



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 3, 2017 – 01:59 PM EDT

PDB ID : 4BKT
Title : von Hippel Lindau protein:ElonginB:ElonginC complex, in complex with (2S, 4R)-N-methyl-1-[2-(3-methyl-1,2-oxazol-5-yl)ethanoyl]-4-oxidanyl-pyrrolidine-2-carboxamide
Authors : Van Molle, I.; Dias, D.M.; Baud, M.; Galdeano, C.; Geraldès, C.F.G.C.; Ciulli, A.
Deposited on : unknown
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

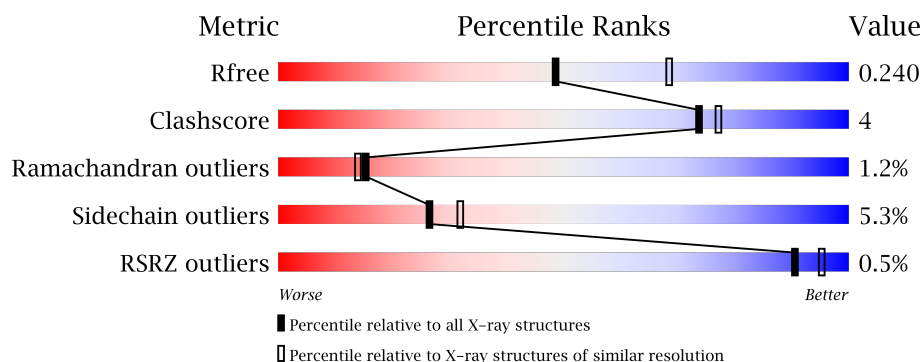
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	104	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 88%, yellow 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 1% 88% 12% </div> </div>
1	D	104	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 85%, yellow 10%, orange 3%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 1% 85% 10% 3% 2% </div> </div>
1	G	104	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 91%, yellow 7%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 91% 7% 2% </div> </div>
1	J	104	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 92%, yellow 6%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 92% 6% 2% </div> </div>
2	B	97	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 73%, yellow 16%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 73% 16% 10% </div> </div>

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Mol	Chain	Length	Quality of chain
2	E	97	
2	H	97	
2	K	97	
3	C	162	
3	F	162	
3	I	162	
3	L	162	

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	QD0	C	301	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10972 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	104	Total	As	C	N	O	S	0	0	0
			808	1	514	137	152	4			
1	D	102	Total	As	C	N	O	S	0	0	0
			783	1	498	135	146	3			
1	G	103	Total	As	C	N	O	S	0	0	0
			806	1	510	132	158	5			
1	J	103	Total	As	C	N	O	S	0	0	0
			803	1	510	136	152	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	87	Total	C	N	O	S	0	0	0
			687	443	110	128	6			
2	E	87	Total	C	N	O	S	0	0	0
			692	446	111	129	6			
2	H	87	Total	C	N	O	S	0	0	0
			677	438	108	125	6			
2	K	87	Total	C	N	O	S	0	0	0
			690	446	108	129	7			

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 Q15369

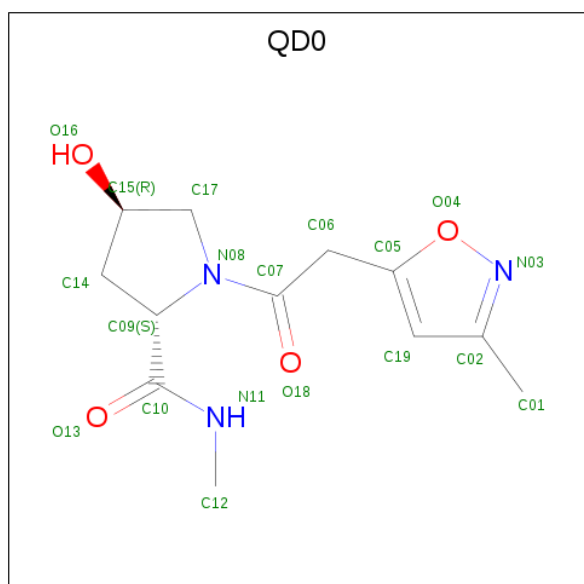
- Molecule 3 is a protein called VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	138	Total	As	C	N	O	S	0	0	0
			1082	1	697	190	192	2			
3	F	141	Total	As	C	N	O	S	0	0	0
			1116	1	712	201	200	2			
3	I	143	Total	As	C	N	O	S	0	0	0
			1159	1	739	207	210	2			
3	L	144	Total	As	C	N	O	S	0	0	0
			1154	1	735	207	209	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	52	GLY	-	expression tag	UNP P40337
C	53	SER	-	expression tag	UNP P40337
F	52	GLY	-	expression tag	UNP P40337
F	53	SER	-	expression tag	UNP P40337
I	52	GLY	-	expression tag	UNP P40337
I	53	SER	-	expression tag	UNP P40337
L	52	GLY	-	expression tag	UNP P40337
L	53	SER	-	expression tag	UNP P40337

