



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 12:24 PM EST

PDB ID : 2J9J
Title : Atomic-resolution Crystal Structure of Chemically-Synthesized HIV-1 Protease Complexed with Inhibitor JG-365
Authors : Malito, E.; Shen, Y.; Johnson, E.C.B.; Tang, W.J.
Deposited on : 2006-11-11
Resolution : 1.04 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

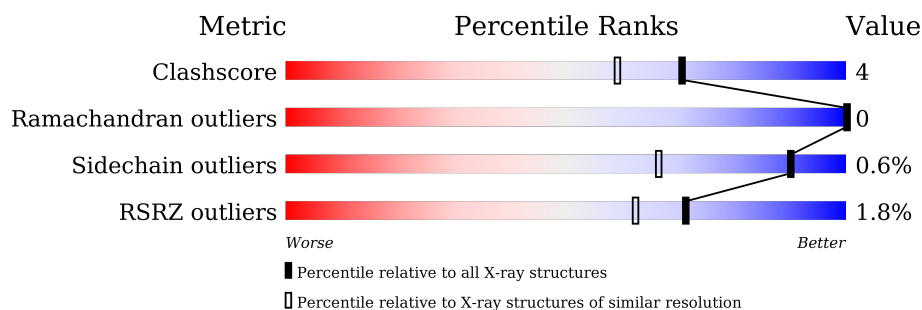
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.04 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))
Clashscore	102246	1109 (1.10-0.98)
Ramachandran outliers	100387	1041 (1.10-0.98)
Sidechain outliers	100360	1039 (1.10-0.98)
RSRZ outliers	91569	1034 (1.10-0.98)

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	1-A	99	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>
1	2-A	99	<div> <div>%</div> <div> <div></div> <div>95%</div> <div></div> <div>..</div> </div> </div>
2	1-B	99	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
2	2-B	99	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>7%</div> <div>.</div> </div> </div>
3	1-C	7	<div> <div></div> <div> <div>29%</div> <div>57%</div> <div>14%</div> </div> </div>
3	2-C	7	<div> <div></div> <div> <div>43%</div> <div>43%</div> <div>14%</div> </div> </div>

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
3	JG3	1-C	4[A]	X	-	-	-
3	JG3	2-C	4[C]	X	-	-	-
4	SO4	1-B	1105[A]	-	-	-	X
4	SO4	2-B	1105[C]	-	-	-	X
5	GOL	1-A	1107[A]	-	-	-	X
5	GOL	1-A	1108[A]	-	-	-	X
5	GOL	2-A	1107[C]	-	-	-	X
5	GOL	2-A	1108[C]	-	-	-	X
6	ACT	1-B	1106[A]	-	-	-	X
6	ACT	2-B	1106[C]	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3784 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 PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	99	Total	C	N	O	S	0	99	0
			784	512	134	137	1			
1	2-A	99	Total	C	N	O	S	0	99	0
			784	512	134	137	1			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LYS	GLN	CONFLICT	UNP O38907
A	36	NLE	MET	CONFLICT	UNP O38907
A	41	SLZ	ARG	CONFLICT	UNP O38907
A	46	NLE	MET	CONFLICT	UNP O38907
A	62	ILE	VAL	CONFLICT	UNP O38907
A	64	VAL	ILE	CONFLICT	UNP O38907
A	93	ILE	LEU	CONFLICT	UNP O38907

- Molecule 2 is a protein called PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1-B	99	Total	C	N	O	S	0	99	0
			779	509	133	136	1			
2	2-B	99	Total	C	N	O	S	0	99	0
			779	509	133	136	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	LYS	GLN	CONFLICT	UNP O38907
B	18	ASN	GLN	CONFLICT	UNP O38907
B	36	NLE	MET	CONFLICT	UNP O38907
B	41	SLZ	ARG	CONFLICT	UNP O38907
B	46	NLE	MET	CONFLICT	UNP O38907

Continued on next page...

