Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:34 PM GMT

PDB ID	:	3ZUN
Title	:	pVHL54-213-EloB-EloC complex_(2S,4R)-4-hydroxy-1-(2-(3-methylisoxazol-5-yl)acetyl)-N-(4-nitrobenzyl)pyrrolidine-2-carboxamide bound
Authors	:	Vanmolle, I.; Buckley, D.; Crews, C.M.; Ciulli, A.
Deposited on	:	2011-07-19
Resolution	:	2.50 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 ①) were used in the production of this report:

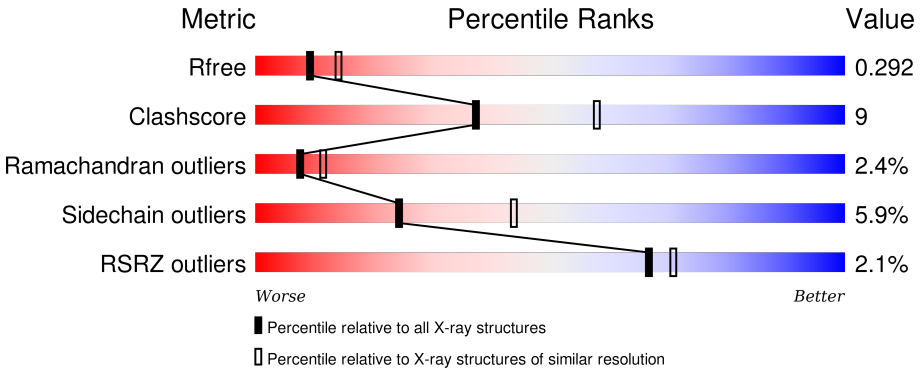
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 <=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	118	3% 66% 18% • 14%
1	D	118	3% 66% 14% • • 14%
1	G	118	3% 58% 24% 5% 13%
1	J	118	2% 67% 16% • • 12%
2	B	97	% 65% 22% • 11%

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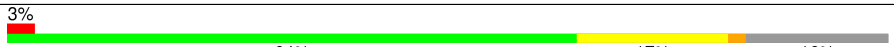
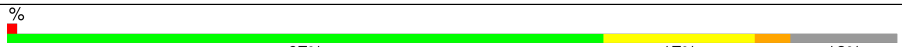
Mol	Chain	Length	Quality of chain
2	E	97	
2	H	97	
2	K	97	
3	C	163	
3	F	163	
3	I	163	
3	L	163	

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
4	GOL	B	1113	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10609 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 TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	S	0	0	0
			787	502	132	149	4			
1	D	101	Total	C	N	O	S	0	0	0
			762	486	128	144	4			
1	G	103	Total	C	N	O	S	0	0	0
			787	500	134	148	5			
1	J	104	Total	C	N	O	S	0	0	0
			799	507	137	151	4			

- Molecule 2 is a protein called TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	86	Total	C	N	O	S	0	0	0
			673	436	105	126	6			
2	E	87	Total	C	N	O	S	0	0	0
			673	437	107	123	6			
2	H	87	Total	C	N	O	S	0	0	0
			680	441	109	124	6			
2	K	86	Total	C	N	O	S	0	0	0
			674	438	106	124	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	EXPRESSION TAG	UNP Q15369
E	16	MET	-	EXPRESSION TAG	UNP Q15369
H	16	MET	-	EXPRESSION TAG	UNP Q15369
K	16	MET	-	EXPRESSION TAG	UNP E5RGD9

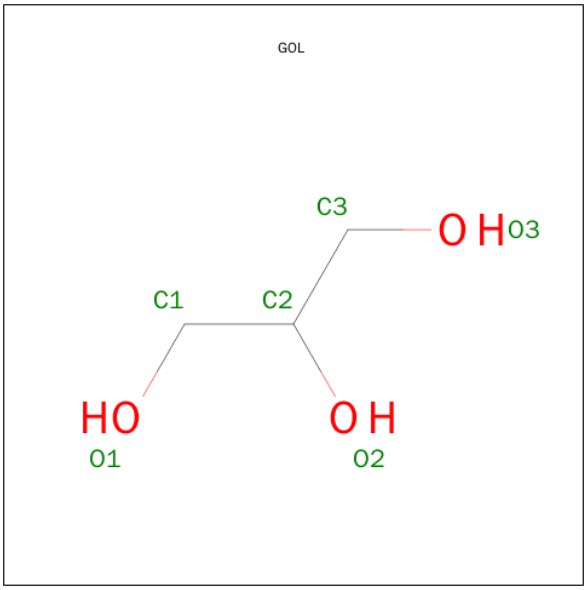
- Molecule 3 is a protein called VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	137	Total	C	N	O	S	0	0	0
			1062	679	187	194	2			
3	F	143	Total	C	N	O	S	0	0	0
			1128	722	198	206	2			
3	I	144	Total	C	N	O	S	0	0	0
			1127	718	202	205	2			
3	L	139	Total	C	N	O	S	0	0	0
			1116	714	198	202	2			

There are 12 discrepancies between the modelled and reference sequences:

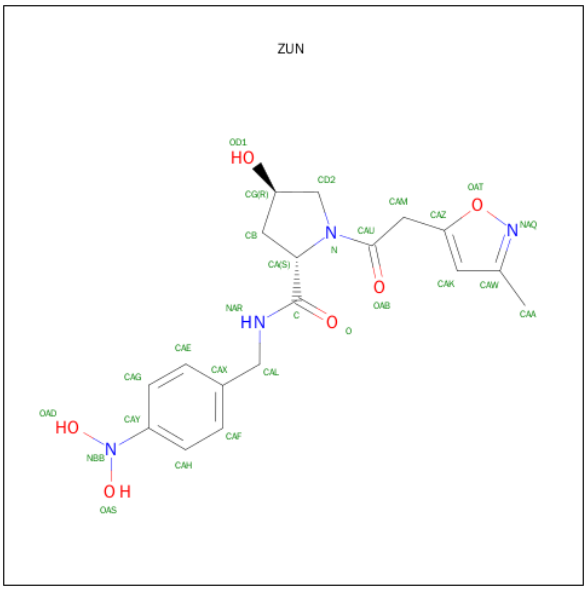
Chain	Residue	Modelled	Actual	Comment	Reference
C	51	GLY	-	EXPRESSION TAG	UNP P40337
C	52	SER	-	EXPRESSION TAG	UNP P40337
C	53	HIS	-	EXPRESSION TAG	UNP P40337
F	51	GLY	-	EXPRESSION TAG	UNP P40337
F	52	SER	-	EXPRESSION TAG	UNP P40337
F	53	HIS	-	EXPRESSION TAG	UNP P40337
I	51	GLY	-	EXPRESSION TAG	UNP P40337
I	52	SER	-	EXPRESSION TAG	UNP P40337
I	53	HIS	-	EXPRESSION TAG	UNP P40337
L	51	GLY	-	EXPRESSION TAG	UNP P40337
L	52	SER	-	EXPRESSION TAG	UNP P40337
L	53	HIS	-	EXPRESSION TAG	UNP P40337