- Molecule 4 is (2S,4R)-N-methyl-1-[2-(3-methyl-1,2-oxazol-5-yl)ethanoyl]-4-oxidanyl-pyrrolidine-2-carboxamide (three-letter code: QD0) (formula: C₁₂H₁₇N₃O₄).



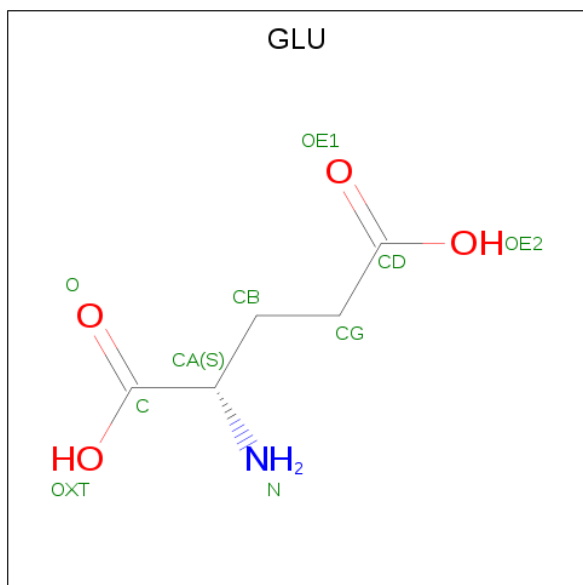
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			19	12	3	4		

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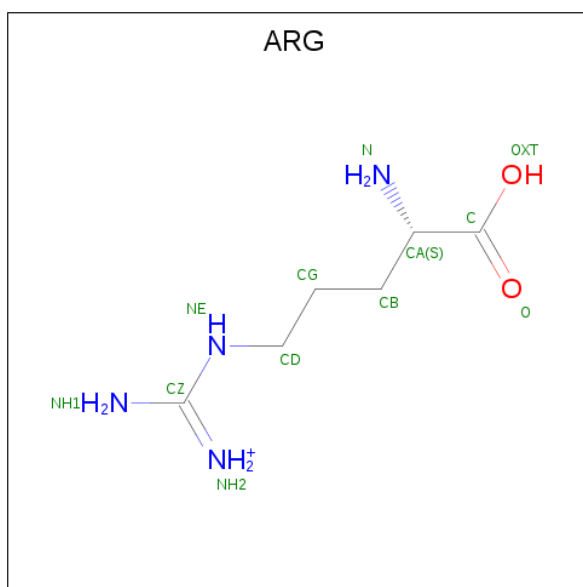
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	N	O	0	0
			19	12	3	4		
4	I	1	Total	C	N	O	0	0
			19	12	3	4		
4	L	1	Total	C	N	O	0	0
			19	12	3	4		

- Molecule 5 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 6 is ARGinine (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	I	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	57	Total	O	0	0
			57	57		
7	B	21	Total	O	0	0
			21	21		
7	C	32	Total	O	0	0
			32	32		
7	D	26	Total	O	0	0
			26	26		
7	E	28	Total	O	0	0
			28	28		
7	F	35	Total	O	0	0
			35	35		
7	G	28	Total	O	0	0
			28	28		
7	H	24	Total	O	0	0
			24	24		
7	I	35	Total	O	0	0
			35	35		
7	J	59	Total	O	0	0
			59	59		
7	K	32	Total	O	0	0
			32	32		

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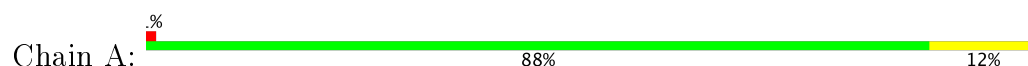
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	52	Total	O	0	0
			52	52		

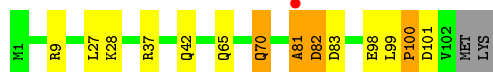
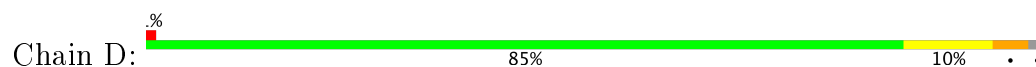
3 Residue-property plots [i](#)

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.