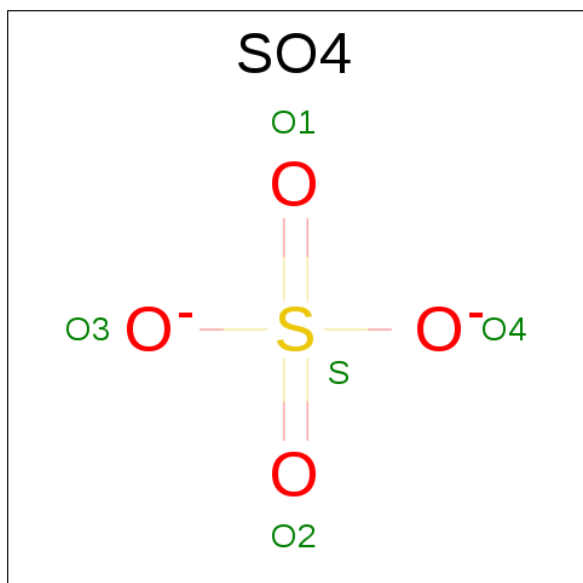
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	62	ILE	VAL	CONFLICT	UNP O38907
B	64	VAL	ILE	CONFLICT	UNP O38907
B	93	ILE	LEU	CONFLICT	UNP O38907

- Molecule 3 is a protein called INHIBITOR MOLECULE JG365.

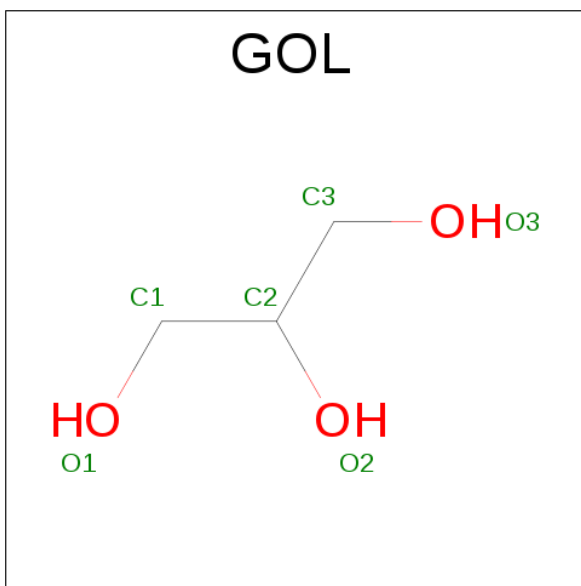
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	1-C	6	Total	C	N	O	0	6	0
			58	40	8	10			
3	2-C	6	Total	C	N	O	0	6	0
			58	40	8	10			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



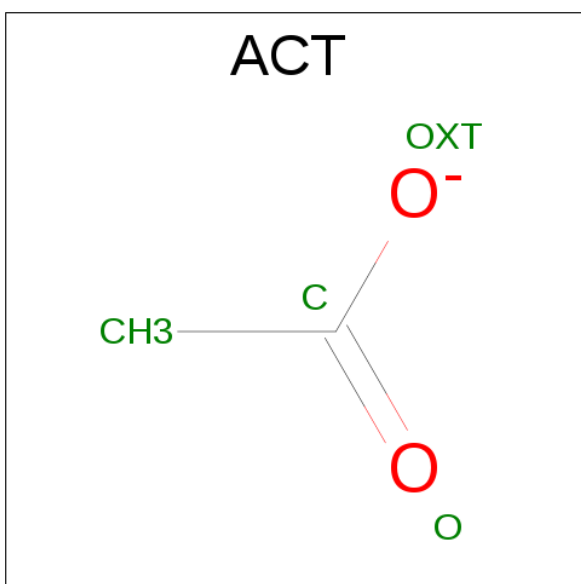
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	1-A	1	Total	O	S	0	1
			5	4	1		
4	2-A	1	Total	O	S	0	1
			5	4	1		
4	1-A	1	Total	O	S	0	1
			5	4	1		
4	2-A	1	Total	O	S	0	1
			5	4	1		
4	1-B	1	Total	O	S	0	1
			5	4	1		
4	2-B	1	Total	O	S	0	1
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	1-A	1	Total	C	O	0	1
			6	3	3		
5	2-A	1	Total	C	O	0	1
			6	3	3		
5	1-A	1	Total	C	O	0	1
			6	3	3		
5	2-A	1	Total	C	O	0	1
			6	3	3		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1-B	1	Total C O 4 2 2	0	1
6	2-B	1	Total C O 4 2 2	0	1