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is (4R)-N-[4-(DIHYDROXYAMINO)BENZYL]-4-HYDROXY-1-[(3-METHYLISOXAZOL-5-YL)ACETYL]-L-PROLINAMIDE (three-letter code: ZUN) (formula: $C_{18}H_{22}N_4O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 28 18 4 6	0	0
5	F	1	Total C N O 28 18 4 6	0	0
5	I	1	Total C N O 28 18 4 6	0	0
5	L	1	Total C N O 28 18 4 6	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	23	Total O 23 23	0	0
6	B	15	Total O 15 15	0	0
6	C	23	Total O 23 23	0	0
6	D	17	Total O 17 17	0	0

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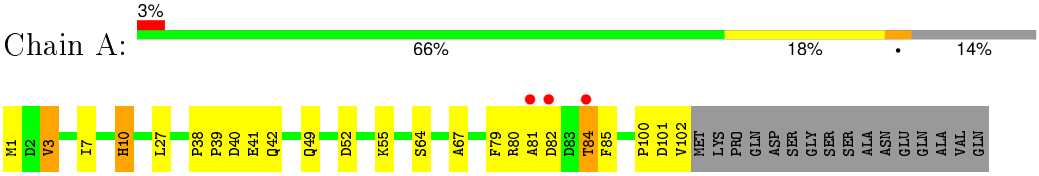
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	15	Total O 15 15	0	0
6	F	33	Total O 33 33	0	0
6	G	11	Total O 11 11	0	0
6	H	10	Total O 10 10	0	0
6	I	14	Total O 14 14	0	0
6	J	29	Total O 29 29	0	0
6	K	12	Total O 12 12	0	0
6	L	21	Total O 21 21	0	0

3 Residue-property plots (i)

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

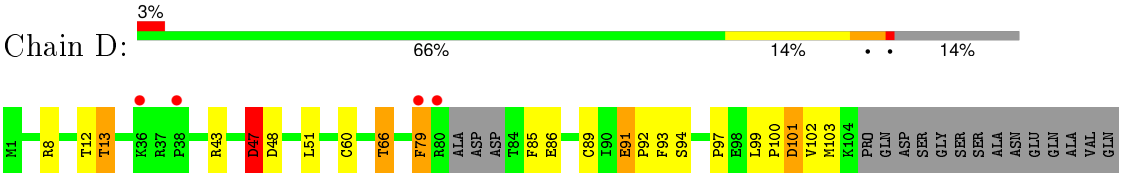
• Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

Chain A:



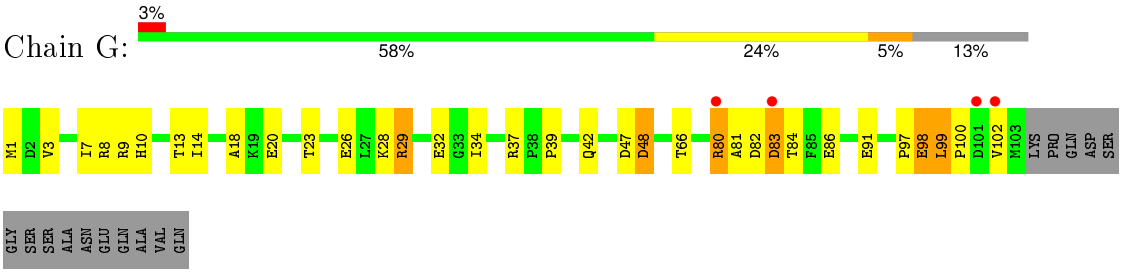
• Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

Chain D:



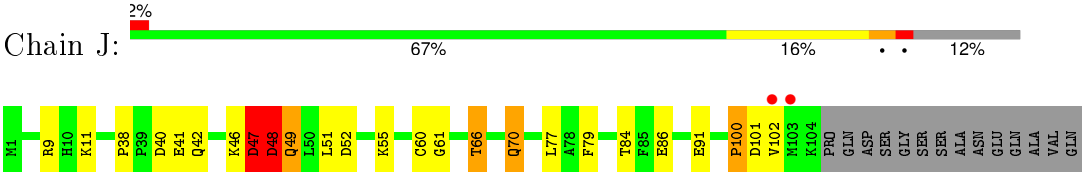
• Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

Chain G:



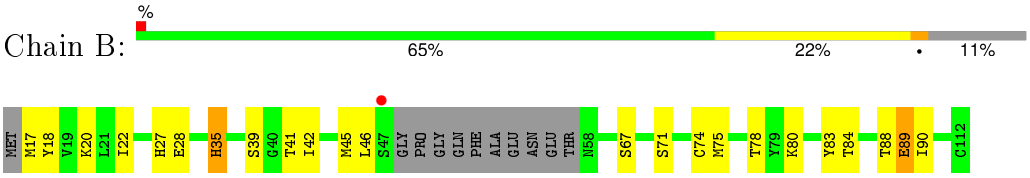
• Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

Chain J:



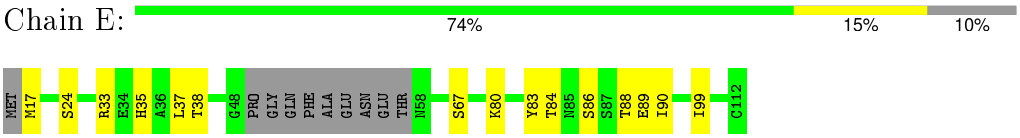
• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

Chain B:



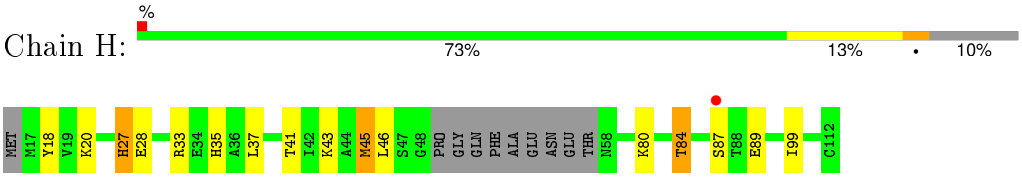
• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

Chain E:



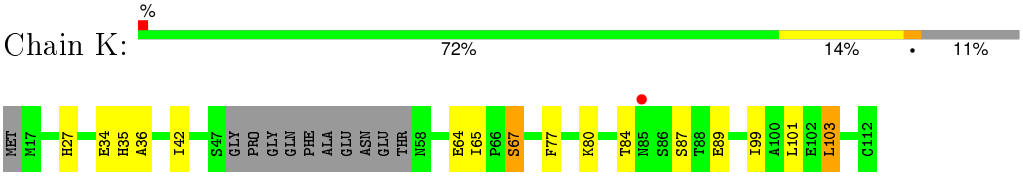
• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

Chain H:



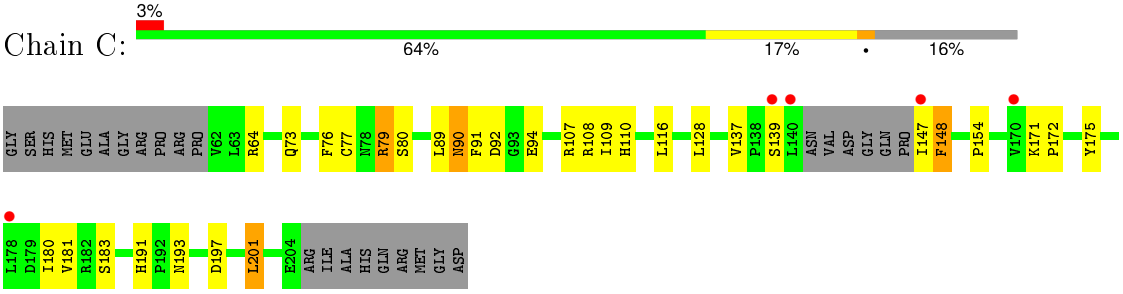
• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

Chain K:



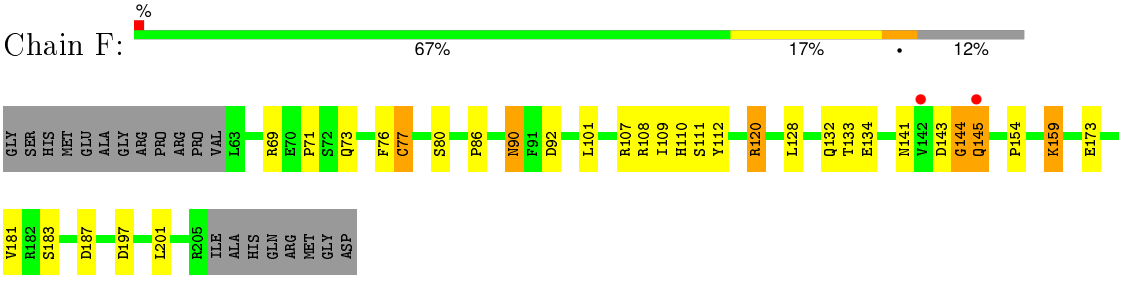
• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR

Chain C:



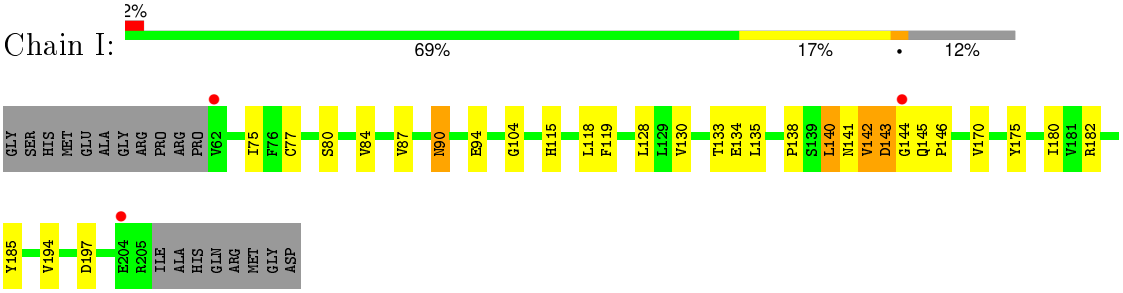
• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR

Chain F:



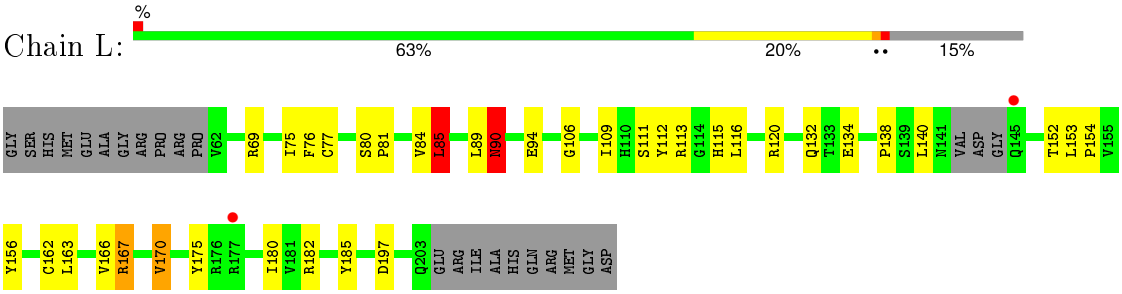
• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR

Chain I:



• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	93.40Å 93.40Å 362.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.50 – 2.50 41.50 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.50-2.50) 99.5 (41.50-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.229 , 0.302 0.226 , 0.292	Depositor DCC
R_{free} test set	2417 reflections (4.48%)	DCC
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	2 of 56349 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10609	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.12 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6362e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.69	0/803	0.80	0/1087
1	D	0.63	0/777	0.68	0/1054
1	G	0.63	0/803	0.78	0/1088
1	J	0.68	0/815	0.89	3/1104 (0.3%)
2	B	0.70	0/687	0.74	0/929
2	E	0.67	0/687	0.76	0/928
2	H	0.72	0/694	0.74	0/936
2	K	0.75	0/688	0.84	0/929
3	C	0.73	1/1089 (0.1%)	0.83	1/1493 (0.1%)
3	F	0.80	3/1158 (0.3%)	0.78	0/1587
3	I	0.65	0/1157	0.78	0/1586
3	L	0.64	0/1145	0.84	3/1566 (0.2%)
All	All	0.69	4/10503 (0.0%)	0.79	7/14287 (0.0%)