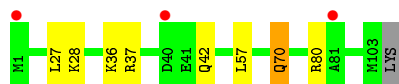
- Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2



- Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2



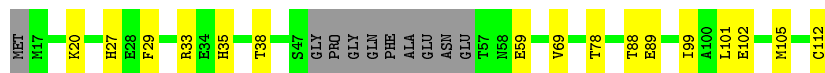
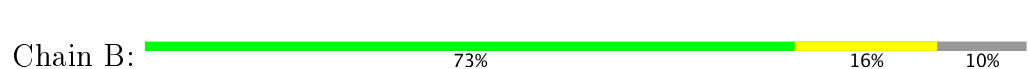
- Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2



- Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

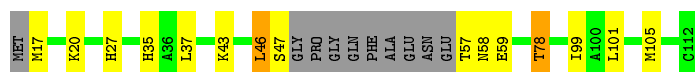


- Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

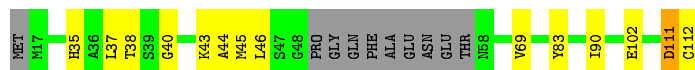


- Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

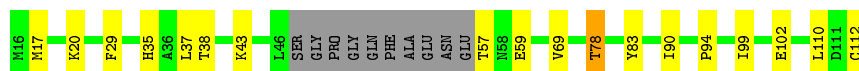




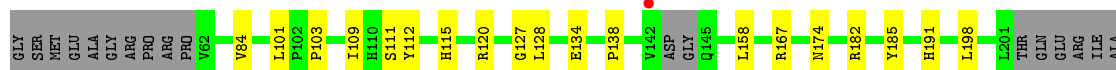
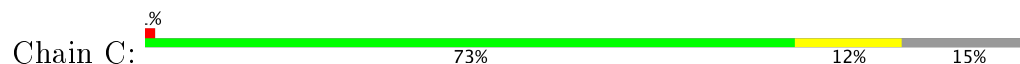
- Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1



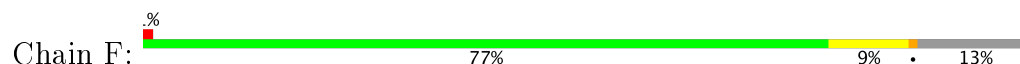
- Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1



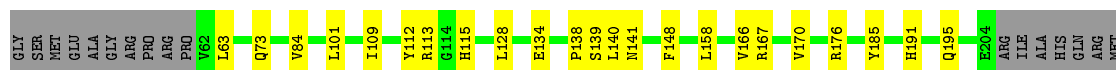
- Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR



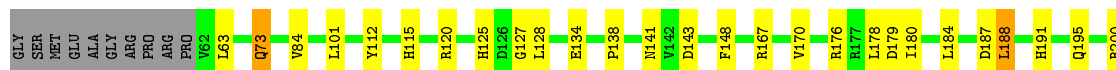
- Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR



- Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR



- Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR



R20s
ILE
ALA
HIS
GLN
ARG
MET
GLY
ASP

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	93.18 Å 93.18 Å 364.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.59 – 2.35 46.59 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.59-2.35) 100.0 (46.59-2.35)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.34 Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.190 , 0.228 0.205 , 0.240	Depositor DCC
R_{free} test set	3454 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10972	wwPDB-VP
Average B, all atoms (Å ²)	54.0	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 29.66 % 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 1.4921e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: CAS, QD0