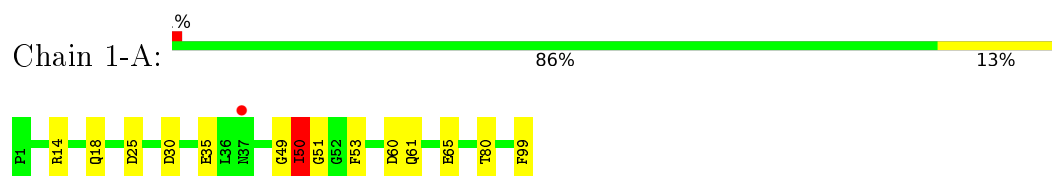
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	1-A	123	Total O 123 123	0	123
7	2-A	123	Total O 123 123	0	123
7	1-B	116	Total O 116 116	0	116
7	2-B	116	Total O 116 116	0	116
7	1-C	1	Total O 1 1	0	1
7	2-C	1	Total O 1 1	0	1

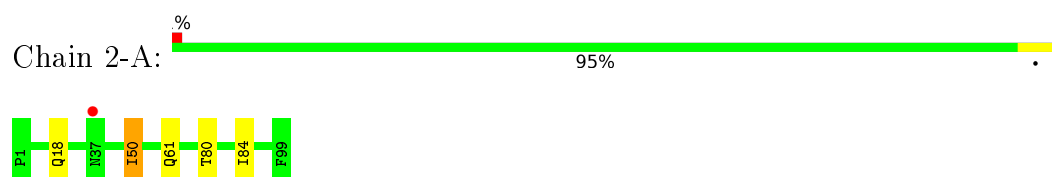
3 Residue-property plots

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

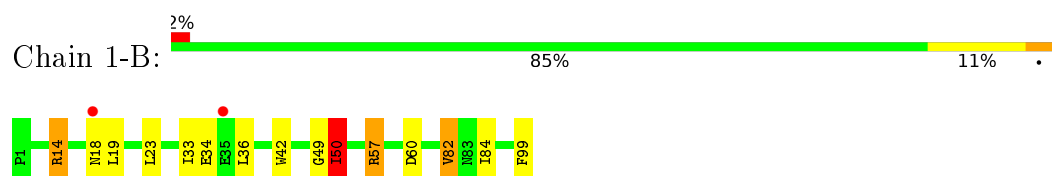
- Molecule 1: PROTEASE



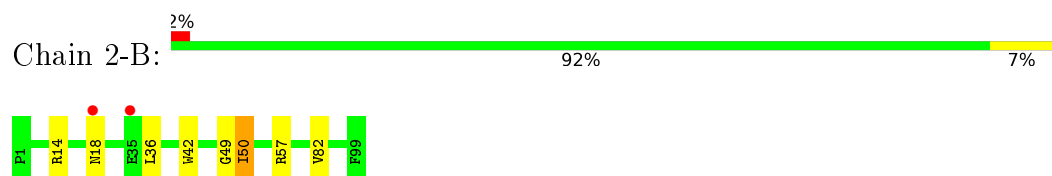
- Molecule 1: PROTEASE



- Molecule 2: PROTEASE



- Molecule 2: PROTEASE



- Molecule 3: INHIBITOR MOLECULE JG365



- Molecule 3: INHIBITOR MOLECULE JG365



ACE
S1
L2
N3
?4
I5
?6

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.55Å 58.81Å 60.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.04 9.98 – 1.04	Depositor EDS
% Data completeness (in resolution range)	84.5 (10.00-1.04) 81.6 (9.98-1.04)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.04Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.131 , 0.191 0.150 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	10.4	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,l,k	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	3784	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SLZ, ABA, VME, NLE, SO4, ACT, JG3

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	1-A	1.24	4/759 (0.5%)	2.34	19/1022 (1.9%)
2	1-B	1.99	3/754 (0.4%)	2.41	20/1016 (2.0%)
3	1-C	1.27	0/28	1.47	0/35
All	All	1.65	7/1541 (0.5%)	2.36	39/2073 (1.9%)

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	1-A	0	3
1	2-A	0	3
2	1-B	0	3
2	2-B	0	3
3	1-C	1	1
3	2-C	1	1
All	All	2	14