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	G	0	1
3	I	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	77	CYS	CB-SG	10.76	2.00	1.82
3	C	77	CYS	CB-SG	8.57	1.96	1.82
3	F	145	GLN	C-N	7.16	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	144	GLY	C-N	6.03	1.48	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	48	ASP	N-CA-C	6.95	129.78	111.00
1	J	48	ASP	C-N-CA	6.74	138.54	121.70
3	C	201	LEU	CA-CB-CG	6.07	129.27	115.30
1	J	70	GLN	CB-CA-C	-5.38	99.65	110.40
3	L	85	LEU	CA-CB-CG	5.31	127.52	115.30
3	L	167	ARG	NE-CZ-NH2	5.18	122.89	120.30
3	L	90	ASN	N-CA-CB	-5.06	101.49	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	PRO	Peptide
1	G	98	GLU	Peptide
3	I	104	GLY	Peptide
3	I	144	GLY	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	787	0	780	13	0
1	D	762	0	733	15	0
1	G	787	0	770	27	0
1	J	799	0	787	16	0
2	B	673	0	659	11	0
2	E	673	0	665	10	0
2	H	680	0	676	7	0
2	K	674	0	668	10	0
3	C	1062	0	1009	25	0
3	F	1128	0	1092	20	0
3	I	1127	0	1079	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1116	0	1095	24	0
4	B	6	0	8	0	0
5	C	28	0	22	0	0
5	F	28	0	22	1	0
5	I	28	0	22	0	0
5	L	28	0	22	0	0
6	A	23	0	0	1	0
6	B	15	0	0	0	0
6	C	23	0	0	1	0
6	D	17	0	0	0	0
6	E	15	0	0	0	0
6	F	33	0	0	5	0
6	G	11	0	0	1	0
6	H	10	0	0	0	0
6	I	14	0	0	0	0
6	J	29	0	0	2	0
6	K	12	0	0	0	0
6	L	21	0	0	2	0
All	All	10609	0	10109	191	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 (191) 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)
3:C:89:LEU:HD12	3:C:116:LEU:HD23	1.41	1.01
3:C:79:ARG:HG2	3:C:79:ARG:HH11	1.30	0.96
3:L:120:ARG:HD2	6:L:2008:HOH:O	1.64	0.95
1:G:29:ARG:HH11	1:G:29:ARG:HG3	1.32	0.93
3:C:73:GLN:NE2	3:C:108:ARG:HH11	1.68	0.92
1:A:101:ASP:O	1:A:102:VAL:HG23	1.76	0.85
1:D:101:ASP:HA	1:D:103:MET:N	1.96	0.81
3:L:120:ARG:CD	6:L:2008:HOH:O	2.24	0.80
3:F:133:THR:HG22	3:F:134:GLU:H	1.46	0.79
3:I:133:THR:HG22	3:I:134:GLU:H	1.46	0.79
2:E:88:THR:HG22	2:E:89:GLU:H	1.51	0.75
1:G:29:ARG:HG3	1:G:29:ARG:NH1	1.99	0.74
1:J:46:LYS:O	1:J:49:GLN:HB3	1.86	0.74
3:L:90:ASN:HB2	3:L:94:GLU:O	1.89	0.73
1:G:98:GLU:HA	1:G:99:LEU:CB	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:LEU:H	1:G:100:PRO:HD3	1.52	0.73
3:I:182:ARG:HA	3:I:185:TYR:CD2	2.27	0.69
1:J:79:PHE:O	1:J:86:GLU:HG2	1.94	0.68
1:G:83:ASP:OD1	1:G:84:THR:HA	1.94	0.68
1:A:101:ASP:O	1:A:102:VAL:CG2	2.41	0.68
2:H:80:LYS:O	2:H:84:THR:HB	1.95	0.67
1:J:47:ASP:O	1:J:48:ASP:HB2	1.94	0.67
1:G:99:LEU:N	1:G:100:PRO:HD3	2.10	0.67
1:J:38:PRO:HD2	1:J:41:GLU:OE1	1.95	0.66
3:L:115:HIS:O	3:L:138:PRO:HD2	1.95	0.66
1:D:99:LEU:HD22	1:D:99:LEU:H	1.60	0.66
1:J:52:ASP:HB2	1:J:55:LYS:HG2	1.77	0.66
6:G:2003:HOH:O	2:H:27:HIS:HD2	1.79	0.65
3:L:182:ARG:HA	3:L:185:TYR:CD2	2.31	0.65
2:B:35:HIS:HD2	2:B:78:THR:HG22	1.63	0.64
1:G:28:LYS:HA	1:G:42:GLN:HE22	1.61	0.64
3:C:73:GLN:NE2	3:C:108:ARG:HD2	2.12	0.63
2:K:80:LYS:O	2:K:84:THR:HG23	1.99	0.63
1:D:101:ASP:HA	1:D:103:MET:H	1.63	0.62
1:G:66:THR:HG22	1:G:66:THR:O	1.99	0.62
1:J:61:GLY:O	1:J:66:THR:HG21	1.99	0.62
1:A:84:THR:O	1:A:85:PHE:HB2	2.00	0.62
1:G:8:ARG:HG2	1:G:13:THR:HG23	1.81	0.62
1:A:38:PRO:HG2	1:A:41:GLU:HG3	1.82	0.61
2:E:88:THR:HG22	2:E:89:GLU:N	2.16	0.60
3:I:90:ASN:HB2	3:I:94:GLU:O	2.01	0.60
2:B:71:SER:O	2:B:75:MET:HG3	2.01	0.59
1:G:3:VAL:HG12	1:G:18:ALA:O	2.03	0.59
3:L:162:CYS:O	3:L:166:VAL:HG23	2.03	0.59
1:G:98:GLU:CA	1:G:99:LEU:CB	2.81	0.58
3:C:90:ASN:HB3	3:C:92:ASP:H	1.69	0.58
3:F:109:ILE:HD12	5:F:1206:ZUN:HAG	1.84	0.58
1:A:52:ASP:HB2	1:A:55:LYS:HG3	1.84	0.58
3:I:141:ASN:O	3:I:145:GLN:HB2	2.03	0.57
3:F:181:VAL:HG12	3:F:183:SER:H	1.68	0.57
2:E:80:LYS:O	2:E:84:THR:HG22	2.04	0.56
1:G:47:ASP:O	1:G:48:ASP:CB	2.53	0.56
3:I:170:VAL:HG13	3:I:175:TYR:CE1	2.41	0.56
2:E:83:TYR:HB3	2:E:90:ILE:HG12	1.86	0.56
3:C:79:ARG:CG	3:C:79:ARG:HH11	2.13	0.56
3:I:115:HIS:O	3:I:138:PRO:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:GLU:OE1	1:G:39:PRO:HD3	2.05	0.56
1:J:9:ARG:HD2	1:J:86:GLU:OE2	2.06	0.55
3:I:118:LEU:HD23	3:I:135:LEU:HD23	1.87	0.55
3:I:142:VAL:O	3:I:143:ASP:O	2.25	0.55
3:I:84:VAL:HG22	3:I:128:LEU:HD13	1.88	0.54
3:C:116:LEU:HD12	3:C:137:VAL:HG22	1.89	0.54
3:L:89:LEU:HD12	3:L:116:LEU:HD23	1.88	0.54
2:K:87:SER:HB3	3:L:132:GLN:HE21	1.73	0.54
2:B:17:MET:HG3	2:B:18:TYR:CD1	2.43	0.54
1:G:29:ARG:HH11	1:G:29:ARG:CG	2.14	0.54
3:C:73:GLN:HE21	3:C:108:ARG:HD2	1.71	0.54
1:G:66:THR:CG2	1:G:66:THR:O	2.56	0.53
1:D:93:PHE:HB3	2:E:67:SER:HB3	1.90	0.53
2:B:80:LYS:O	2:B:84:THR:HG23	2.09	0.52
1:J:52:ASP:HB3	6:J:2022:HOH:O	2.08	0.52
3:F:133:THR:CG2	6:F:2019:HOH:O	2.56	0.52
1:G:97:PRO:O	1:G:98:GLU:CB	2.58	0.52
3:F:69:ARG:O	3:F:71:PRO:HD3	2.10	0.52
1:A:7:ILE:HD11	1:A:27:LEU:HD11	1.92	0.52
3:C:181:VAL:HG12	3:C:183:SER:H	1.75	0.52
3:F:133:THR:HG22	3:F:134:GLU:N	2.20	0.52
3:C:73:GLN:HE22	3:C:108:ARG:HH11	1.55	0.51
3:I:182:ARG:HA	3:I:185:TYR:HD2	1.73	0.51
3:C:64:ARG:HD3	3:C:91:PHE:O	2.11	0.51
2:K:103:LEU:HB3	3:L:162:CYS:SG	2.51	0.51
3:L:170:VAL:HG22	3:L:175:TYR:CD1	2.45	0.51
6:J:2007:HOH:O	2:K:27:HIS:HD2	1.92	0.51
3:C:107:ARG:HD2	3:C:109:ILE:HD11	1.93	0.50
1:A:1:MET:HG2	1:A:64:SER:HB3	1.93	0.50
2:B:74:CYS:O	2:B:78:THR:HG23	2.11	0.50