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	0.49	0/814	0.77	1/1099 (0.1%)
1	D	0.48	0/788	0.88	3/1066 (0.3%)
1	G	0.45	0/812	0.71	0/1099
1	J	0.51	0/809	0.71	0/1094
2	B	0.49	0/701	0.68	0/947
2	E	0.54	0/706	0.70	0/952
2	H	0.46	0/691	0.65	0/933
2	K	0.49	0/704	0.67	0/950
3	C	0.50	0/1101	0.74	1/1508 (0.1%)
3	F	0.48	0/1135	0.71	0/1552
3	I	0.48	0/1179	0.69	0/1610
3	L	0.50	0/1174	0.73	0/1605
All	All	0.49	0/10614	0.72	5/14415 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	81	ALA	C-N-CA	7.37	140.12	121.70
1	D	100	PRO	N-CA-CB	7.12	111.85	103.30
1	D	82	ASP	C-N-CA	6.00	136.71	121.70
1	A	82	ASP	C-N-CA	5.79	136.19	121.70
3	C	103	PRO	N-CA-C	5.50	126.39	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	808	0	798	4	0
1	D	783	0	766	3	0
1	G	806	0	787	4	0
1	J	803	0	794	4	0
2	B	687	0	682	6	0
2	E	692	0	690	9	0
2	H	677	0	672	14	0
2	K	690	0	688	7	0
3	C	1082	0	1037	10	0
3	F	1116	0	1088	14	0
3	I	1159	0	1142	8	0
3	L	1154	0	1122	12	0
4	C	19	0	17	0	0
4	F	19	0	17	0	0
4	I	19	0	17	0	0
4	L	19	0	17	0	0
5	F	5	0	1	0	0
6	I	5	0	1	0	0
7	A	57	0	0	1	0
7	B	21	0	0	0	0
7	C	32	0	0	0	0
7	D	26	0	0	1	0
7	E	28	0	0	1	0
7	F	35	0	0	0	0
7	G	28	0	0	0	0
7	H	24	0	0	0	0
7	I	35	0	0	0	0
7	J	59	0	0	1	0
7	K	32	0	0	0	0
7	L	52	0	0	0	0
All	All	10972	0	10336	80	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 4.

