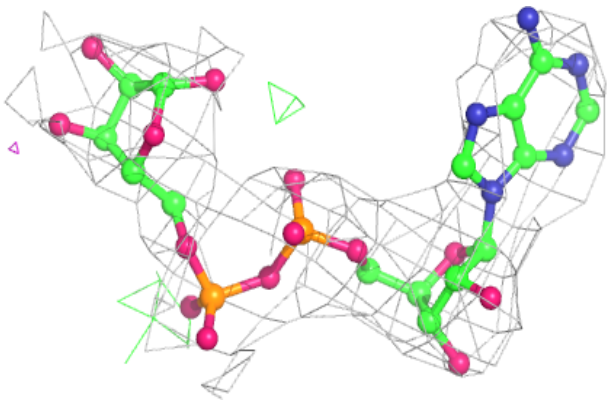


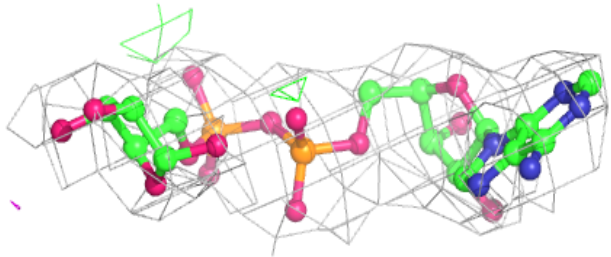


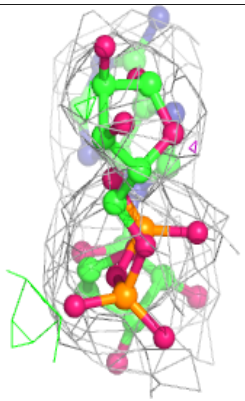


Electron density around APR D 477:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.