3:C:110:HIS:HD2	6:C:2002:HOH:O	1.95	0.50
2:E:33:ARG:O	2:E:37:LEU:HG	2.11	0.50
3:L:182:ARG:HA	3:L:185:TYR:HD2	1.74	0.50
3:I:118:LEU:HD23	3:I:135:LEU:CD2	2.42	0.50
3:F:197:ASP:O	3:F:201:LEU:HB2	2.11	0.49
1:G:10:HIS:O	1:G:91:GLU:HB2	2.12	0.49
3:I:90:ASN:HB3	3:I:94:GLU:H	1.77	0.49
1:A:80:ARG:HA	1:A:85:PHE:HA	1.94	0.49
3:L:76:PHE:O	3:L:106:GLY:HA2	2.12	0.49
3:C:79:ARG:NH1	3:C:79:ARG:HG2	2.09	0.49
2:B:22:ILE:HG12	2:B:28:GLU:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:HIS:HD2	6:A:2005:HOH:O	1.95	0.49
3:F:133:THR:HG22	6:F:2019:HOH:O	2.13	0.48
1:J:51:LEU:HD22	1:J:60:CYS:SG	2.53	0.48
3:F:73:GLN:OE1	3:F:110:HIS:CD2	2.66	0.48
1:D:8:ARG:HG2	1:D:13:THR:HB	1.96	0.48
3:C:172:PRO:HA	3:C:175:TYR:CZ	2.49	0.48
1:D:91:GLU:HG3	1:D:92:PRO:HD2	1.95	0.48
3:I:84:VAL:HG22	3:I:128:LEU:CD1	2.43	0.48
2:K:64:GLU:HG2	2:K:65:ILE:HG13	1.96	0.48
3:F:141:ASN:ND2	6:F:2006:HOH:O	2.46	0.48
3:C:147:ILE:HG22	3:C:148:PHE:N	2.29	0.48
1:A:101:ASP:C	1:A:102:VAL:HG23	2.35	0.47
3:L:84:VAL:HG12	3:L:85:LEU:N	2.29	0.47
3:C:128:LEU:HA	3:C:154:PRO:HD3	1.96	0.47
3:I:133:THR:HG22	3:I:134:GLU:N	2.21	0.47
3:F:128:LEU:HA	3:F:154:PRO:HD3	1.96	0.47
2:B:20:LYS:HD3	2:B:28:GLU:HG2	1.97	0.47
1:G:99:LEU:N	1:G:100:PRO:CD	2.76	0.47
1:G:37:ARG:NH2	1:G:80:ARG:O	2.46	0.46
2:K:34:GLU:N	2:K:34:GLU:OE1	2.36	0.46
1:D:66:THR:O	1:D:66:THR:CG2	2.62	0.46
3:L:109:ILE:C	3:L:109:ILE:HD12	2.36	0.46
1:J:70:GLN:NE2	1:J:70:GLN:H	2.13	0.46
2:B:39:SER:HB3	2:B:42:ILE:HB	1.97	0.46
2:H:33:ARG:O	2:H:37:LEU:HG	2.16	0.45
3:F:159:LYS:NZ	3:F:187:ASP:OD2	2.49	0.45
1:J:42:GLN:HB3	1:J:77:LEU:HD11	1.97	0.45
3:I:170:VAL:HG13	3:I:175:TYR:HE1	1.80	0.45
3:I:130:VAL:HG13	3:I:130:VAL:O	2.17	0.45
1:J:46:LYS:HD3	1:J:60:CYS:O	2.17	0.45
1:D:100:PRO:O	1:D:101:ASP:CB	2.65	0.45
3:I:119:PHE:CE1	3:I:130:VAL:HG21	2.51	0.45
3:L:84:VAL:CG1	3:L:85:LEU:N	2.80	0.45
3:F:145:GLN:NE2	2:H:43:LYS:HD3	2.31	0.45
3:F:76:PHE:CE2	3:F:109:ILE:HG13	2.52	0.45
1:D:43:ARG:HG3	1:D:85:PHE:CZ	2.52	0.44
3:C:79:ARG:CG	3:C:79:ARG:NH1	2.78	0.44
1:D:94:SER:H	2:E:67:SER:HB2	1.82	0.44
3:L:111:SER:C	3:L:112:TYR:CD1	2.91	0.44
3:C:90:ASN:ND2	3:C:94:GLU:HB2	2.32	0.44
3:L:89:LEU:HD12	3:L:116:LEU:CD2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:120:ARG:HD2	6:F:2014:HOH:O	2.16	0.44
3:L:111:SER:OG	3:L:112:TYR:N	2.51	0.44
3:F:120:ARG:CD	6:F:2014:HOH:O	2.65	0.44
3:F:111:SER:C	3:F:112:TYR:CD1	2.91	0.44
3:F:90:ASN:HB3	3:F:92:ASP:H	1.82	0.43
3:C:76:PHE:CE2	3:C:109:ILE:HG13	2.52	0.43
3:L:81:PRO:HD2	3:L:153:LEU:HG	2.00	0.43
3:C:90:ASN:HB2	3:C:94:GLU:H	1.83	0.43
2:E:88:THR:CG2	2:E:89:GLU:H	2.25	0.43
3:F:143:ASP:HA	3:F:144:GLY:HA2	1.81	0.43
2:H:41:THR:O	2:H:45:MET:HB2	2.17	0.43
1:G:81:ALA:C	1:G:83:ASP:H	2.20	0.43
1:J:100:PRO:C	1:J:102:VAL:H	2.21	0.43
1:D:51:LEU:HD22	1:D:60:CYS:SG	2.58	0.43
1:A:80:ARG:HG2	1:A:80:ARG:HH11	1.82	0.43
1:J:11:LYS:HG3	1:J:91:GLU:HG3	2.01	0.43
2:K:87:SER:HA	3:L:132:GLN:HE22	1.83	0.42
3:F:108:ARG:O	3:F:109:ILE:HD13	2.20	0.42
1:A:3:VAL:HG22	1:A:67:ALA:HB3	2.01	0.42
3:C:197:ASP:O	3:C:201:LEU:HB2	2.19	0.42
1:D:79:PHE:H	1:D:86:GLU:HG2	1.83	0.42
3:C:89:LEU:O	3:C:90:ASN:O	2.38	0.42
2:K:36:ALA:HB1	2:K:42:ILE:HG21	2.01	0.42
3:L:163:LEU:O	3:L:167:ARG:HG3	2.18	0.42
3:I:140:LEU:HD12	3:I:140:LEU:HA	1.80	0.42
2:B:88:THR:O	2:B:89:GLU:O	2.36	0.42
2:K:35:HIS:HB3	2:K:77:PHE:HB3	2.02	0.42
1:J:49:GLN:HA	1:J:49:GLN:OE1	2.18	0.42
3:C:172:PRO:HA	3:C:175:TYR:CE1	2.54	0.42
1:D:99:LEU:H	1:D:99:LEU:CD2	2.31	0.41
3:C:171:LYS:HA	3:C:172:PRO:HD3	1.84	0.41
1:G:80:ARG:HG3	1:G:80:ARG:HH11	1.84	0.41
2:B:41:THR:O	2:B:45:MET:HG3	2.19	0.41
3:L:154:PRO:HD2	3:L:156:TYR:CZ	2.55	0.41
3:L:113:ARG:NE	3:L:140:LEU:HB2	2.35	0.41
3:I:87:VAL:HB	3:I:118:LEU:HD12	2.02	0.41
1:D:47:ASP:HB3	1:D:48:ASP:H	1.56	0.41
3:L:132:GLN:HA	3:L:132:GLN:OE1	2.20	0.41
1:G:1:MET:HB3	1:G:20:GLU:HG3	2.02	0.41
1:G:9:ARG:HD2	1:G:86:GLU:OE2	2.20	0.41
1:J:46:LYS:O	1:J:47:ASP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:ILE:HB	1:G:14:ILE:HB	2.03	0.41
1:G:23:THR:OG1	1:G:26:GLU:HG3	2.21	0.41
3:I:75:ILE:HD12	3:I:146:PRO:HB2	2.02	0.41
1:G:34:ILE:HD11	2:H:18:TYR:CZ	2.55	0.41
1:D:93:PHE:CB	2:E:67:SER:HB3	2.50	0.40
2:E:88:THR:CG2	2:E:89:GLU:N	2.84	0.40
1:G:81:ALA:O	1:G:83:ASP:N	2.55	0.40
3:I:141:ASN:ND2	3:I:145:GLN:O	2.55	0.40
2:K:101:LEU:HD23	2:K:101:LEU:HA	1.88	0.40
1:A:42:GLN:HG2	1:A:79:PHE:HE1	1.86	0.40
2:B:83:TYR:HB3	2:B:90:ILE:CG1	2.52	0.40
2:H:20:LYS:HD3	2:H:28:GLU:HG2	2.04	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	100/118 (85%)	90 (90%)	5 (5%)	5 (5%)	3 3
1	D	97/118 (82%)	89 (92%)	4 (4%)	4 (4%)	3 4
1	G	101/118 (86%)	90 (89%)	6 (6%)	5 (5%)	3 3
1	J	102/118 (86%)	91 (89%)	6 (6%)	5 (5%)	3 3
2	B	82/97 (84%)	78 (95%)	3 (4%)	1 (1%)	16 29
2	E	83/97 (86%)	80 (96%)	2 (2%)	1 (1%)	16 29
2	H	83/97 (86%)	78 (94%)	3 (4%)	2 (2%)	7 11
2	K	82/97 (84%)	75 (92%)	5 (6%)	2 (2%)	7 11
3	C	133/163 (82%)	124 (93%)	8 (6%)	1 (1%)	24 41
3	F	141/163 (86%)	130 (92%)	10 (7%)	1 (1%)	26 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	I	142/163 (87%)	129 (91%)	10 (7%)	3 (2%)	9 14
3	L	135/163 (83%)	126 (93%)	8 (6%)	1 (1%)	26 46
All	All	1281/1512 (85%)	1180 (92%)	70 (6%)	31 (2%)	7 11