All (80) 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)
2:E:57:THR:HA	2:E:59:GLU:H	1.33	0.93
2:E:37:LEU:HD22	2:E:43:LYS:HG3	1.52	0.90
3:I:73:GLN:H	3:I:141:ASN:HD21	1.30	0.80
3:L:73:GLN:H	3:L:141:ASN:HD21	1.32	0.78
2:E:46:LEU:O	2:E:47:SER:HB3	1.84	0.77
2:E:46:LEU:O	2:E:47:SER:CB	2.47	0.60
1:G:27:LEU:HD13	1:G:57:LEU:HD11	1.82	0.60
3:L:187:ASP:O	3:L:188:LEU:HB2	2.05	0.57
2:H:37:LEU:HD21	2:H:46:LEU:HD11	1.86	0.57
2:B:101:LEU:O	2:B:105:MET:HG3	2.05	0.57
3:F:148:PHE:HE1	2:H:44:ALA:HB3	1.70	0.56
2:E:101:LEU:O	2:E:105:MET:HG3	2.07	0.54
3:L:115:HIS:O	3:L:138:PRO:HD2	2.07	0.54
1:G:70:GLN:NE2	1:G:70:GLN:H	2.05	0.53
1:D:70:GLN:H	1:D:70:GLN:NE2	2.05	0.53
3:F:148:PHE:HE1	2:H:44:ALA:CB	2.21	0.53
2:H:40:GLY:H	2:H:111:ASP:HB2	1.74	0.53
2:H:112:CYS:HB3	3:I:158:LEU:HB3	1.91	0.53
1:A:102:VAL:HG21	3:C:174:ASN:CB	2.40	0.52
3:F:166:VAL:O	3:F:170:VAL:HG12	2.11	0.51
3:C:182:ARG:HA	3:C:185:TYR:CD2	2.46	0.51
3:I:166:VAL:O	3:I:170:VAL:HG12	2.12	0.50
7:J:225:HOH:O	2:K:78:THR:HG21	2.13	0.49
3:L:167:ARG:HD3	3:L:191:HIS:HD2	1.78	0.49
1:G:70:GLN:H	1:G:70:GLN:HE21	1.61	0.49
1:J:63:THR:H	1:J:66:THR:HG22	1.78	0.49
1:A:102:VAL:HG21	3:C:174:ASN:HB2	1.93	0.48
2:H:37:LEU:HD22	2:H:43:LYS:HG3	1.95	0.48
2:E:78:THR:HG22	7:E:204:HOH:O	2.13	0.48
3:L:120:ARG:HD3	3:L:127:GLY:HA2	1.96	0.48
3:F:148:PHE:CZ	2:H:45:MET:HG3	2.49	0.48
2:B:112:CYS:HB3	3:C:158:LEU:HB3	1.95	0.47
3:F:148:PHE:CE1	2:H:44:ALA:CB	2.97	0.47
2:K:37:LEU:HD22	2:K:43:LYS:HG3	1.95	0.47
1:D:70:GLN:H	1:D:70:GLN:HE21	1.63	0.47
1:A:41:GLU:HA	1:A:80:ARG:HG2	1.96	0.46
3:I:167:ARG:HD3	3:I:191:HIS:HD2	1.81	0.46
1:D:28:LYS:HA	1:D:42:GLN:HE22	1.81	0.46
3:F:148:PHE:CD1	2:H:44:ALA:HB1	2.51	0.46
3:C:115:HIS:O	3:C:138:PRO:HD2	2.16	0.46
3:F:148:PHE:HZ	2:H:45:MET:HG3	1.81	0.46
3:I:84:VAL:HG22	3:I:128:LEU:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:148:PHE:CE1	2:H:44:ALA:HB1	2.51	0.45
2:E:20:LYS:HB3	2:E:59:GLU:HG2	1.99	0.45
3:L:84:VAL:HG22	3:L:128:LEU:CD1	2.47	0.45
3:F:84:VAL:HG22	3:F:128:LEU:CD1	2.46	0.45
3:C:120:ARG:HD3	3:C:127:GLY:HA2	1.99	0.45
2:B:20:LYS:HB3	2:B:59:GLU:HG2	1.99	0.45
3:F:167:ARG:HD3	3:F:191:HIS:HD2	1.81	0.45
3:C:84:VAL:HG22	3:C:128:LEU:CD1	2.47	0.44
1:G:28:LYS:HA	1:G:42:GLN:HE22	1.81	0.44
2:K:20:LYS:HB3	2:K:59:GLU:HG2	1.99	0.44
3:L:167:ARG:HD3	3:L:191:HIS:CD2	2.53	0.43
3:L:120:ARG:HD2	3:L:125:HIS:O	2.19	0.43
3:F:112:TYR:HB2	3:F:115:HIS:CE1	2.54	0.43
1:A:15:PHE:HE1	2:B:29:PHE:HD1	1.67	0.42
3:C:167:ARG:HD3	3:C:191:HIS:HD2	1.84	0.42
3:I:112:TYR:HB2	3:I:115:HIS:CE1	2.54	0.42
1:J:70:GLN:HG3	2:K:94:PRO:HD3	2.02	0.42
2:K:83:TYR:HB3	2:K:90:ILE:HG12	2.02	0.42
3:L:184:LEU:O	3:L:187:ASP:O	2.38	0.42
7:A:203:HOH:O	2:B:27:HIS:HD2	2.03	0.42
2:E:57:THR:HA	2:E:59:GLU:N	2.17	0.42
3:F:73:GLN:HE22	3:F:110:HIS:CG	2.37	0.42
1:J:15:PHE:HE1	2:K:29:PHE:HD1	1.68	0.42
1:J:102:VAL:HG13	3:L:170:VAL:HG13	2.01	0.41
3:C:112:TYR:HB2	3:C:115:HIS:CE1	2.55	0.41
3:F:115:HIS:O	3:F:138:PRO:HD2	2.20	0.41
3:I:115:HIS:O	3:I:138:PRO:HD2	2.20	0.41
3:C:109:ILE:HD12	3:C:111:SER:HB2	2.02	0.41
2:H:83:TYR:HB3	2:H:90:ILE:HG12	2.03	0.41
7:D:205:HOH:O	2:E:27:HIS:HD2	2.03	0.41
2:H:69:VAL:HG21	2:H:102:GLU:HB3	2.02	0.41
3:F:134:GLU:HB3	3:F:135:LEU:HD22	2.02	0.41
2:B:69:VAL:HG21	2:B:102:GLU:HB3	2.02	0.41
2:H:40:GLY:H	2:H:111:ASP:CB	2.33	0.41
3:I:176:ARG:NH1	3:I:185:TYR:HB3	2.36	0.41
3:L:112:TYR:HB2	3:L:115:HIS:CE1	2.55	0.41
2:K:69:VAL:HG21	2:K:102:GLU:HB3	2.01	0.40
3:L:170:VAL:HG21	3:L:178:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	101/104 (97%)	93 (92%)	5 (5%)	3 (3%)	5	2
1	D	99/104 (95%)	88 (89%)	4 (4%)	7 (7%)	1	0
1	G	100/104 (96%)	95 (95%)	5 (5%)	0	100	100
1	J	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
2	B	83/97 (86%)	81 (98%)	1 (1%)	1 (1%)	15	14
2	E	83/97 (86%)	80 (96%)	3 (4%)	0	100	100
2	H	83/97 (86%)	82 (99%)	1 (1%)	0	100	100
2	K	83/97 (86%)	83 (100%)	0	0	100	100
3	C	133/162 (82%)	126 (95%)	6 (4%)	1 (1%)	22	24
3	F	138/162 (85%)	133 (96%)	5 (4%)	0	100	100
3	I	140/162 (86%)	135 (96%)	5 (4%)	0	100	100
3	L	141/162 (87%)	130 (92%)	7 (5%)	4 (3%)	6	3
All	All	1284/1452 (88%)	1220 (95%)	48 (4%)	16 (1%)	15	14