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-B	50[A]	ILE	C-N	-34.35	0.71	1.33
2	1-B	50[B]	ILE	C-N	-34.35	0.71	1.33
1	1-A	50[A]	ILE	C-N	17.23	1.64	1.33
1	1-A	50[B]	ILE	C-N	17.23	1.64	1.33
2	1-B	99[A]	PHE	C-OXT	6.09	1.34	1.23
1	1-A	30[A]	ASP	CG-OD2	-5.50	1.12	1.25
1	1-A	99[A]	PHE	C-OXT	5.13	1.33	1.23

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	50[A]	ILE	O-C-N	-31.58	69.52	123.20
1	1-A	50[B]	ILE	O-C-N	-31.58	69.52	123.20
2	1-B	50[A]	ILE	O-C-N	-30.76	70.91	123.20
2	1-B	50[B]	ILE	O-C-N	-30.76	70.91	123.20
1	1-A	50[A]	ILE	CA-C-N	25.36	166.93	116.20
1	1-A	50[B]	ILE	CA-C-N	25.36	166.93	116.20
2	1-B	50[A]	ILE	CA-C-N	23.94	164.09	116.20
2	1-B	50[B]	ILE	CA-C-N	23.94	164.09	116.20
2	1-B	14[A]	ARG	CD-NE-CZ	17.70	148.38	123.60
2	1-B	50[A]	ILE	C-N-CA	14.47	152.70	122.30
2	1-B	50[B]	ILE	C-N-CA	14.47	152.70	122.30
1	1-A	50[A]	ILE	C-N-CA	13.27	150.16	122.30
1	1-A	50[B]	ILE	C-N-CA	13.27	150.16	122.30
2	1-B	14[A]	ARG	NE-CZ-NH2	9.76	125.18	120.30
2	1-B	57[A]	ARG	NE-CZ-NH1	-9.35	115.62	120.30
2	1-B	57[A]	ARG	CD-NE-CZ	8.93	136.10	123.60
1	1-A	35[A]	GLU	CB-CG-CD	8.35	136.74	114.20
1	1-A	14[A]	ARG	NE-CZ-NH2	-8.27	116.17	120.30
2	1-B	60[A]	ASP	CB-CG-OD1	7.81	125.33	118.30
1	1-A	60[A]	ASP	CB-CG-OD2	-7.36	111.67	118.30
1	1-A	30[A]	ASP	CB-CG-OD2	7.25	124.82	118.30
2	1-B	57[A]	ARG	NH1-CZ-NH2	6.90	126.99	119.40
1	1-A	49[A]	GLY	O-C-N	6.75	133.50	122.70
1	1-A	53[A]	PHE	CB-CG-CD2	-6.71	116.10	120.80
2	1-B	82[A]	VAL	CG1-CB-CG2	-6.33	100.78	110.90
1	1-A	53[A]	PHE	CB-CG-CD1	6.32	125.23	120.80
2	1-B	57[A]	ARG	CG-CD-NE	5.95	124.29	111.80
1	1-A	60[A]	ASP	CB-CG-OD1	5.93	123.64	118.30
2	1-B	57[A]	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	1-A	65[A]	GLU	CG-CD-OE2	5.82	129.94	118.30
1	1-A	65[A]	GLU	CG-CD-OE1	-5.54	107.22	118.30
2	1-B	23[A]	LEU	CA-CB-CG	5.26	127.39	115.30
2	1-B	33[A]	ILE	C-N-CA	-5.18	108.75	121.70
2	1-B	33[B]	ILE	C-N-CA	-5.18	108.75	121.70
1	1-A	25[A]	ASP	CB-CG-OD1	5.17	122.95	118.30
1	1-A	51[A]	GLY	C-N-CA	-5.14	111.50	122.30
1	1-A	51[B]	GLY	C-N-CA	-5.14	111.50	122.30
2	1-B	14[A]	ARG	NH1-CZ-NH2	-5.08	113.81	119.40
2	1-B	34[A]	GLU	CG-CD-OE2	5.03	128.36	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	1-C	4[A]	JG3	C1
3	2-C	4[C]	JG3	C1