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	84	THR
2	B	89	GLU
3	C	90	ASN
1	D	97	PRO
1	D	101	ASP
3	F	90	ASN
3	I	142	VAL
3	I	143	ASP
1	J	49	GLN
3	L	90	ASN
1	A	100	PRO
1	D	102	VAL
1	G	82	ASP
1	G	102	VAL
1	J	47	ASP
1	J	48	ASP
1	J	101	ASP
2	K	89	GLU
1	D	47	ASP
1	G	83	ASP
3	I	90	ASN
1	J	100	PRO
1	A	81	ALA
1	A	82	ASP
1	G	48	ASP
2	H	45	MET
2	E	38	THR
1	G	99	LEU
2	H	89	GLU
2	K	67	SER

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	84/103 (82%)	81 (96%)	3 (4%)	42	69
1	D	79/103 (77%)	72 (91%)	7 (9%)	12	23
1	G	83/103 (81%)	81 (98%)	2 (2%)	57	82
1	J	85/103 (82%)	81 (95%)	4 (5%)	32	56
2	B	74/86 (86%)	70 (95%)	4 (5%)	27	49
2	E	73/86 (85%)	68 (93%)	5 (7%)	20	36
2	H	74/86 (86%)	68 (92%)	6 (8%)	15	27
2	K	74/86 (86%)	71 (96%)	3 (4%)	37	63
3	C	114/149 (76%)	107 (94%)	7 (6%)	23	42
3	F	124/149 (83%)	115 (93%)	9 (7%)	17	32
3	I	122/149 (82%)	116 (95%)	6 (5%)	31	55
3	L	125/149 (84%)	115 (92%)	10 (8%)	15	28
All	All	1111/1352 (82%)	1045 (94%)	66 (6%)	24	44