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	THR
1	A	103	MET
1	D	81	ALA
1	D	82	ASP
1	D	98	GLU
1	D	99	LEU
1	D	100	PRO
3	L	143	ASP
3	L	179	ASP
3	L	180	ILE
3	L	188	LEU
1	A	83	ASP

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Mol	Chain	Res	Type
3	C	198	LEU
1	D	83	ASP
1	D	101	ASP
2	B	88	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/91 (93%)	81 (95%)	4 (5%)	30	38
1	D	81/91 (89%)	76 (94%)	5 (6%)	21	24
1	G	88/91 (97%)	84 (96%)	4 (4%)	32	40
1	J	86/91 (94%)	83 (96%)	3 (4%)	41	52
2	B	77/86 (90%)	71 (92%)	6 (8%)	15	16
2	E	78/86 (91%)	72 (92%)	6 (8%)	15	16
2	H	75/86 (87%)	72 (96%)	3 (4%)	36	46
2	K	78/86 (91%)	70 (90%)	8 (10%)	8	8
3	C	115/147 (78%)	113 (98%)	2 (2%)	66	77
3	F	122/147 (83%)	119 (98%)	3 (2%)	53	66
3	I	130/147 (88%)	121 (93%)	9 (7%)	18	19
3	L	127/147 (86%)	119 (94%)	8 (6%)	21	23
All	All	1142/1296 (88%)	1081 (95%)	61 (5%)	26	32

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	49	GLN
1	A	65	GLN
1	A	68	ARG
2	B	33	ARG
2	B	35	HIS

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Mol	Chain	Res	Type
2	B	38	THR
2	B	78	THR
2	B	89	GLU
2	B	99	ILE
3	C	101	LEU
3	C	134	GLU
1	D	9	ARG
1	D	27	LEU
1	D	37	ARG
1	D	65	GLN
1	D	70	GLN
2	E	17	MET
2	E	35	HIS
2	E	46	LEU
2	E	58	ASN
2	E	78	THR
2	E	99	ILE
3	F	63	LEU
3	F	120	ARG
3	F	148	PHE
1	G	36	LYS
1	G	37	ARG
1	G	70	GLN
1	G	80	ARG
2	H	35	HIS
2	H	38	THR
2	H	111	ASP
3	I	63	LEU
3	I	101	LEU
3	I	109	ILE
3	I	113	ARG
3	I	134	GLU
3	I	139	SER
3	I	140	LEU
3	I	148	PHE
3	I	195	GLN
1	J	27	LEU
1	J	84	THR
1	J	102	VAL
2	K	17	MET
2	K	35	HIS
2	K	38	THR

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Mol	Chain	Res	Type
2	K	57	THR
2	K	78	THR
2	K	99	ILE
2	K	110	LEU
2	K	112	CYS
3	L	63	LEU
3	L	73	GLN
3	L	101	LEU
3	L	134	GLU
3	L	148	PHE
3	L	176	ARG
3	L	195	GLN
3	L	200	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
2	B	27	HIS
3	C	67	ASN
3	C	174	ASN
1	D	42	GLN
1	D	65	GLN
1	D	70	GLN
3	F	73	GLN
1	G	42	GLN
1	G	70	GLN
2	H	27	HIS
3	I	141	ASN
3	L	141	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CAS	A	89	1	6,8,9	1.22	0	2,9,11	1.24	0
3	CAS	C	77	3	6,8,9	1.40	1 (16%)	2,9,11	1.20	0
1	CAS	D	89	1	6,8,9	1.30	0	2,9,11	1.15	0
3	CAS	F	77	3	6,8,9	1.06	0	2,9,11	1.71	1 (50%)
1	CAS	G	89	1	6,8,9	1.22	0	2,9,11	1.45	1 (50%)
3	CAS	I	77	3	6,8,9	0.91	0	2,9,11	1.55	1 (50%)
1	CAS	J	89	1	6,8,9	1.04	0	2,9,11	1.42	0
3	CAS	L	77	3	6,8,9	1.55	2 (33%)	2,9,11	1.37	0