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	50[A]	ILE	Mainchain,Peptide
1	1-A	50[B]	ILE	Mainchain
2	1-B	50[A]	ILE	Mainchain,Peptide
2	1-B	50[B]	ILE	Mainchain
3	1-C	3[A]	ASN	Peptide
1	2-A	50[C]	ILE	Mainchain,Peptide
1	2-A	50[D]	ILE	Mainchain
2	2-B	50[C]	ILE	Mainchain,Peptide
2	2-B	50[D]	ILE	Mainchain
3	2-C	3[C]	ASN	Peptide

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	1-A	784	0	842	4	0
1	2-A	784	0	842	6	0
2	1-B	779	0	834	10	0
2	2-B	779	0	834	9	0
3	1-C	58	0	63	4	0
3	2-C	58	0	63	4	0
4	1-A	10	0	0	0	0
4	1-B	5	0	0	0	0
4	2-A	10	0	0	0	0
4	2-B	5	0	0	0	0
5	1-A	12	0	14	1	0
5	2-A	12	0	14	1	0
6	1-B	4	0	3	0	0
6	2-B	4	0	3	0	0
7	1-A	123	0	0	3	0
7	1-B	116	0	0	3	0
7	1-C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	2-A	123	0	0	3	0
7	2-B	116	0	0	3	0
7	2-C	1	0	0	0	0
All	All	3784	0	3512	30	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 (30) 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:4[A]:JG3:O	3:C:5[A]:ILE:HD13	1.85	0.76
2:B:18[A]:ASN:HD22	2:B:18[A]:ASN:N	2.01	0.58
2:B:18[C]:ASN:N	2:B:18[C]:ASN:HD22	2.01	0.58
1:A:84[C]:ILE:CD1	3:C:5[C]:ILE:HG13	2.35	0.56
2:B:82[A]:VAL:HG23	7:B:2024[A]:HOH:O	2.06	0.56
2:B:82[C]:VAL:HG23	7:B:2024[C]:HOH:O	2.06	0.56
2:B:42[A]:TRP:CE2	2:B:57[A]:ARG:HD2	2.43	0.54
2:B:42[C]:TRP:CE2	2:B:57[C]:ARG:HD2	2.43	0.54
1:A:84[C]:ILE:HD11	3:C:5[C]:ILE:HG13	1.88	0.54
2:B:84[A]:ILE:CD1	3:C:5[A]:ILE:HG13	2.41	0.50
1:A:80[A]:THR:CB	2:B:50[A]:ILE:HD11	2.42	0.50
1:A:80[C]:THR:CB	2:B:50[C]:ILE:HD11	2.42	0.50
2:B:50[C]:ILE:HG13	3:C:5[C]:ILE:CD1	2.43	0.48
2:B:57[A]:ARG:NH1	7:B:2073[A]:HOH:O	2.49	0.46
2:B:57[C]:ARG:NH1	7:B:2073[C]:HOH:O	2.49	0.46
1:A:18[A]:GLN:HA	7:A:2032[A]:HOH:O	2.16	0.45
2:B:36[A]:NLE:O	2:B:57[A]:ARG:NH2	2.50	0.45
1:A:18[C]:GLN:HA	7:A:2032[C]:HOH:O	2.16	0.45
2:B:36[C]:NLE:O	2:B:57[C]:ARG:NH2	2.50	0.45
1:A:61[A]:GLN:HG3	7:A:2080[A]:HOH:O	2.16	0.45
1:A:61[C]:GLN:HG3	7:A:2080[C]:HOH:O	2.16	0.45
5:A:1108[A]:GOL:H31	7:A:2124[A]:HOH:O	2.17	0.45
5:A:1108[C]:GOL:H31	7:A:2124[C]:HOH:O	2.17	0.45
7:B:2115[C]:HOH:O	3:C:1[C]:SER:HB2	2.17	0.44
2:B:14[A]:ARG:HA	2:B:18[A]:ASN:O	2.18	0.44
2:B:14[C]:ARG:HA	2:B:18[C]:ASN:O	2.18	0.44
1:A:50[A]:ILE:HG22	2:B:49[A]:GLY:HA3	2.01	0.42
2:B:84[A]:ILE:HD11	3:C:5[A]:ILE:HG13	2.01	0.42
1:A:50[C]:ILE:HG22	2:B:49[C]:GLY:HA3	2.01	0.42
7:B:2106[A]:HOH:O	3:C:6[A]:VME:HMC3	2.21	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	1-A	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
1	2-A	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
2	1-B	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
2	2-B	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
3	1-C	3/7 (43%)	3 (100%)	0	0	100	100
3	2-C	3/7 (43%)	3 (100%)	0	0	100	100
All	All	390/410 (95%)	382 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1-A	81/78 (104%)	81 (100%)	0	100	100
2	1-B	80/78 (103%)	79 (99%)	1 (1%)	76	41
3	1-C	4/4 (100%)	4 (100%)	0	100	100
All	All	165/160 (103%)	164 (99%)	1 (1%)	90	66