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	10	HIS
1	A	49	GLN
2	B	27	HIS
2	B	35	HIS
2	B	46	LEU
2	B	67	SER
3	C	79	ARG
3	C	80	SER
3	C	139	SER
3	C	148	PHE
3	C	180	ILE
3	C	191	HIS
3	C	193	ASN

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Mol	Chain	Res	Type
1	D	12	THR
1	D	13	THR
1	D	47	ASP
1	D	66	THR
1	D	79	PHE
1	D	89	CYS
1	D	91	GLU
2	E	17	MET
2	E	24	SER
2	E	35	HIS
2	E	86	SER
2	E	99	ILE
3	F	77	CYS
3	F	80	SER
3	F	86	PRO
3	F	101	LEU
3	F	107	ARG
3	F	120	ARG
3	F	132	GLN
3	F	159	LYS
3	F	173	GLU
1	G	29	ARG
1	G	80	ARG
2	H	27	HIS
2	H	35	HIS
2	H	46	LEU
2	H	84	THR
2	H	87	SER
2	H	99	ILE
3	I	77	CYS
3	I	80	SER
3	I	140	LEU
3	I	180	ILE
3	I	194	VAL
3	I	197	ASP
1	J	40	ASP
1	J	47	ASP
1	J	66	THR
1	J	84	THR
2	K	67	SER
2	K	99	ILE
2	K	103	LEU

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Mol	Chain	Res	Type
3	L	69	ARG
3	L	75	ILE
3	L	77	CYS
3	L	80	SER
3	L	85	LEU
3	L	134	GLU
3	L	152	THR
3	L	170	VAL
3	L	180	ILE
3	L	197	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
2	B	35	HIS
3	C	73	GLN
3	C	110	HIS
1	D	10	HIS
3	F	110	HIS
3	F	132	GLN
3	F	141	ASN
3	F	174	ASN
1	G	42	GLN
2	H	27	HIS
2	H	35	HIS
3	I	191	HIS
3	I	195	GLN
1	J	70	GLN
3	L	174	ASN
3	L	191	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
4	GOL	B	1113	-	5,5,5	0.32	0	5,5,5	0.42	0
5	ZUN	C	1205	-	25,30,30	1.36	4 (16%)	34,42,42	2.83	9 (26%)
5	ZUN	F	1206	-	25,30,30	1.21	3 (12%)	34,42,42	2.85	8 (23%)
5	ZUN	I	1206	-	25,30,30	1.10	4 (16%)	34,42,42	2.68	8 (23%)
5	ZUN	L	1204	-	25,30,30	1.10	4 (16%)	34,42,42	3.09	10 (29%)