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
1	CAS	A	89	1	-	0/0/7/9	0/0/0/0
3	CAS	C	77	3	-	0/0/7/9	0/0/0/0
1	CAS	D	89	1	-	0/0/7/9	0/0/0/0
3	CAS	F	77	3	-	0/0/7/9	0/0/0/0
1	CAS	G	89	1	-	0/0/7/9	0/0/0/0
3	CAS	I	77	3	-	0/0/7/9	0/0/0/0
1	CAS	J	89	1	-	0/0/7/9	0/0/0/0
3	CAS	L	77	3	-	0/0/7/9	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	77	CAS	AS-CE2	2.24	2.01	1.96
3	L	77	CAS	AS-CE1	2.28	2.02	1.96
3	C	77	CAS	CA-C	2.52	1.53	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	77	CAS	O-C-CA	-2.24	118.84	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	77	CAS	O-C-CA	-2.17	119.03	125.02
1	G	89	CAS	O-C-CA	-2.04	119.37	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	QD0	C	301	-	17,20,20	2.64	4 (23%)	23,28,28	1.93	7 (30%)
5	GLU	F	301	-	4,4,9	1.40	1 (25%)	1,4,11	0.02	0
4	QD0	F	302	-	17,20,20	2.46	4 (23%)	23,28,28	2.41	10 (43%)
6	ARG	I	301	-	4,4,11	1.47	1 (25%)	1,4,13	0.06	0
4	QD0	I	302	-	17,20,20	2.53	4 (23%)	23,28,28	2.14	9 (39%)
4	QD0	L	301	-	17,20,20	2.54	4 (23%)	23,28,28	2.20	8 (34%)

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	QD0	C	301	-	-	0/12/26/26	0/1/2/2
5	GLU	F	301	-	-	0/0/2/9	0/0/0/0
4	QD0	F	302	-	-	0/12/26/26	0/1/2/2
6	ARG	I	301	-	-	0/0/2/11	0/0/0/0
4	QD0	I	302	-	-	0/12/26/26	0/1/2/2
4	QD0	L	301	-	-	0/12/26/26	0/1/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	302	QD0	C14-C09	-2.88	1.47	1.53
4	F	302	QD0	C14-C09	-2.53	1.48	1.53
4	L	301	QD0	C14-C09	-2.48	1.48	1.53
4	C	301	QD0	C14-C09	-2.47	1.48	1.53
4	C	301	QD0	C14-C15	-2.46	1.47	1.52
4	L	301	QD0	C14-C15	-2.28	1.48	1.52
4	F	302	QD0	C14-C15	-2.26	1.48	1.52
4	I	302	QD0	C14-C15	-2.12	1.48	1.52
5	F	301	GLU	CA-C	2.61	1.53	1.50
6	I	301	ARG	CA-C	2.78	1.53	1.50
4	I	302	QD0	C07-N08	4.67	1.46	1.35
4	F	302	QD0	C07-N08	4.93	1.47	1.35
4	L	301	QD0	C07-N08	4.94	1.47	1.35
4	C	301	QD0	C07-N08	5.00	1.47	1.35
4	F	302	QD0	C10-N11	7.43	1.43	1.32
4	I	302	QD0	C10-N11	7.74	1.44	1.32
4	L	301	QD0	C10-N11	7.84	1.44	1.32
4	C	301	QD0	C10-N11	8.21	1.44	1.32