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1-B	19[A]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	98[A]	ASN
2	1-B	2[A]	GLN
2	1-B	18[A]	ASN
2	1-B	69[A]	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

26 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	NLE	1-A	36[A]	1	5,7,8	0.50	0	5,7,9	1.26	1 (20%)
1	SLZ	1-A	41[A]	1	6,8,9	0.53	0	4,8,10	2.35	1 (25%)
1	NLE	1-A	46[A]	1	5,7,8	1.16	1 (20%)	5,7,9	1.07	1 (20%)
1	ABA	1-A	67[A]	1	3,5,6	0.68	0	3,5,7	2.18	2 (66%)
1	ABA	1-A	67[B]	-	2,2,6	0.23	0	0,1,7	0.00	-
1	ABA	1-A	95[A]	1	3,5,6	0.45	0	3,5,7	0.98	0
2	NLE	1-B	36[A]	2	5,7,8	0.97	0	5,7,9	2.34	2 (40%)
2	SLZ	1-B	41[A]	2	6,8,9	0.56	0	4,8,10	2.46	2 (50%)
2	NLE	1-B	46[A]	2	5,7,8	0.66	0	5,7,9	1.42	1 (20%)
2	ABA	1-B	67[A]	2	3,5,6	1.20	0	3,5,7	1.96	1 (33%)
2	ABA	1-B	95[A]	2	3,5,6	0.51	0	3,5,7	0.66	0
3	JG3	1-C	4[A]	3	18,20,21	2.54	3 (16%)	18,26,28	4.41	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	VME	1-C	6[A]	-	7,8,8	2.05	2 (28%)	6,10,10	1.51	2 (33%)
1	NLE	2-A	36[C]	-	5,7,8	0.50	0	5,7,9	1.26	1 (20%)
1	SLZ	2-A	41[C]	-	6,8,9	0.53	0	4,8,10	2.35	1 (25%)
1	NLE	2-A	46[C]	-	5,7,8	1.16	1 (20%)	5,7,9	1.07	1 (20%)
1	ABA	2-A	67[C]	-	3,5,6	0.68	0	3,5,7	2.18	2 (66%)
1	ABA	2-A	67[D]	-	2,2,6	0.23	0	0,1,7	0.00	-
1	ABA	2-A	95[C]	-	3,5,6	0.45	0	3,5,7	0.98	0
2	NLE	2-B	36[C]	-	5,7,8	0.97	0	5,7,9	2.34	2 (40%)
2	SLZ	2-B	41[C]	-	6,8,9	0.56	0	4,8,10	2.46	2 (50%)
2	NLE	2-B	46[C]	-	5,7,8	0.66	0	5,7,9	1.42	1 (20%)
2	ABA	2-B	67[C]	-	3,5,6	1.20	0	3,5,7	1.96	1 (33%)
2	ABA	2-B	95[C]	-	3,5,6	0.51	0	3,5,7	0.66	0
3	JG3	2-C	4[C]	-	18,20,21	2.49	4 (22%)	18,26,28	5.89	9 (50%)
3	VME	2-C	6[C]	-	7,8,8	1.69	2 (28%)	6,10,10	0.72	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	NLE	1-A	36[A]	1	-	0/4/6/8	0/0/0/0
1	SLZ	1-A	41[A]	1	-	0/5/7/9	0/0/0/0
1	NLE	1-A	46[A]	1	-	0/4/6/8	0/0/0/0
1	ABA	1-A	67[A]	1	-	0/2/4/6	0/0/0/0
1	ABA	1-A	67[B]	-	-	0/0/0/6	0/0/0/0
1	ABA	1-A	95[A]	1	-	0/2/4/6	0/0/0/0
2	NLE	1-B	36[A]	2	-	0/4/6/8	0/0/0/0
2	SLZ	1-B	41[A]	2	-	0/5/7/9	0/0/0/0
2	NLE	1-B	46[A]	2	-	0/4/6/8	0/0/0/0
2	ABA	1-B	67[A]	2	-	0/2/4/6	0/0/0/0
2	ABA	1-B	95[A]	2	-	0/2/4/6	0/0/0/0
3	JG3	1-C	4[A]	3	1/1/4/5	0/12/24/26	0/2/2/2
3	VME	1-C	6[A]	-	-	0/10/10/10	0/0/0/0
1	NLE	2-A	36[C]	-	-	0/4/6/8	0/0/0/0
1	SLZ	2-A	41[C]	-	-	0/5/7/9	0/0/0/0
1	NLE	2-A	46[C]	-	-	0/4/6/8	0/0/0/0
1	ABA	2-A	67[C]	-	-	0/2/4/6	0/0/0/0
1	ABA	2-A	67[D]	-	-	0/0/0/6	0/0/0/0
1	ABA	2-A	95[C]	-	-	0/2/4/6	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NLE	2-B	36[C]	-	-	0/4/6/8	0/0/0/0
2	SLZ	2-B	41[C]	-	-	0/5/7/9	0/0/0/0
2	NLE	2-B	46[C]	-	-	0/4/6/8	0/0/0/0
2	ABA	2-B	67[C]	-	-	0/2/4/6	0/0/0/0
2	ABA	2-B	95[C]	-	-	0/2/4/6	0/0/0/0
3	JG3	2-C	4[C]	-	1/1/4/5	0/12/24/26	0/2/2/2
3	VME	2-C	6[C]	-	-	0/10/10/10	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-C	4[A]	JG3	O1-C1	-7.74	1.26	1.43
3	2-C	4[C]	JG3	O1-C1	-7.21	1.27	1.43
3	2-C	4[C]	JG3	C4-N2	-5.89	1.34	1.47
3	1-C	4[A]	JG3	C4-N2	-5.21	1.35	1.47
3	1-C	4[A]	JG3	C1-C8	-4.25	1.48	1.53
3	2-C	4[C]	JG3	C1-C8	-3.21	1.49	1.53
3	2-C	6[C]	VME	O2-C	-3.02	1.25	1.33
3	1-C	6[A]	VME	O2-C	-2.96	1.25	1.33
1	2-A	46[C]	NLE	CB-CA	-2.28	1.50	1.53
1	1-A	46[A]	NLE	CB-CA	-2.28	1.50	1.53
3	2-C	4[C]	JG3	C10-C8	-2.02	1.50	1.53
3	2-C	6[C]	VME	O2-CM	3.18	1.53	1.45
3	1-C	6[A]	VME	O2-CM	4.47	1.56	1.45