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
4	GOL	B	1113	-	-	0/4/4/4	0/0/0/0
5	ZUN	C	1205	-	-	0/15/33/33	0/2/3/3
5	ZUN	F	1206	-	-	0/15/33/33	0/2/3/3
5	ZUN	I	1206	-	-	0/15/33/33	0/2/3/3
5	ZUN	L	1204	-	-	0/15/33/33	0/2/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1206	ZUN	CAY-NBB	-3.13	1.32	1.43
5	C	1205	ZUN	CAY-NBB	-2.95	1.33	1.43
5	F	1206	ZUN	CAY-NBB	-2.83	1.33	1.43
5	L	1204	ZUN	CAY-NBB	-2.63	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1206	ZUN	CAK-CAW	-2.35	1.34	1.39
5	L	1204	ZUN	CAK-CAZ	-2.31	1.33	1.39
5	C	1205	ZUN	CAK-CAW	-2.14	1.35	1.39
5	L	1204	ZUN	CAK-CAW	-2.11	1.35	1.39
5	F	1206	ZUN	CAK-CAW	-2.08	1.35	1.39
5	I	1206	ZUN	CAK-CAZ	-2.04	1.34	1.39
5	L	1204	ZUN	CAM-CAU	2.26	1.54	1.52
5	I	1206	ZUN	CAM-CAU	2.26	1.54	1.52
5	C	1205	ZUN	CAM-CAZ	2.45	1.53	1.51
5	F	1206	ZUN	CAM-CAU	2.49	1.55	1.52
5	C	1205	ZUN	CAM-CAU	3.40	1.56	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	1204	ZUN	CAZ-CAM-CAU	-5.66	105.46	112.23
5	I	1206	ZUN	CAZ-CAM-CAU	-4.90	106.36	112.23
5	C	1205	ZUN	CAZ-CAM-CAU	-4.24	107.15	112.23
5	F	1206	ZUN	CAZ-CAM-CAU	-4.08	107.34	112.23
5	L	1204	ZUN	CAH-CAY-NBB	-4.04	116.57	119.31
5	I	1206	ZUN	CAH-CAY-NBB	-3.59	116.88	119.31
5	C	1205	ZUN	OAB-CAU-CAM	-3.14	116.47	121.55
5	F	1206	ZUN	OAB-CAU-CAM	-2.79	117.03	121.55
5	L	1204	ZUN	OD1-CG-CD2	-2.54	105.13	110.58
5	C	1205	ZUN	CAH-CAY-NBB	-2.49	117.62	119.31
5	I	1206	ZUN	CAX-CAL-NAR	-2.44	107.31	112.88
5	C	1205	ZUN	CB-CA-C	-2.30	106.48	111.31
5	L	1204	ZUN	OAB-CAU-CAM	-2.11	118.13	121.55
5	I	1206	ZUN	OAB-CAU-CAM	-2.11	118.14	121.55
5	C	1205	ZUN	CD2-N-CA	-2.08	108.46	111.69
5	L	1204	ZUN	CD2-N-CAU	-2.05	123.90	128.73
5	I	1206	ZUN	CAF-CAX-CAE	2.02	121.37	118.13
5	F	1206	ZUN	CB-CG-CD2	2.22	105.97	103.18
5	C	1205	ZUN	CG-CD2-N	2.46	105.90	103.09
5	F	1206	ZUN	CB-CA-N	2.54	106.91	103.19
5	L	1204	ZUN	CB-CG-CD2	2.80	106.69	103.18
5	F	1206	ZUN	CG-CD2-N	2.91	106.42	103.09
5	F	1206	ZUN	CAG-CAY-NBB	3.12	121.43	119.31
5	L	1204	ZUN	CG-CD2-N	3.17	106.71	103.09
5	I	1206	ZUN	CAG-CAY-NBB	3.19	121.48	119.31
5	C	1205	ZUN	CAG-CAY-NBB	3.58	121.74	119.31
5	L	1204	ZUN	OAD-NBB-CAY	6.36	116.95	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	1204	ZUN	CAG-CAY-NBB	6.36	123.62	119.31
5	C	1205	ZUN	OAS-NBB-CAY	6.46	117.09	108.36
5	I	1206	ZUN	OAS-NBB-CAY	7.07	117.91	108.36
5	F	1206	ZUN	OAS-NBB-CAY	7.85	118.96	108.36
5	I	1206	ZUN	OAD-NBB-CAY	9.91	121.75	108.36
5	L	1204	ZUN	OAS-NBB-CAY	11.43	123.80	108.36
5	F	1206	ZUN	OAD-NBB-CAY	11.70	124.17	108.36
5	C	1205	ZUN	OAD-NBB-CAY	12.03	124.62	108.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1206	ZUN	1	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, 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	102/118 (86%)	0.03	3 (2%) 55 60	18, 35, 61, 69	0
1	D	101/118 (85%)	0.33	4 (3%) 42 47	22, 44, 62, 70	0
1	G	103/118 (87%)	0.23	4 (3%) 43 48	25, 42, 58, 62	0
1	J	104/118 (88%)	0.02	2 (1%) 70 73	17, 34, 56, 65	0
2	B	86/97 (88%)	-0.11	1 (1%) 81 83	20, 33, 49, 55	0
2	E	87/97 (89%)	-0.09	0 100 100	21, 34, 49, 57	0
2	H	87/97 (89%)	-0.09	1 (1%) 82 84	20, 33, 55, 69	0
2	K	86/97 (88%)	-0.23	1 (1%) 81 83	18, 29, 49, 61	0
3	C	137/163 (84%)	-0.07	5 (3%) 46 51	16, 30, 56, 67	0
3	F	143/163 (87%)	-0.08	2 (1%) 78 80	16, 32, 57, 66	0
3	I	144/163 (88%)	-0.01	3 (2%) 67 71	20, 38, 58, 77	0
3	L	139/163 (85%)	-0.04	2 (1%) 78 80	16, 33, 55, 61	0
All	All	1319/1512 (87%)	-0.01	28 (2%) 67 71	16, 35, 58, 77	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	147	ILE	3.9
1	D	38	PRO	3.0
1	D	80	ARG	2.8
3	I	62	VAL	2.7
3	F	145	GLN	2.7
1	G	80	ARG	2.7
1	A	81	ALA	2.6
2	B	47	SER	2.6
3	F	142	VAL	2.6
1	G	102	VAL	2.4
3	L	177	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	83	ASP	2.4
2	H	87	SER	2.4
2	K	85	ASN	2.3
3	I	144	GLY	2.3
3	L	145	GLN	2.3
3	C	170	VAL	2.2
1	D	36	LYS	2.2
3	C	139	SER	2.2
1	A	84	THR	2.2
1	J	103	MET	2.2
1	D	79	PHE	2.2
1	G	101	ASP	2.1
3	C	178	LEU	2.1
3	C	140	LEU	2.1
1	A	82	ASP	2.1
1	J	102	VAL	2.0
3	I	204	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	B	1113	6/6	0.83	0.18	2.55	58,61,62,63	0
5	ZUN	I	1206	28/28	0.93	0.20	1.97	35,43,52,53	0
5	ZUN	F	1206	28/28	0.92	0.19	1.05	31,39,47,50	0
5	ZUN	L	1204	28/28	0.94	0.17	0.99	30,38,46,46	0
5	ZUN	C	1205	28/28	0.96	0.15	0.46	29,37,42,45	0

6.5 Other polymers (i)

There are no such residues in this entry.