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	301	QD0	C05-C06-C07	-4.75	106.06	112.08
4	I	302	QD0	C05-C06-C07	-4.15	106.82	112.08
4	F	302	QD0	C17-N08-C09	-3.55	106.31	111.69
4	F	302	QD0	C05-C06-C07	-3.45	107.70	112.08
4	L	301	QD0	C17-N08-C09	-2.89	107.31	111.69
4	C	301	QD0	C17-N08-C09	-2.72	107.57	111.69
4	F	302	QD0	C15-C14-C09	-2.64	100.38	103.93
4	F	302	QD0	C19-C02-N03	-2.45	106.35	110.86
4	C	301	QD0	C05-C06-C07	-2.42	109.01	112.08
4	I	302	QD0	C17-N08-C09	-2.40	108.06	111.69
4	I	302	QD0	O18-C07-N08	-2.40	117.07	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	302	QD0	C06-C05-C19	-2.36	124.70	131.68
4	L	301	QD0	C19-C02-N03	-2.30	106.63	110.86
4	I	302	QD0	C19-C02-N03	-2.27	106.69	110.86
4	F	302	QD0	O18-C07-C06	-2.18	118.10	121.58
4	C	301	QD0	C19-C02-N03	-2.17	106.86	110.86
4	L	301	QD0	O18-C07-C06	-2.05	118.30	121.58
4	F	302	QD0	O18-C07-N08	-2.01	117.79	121.55
4	C	301	QD0	C14-C15-C17	2.56	106.79	103.38
4	L	301	QD0	C14-C15-C17	2.61	106.86	103.38
4	F	302	QD0	C01-C02-N03	2.94	125.83	120.05
4	C	301	QD0	C01-C02-N03	3.06	126.07	120.05
4	L	301	QD0	C01-C02-N03	3.09	126.12	120.05
4	I	302	QD0	C14-C15-C17	3.13	107.54	103.38
4	I	302	QD0	C06-C07-N08	3.33	122.43	117.90
4	C	301	QD0	C06-C07-N08	3.40	122.53	117.90
4	F	302	QD0	C14-C15-C17	3.47	108.00	103.38
4	L	301	QD0	C06-C07-N08	3.53	122.70	117.90
4	I	302	QD0	C01-C02-N03	3.81	127.54	120.05
4	C	301	QD0	C14-C09-N08	4.43	109.30	103.12
4	F	302	QD0	C06-C07-N08	4.49	124.02	117.90
4	I	302	QD0	C14-C09-N08	4.64	109.59	103.12
4	L	301	QD0	C14-C09-N08	4.91	109.96	103.12
4	F	302	QD0	C14-C09-N08	6.17	111.71	103.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	103/104 (99%)	-0.26	1 (0%) 82 90	31, 46, 88, 114	0
1	D	101/104 (97%)	-0.03	1 (0%) 82 90	38, 62, 98, 122	0
1	G	102/104 (98%)	-0.09	3 (2%) 52 63	38, 59, 84, 101	0
1	J	102/104 (98%)	-0.36	0 100 100	29, 42, 70, 79	0
2	B	87/97 (89%)	-0.22	0 100 100	34, 47, 89, 100	0
2	E	87/97 (89%)	-0.13	0 100 100	37, 55, 83, 94	0
2	H	87/97 (89%)	-0.17	0 100 100	35, 50, 89, 122	0
2	K	87/97 (89%)	-0.23	0 100 100	30, 45, 80, 89	0
3	C	137/162 (84%)	-0.19	1 (0%) 87 93	34, 49, 78, 116	0
3	F	140/162 (86%)	-0.16	1 (0%) 87 93	33, 51, 88, 122	0
3	I	142/162 (87%)	-0.18	0 100 100	34, 52, 79, 102	0
3	L	143/162 (88%)	-0.16	0 100 100	32, 47, 79, 105	0
All	All	1318/1452 (90%)	-0.18	7 (0%) 90 95	29, 50, 86, 122	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	142	VAL	5.6
1	D	81	ALA	3.7
1	A	102	VAL	2.7
1	G	40	ASP	2.6
1	G	1	MET	2.1
3	F	202	THR	2.1
1	G	81	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CAS	L	77	9/10	0.97	0.09	-	36,41,68,70	0
3	CAS	I	77	9/10	0.96	0.09	-	40,43,61,63	3
3	CAS	F	77	9/10	0.96	0.13	-	42,45,62,65	3
3	CAS	C	77	9/10	0.97	0.12	-	45,48,67,71	3
1	CAS	G	89	9/10	0.93	0.13	-	55,58,70,71	3
1	CAS	A	89	9/10	0.93	0.12	-	54,57,77,78	3
1	CAS	J	89	9/10	0.97	0.10	-	43,45,57,58	3
1	CAS	D	89	9/10	0.93	0.10	-	71,75,90,91	3

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	QD0	C	301	19/19	0.95	0.18	3.17	42,46,67,67	0
4	QD0	F	302	19/19	0.94	0.15	0.98	40,46,58,59	0
4	QD0	L	301	19/19	0.95	0.16	0.90	39,46,65,66	0
4	QD0	I	302	19/19	0.93	0.15	0.64	32,45,65,65	0
5	GLU	F	301	5/10	0.78	0.27	-	113,131,137,169	0
6	ARG	I	301	5/12	0.86	0.19	-	84,88,103,123	0

6.5 Other polymers [i](#)

There are no such residues in this entry.