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2-C	4[C]	JG3	C11-CA-C	-5.84	104.13	112.80
1	1-A	41[A]	SLZ	CE-CD-SG	-4.15	101.09	113.88
1	2-A	41[C]	SLZ	CE-CD-SG	-4.15	101.09	113.88
2	2-B	36[C]	NLE	O-C-CA	-3.86	115.37	125.72
2	1-B	36[A]	NLE	O-C-CA	-3.86	115.37	125.72
3	1-C	4[A]	JG3	C11-CA-C	-3.48	107.64	112.80
3	2-C	4[C]	JG3	C13-C5-C12	-3.40	114.09	119.88
2	2-B	41[C]	SLZ	CA-CB-SG	-3.26	105.13	112.84
2	1-B	41[A]	SLZ	CA-CB-SG	-3.26	105.13	112.84
2	2-B	41[C]	SLZ	CE-CD-SG	-2.84	105.13	113.88
2	1-B	41[A]	SLZ	CE-CD-SG	-2.84	105.13	113.88
1	1-A	36[A]	NLE	O-C-CA	-2.78	118.26	125.72
1	2-A	36[C]	NLE	O-C-CA	-2.78	118.26	125.72
2	2-B	46[C]	NLE	O-C-CA	-2.69	118.52	125.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-B	46[A]	NLE	O-C-CA	-2.69	118.52	125.72
3	1-C	6[A]	VME	O2-C-O	-2.61	118.27	123.77
2	1-B	67[A]	ABA	CG-CB-CA	-2.34	107.25	113.48
2	2-B	67[C]	ABA	CG-CB-CA	-2.34	107.25	113.48
3	1-C	6[A]	VME	CM-O2-C	-2.21	110.71	115.97
1	2-A	46[C]	NLE	O-C-CA	-2.11	120.05	125.72
1	1-A	46[A]	NLE	O-C-CA	-2.11	120.05	125.72
3	1-C	4[A]	JG3	C5-C12-C6	-2.02	117.40	120.20
1	1-A	67[A]	ABA	CG-CB-CA	-2.01	108.12	113.48
1	2-A	67[C]	ABA	CG-CB-CA	-2.01	108.12	113.48
3	2-C	4[C]	JG3	C5-C13-C7	2.26	123.34	120.20
3	2-C	4[C]	JG3	C3-N2-C4	2.28	124.78	112.14
2	2-B	36[C]	NLE	CB-CA-N	3.11	119.30	110.54
2	1-B	36[A]	NLE	CB-CA-N	3.11	119.30	110.54
1	1-A	67[A]	ABA	CB-CA-N	3.20	119.54	110.54
1	2-A	67[C]	ABA	CB-CA-N	3.20	119.54	110.54
3	2-C	4[C]	JG3	C5-C12-C6	3.46	125.01	120.20
3	2-C	4[C]	JG3	O1-C1-C4	5.24	122.91	110.47
3	1-C	4[A]	JG3	O1-C1-C4	5.32	123.10	110.47
3	2-C	4[C]	JG3	C3-N2-CA	5.49	115.93	106.62
3	1-C	4[A]	JG3	C3-N2-CA	5.90	116.62	106.62
3	1-C	4[A]	JG3	O1-C1-C8	9.36	122.45	109.13
3	1-C	4[A]	JG3	C1-C4-N2	13.06	134.21	112.06
3	2-C	4[C]	JG3	O1-C1-C8	15.35	130.98	109.13
3	2-C	4[C]	JG3	C1-C4-N2	16.02	139.25	112.06

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	1-C	4[A]	JG3	C1
3	2-C	4[C]	JG3	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1-B	36[A]	NLE	1	0
3	1-C	4[A]	JG3	1	0
3	1-C	6[A]	VME	1	0
2	2-B	36[C]	NLE	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 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	SO4	1-A	1105[A]	-	4,4,4	0.65	0	6,6,6	0.60	0
4	SO4	1-A	1106[A]	-	4,4,4	0.88	0	6,6,6	0.45	0
5	GOL	1-A	1107[A]	-	5,5,5	0.93	0	5,5,5	1.89	2 (40%)
5	GOL	1-A	1108[A]	-	5,5,5	0.69	0	5,5,5	1.81	2 (40%)
4	SO4	1-B	1105[A]	-	4,4,4	1.20	0	6,6,6	1.29	1 (16%)
6	ACT	1-B	1106[A]	-	0,3,3	0.00	-	0,3,3	0.00	-
4	SO4	2-A	1105[C]	-	4,4,4	0.65	0	6,6,6	0.60	0
4	SO4	2-A	1106[C]	-	4,4,4	0.88	0	6,6,6	0.45	0
5	GOL	2-A	1107[C]	-	5,5,5	0.93	0	5,5,5	1.89	2 (40%)
5	GOL	2-A	1108[C]	-	5,5,5	0.69	0	5,5,5	1.81	2 (40%)
4	SO4	2-B	1105[C]	-	4,4,4	1.20	0	6,6,6	1.29	1 (16%)
6	ACT	2-B	1106[C]	-	0,3,3	0.00	-	0,3,3	0.00	-

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	SO4	1-A	1105[A]	-	-	0/0/0/0	0/0/0/0
4	SO4	1-A	1106[A]	-	-	0/0/0/0	0/0/0/0
5	GOL	1-A	1107[A]	-	-	0/4/4/4	0/0/0/0
5	GOL	1-A	1108[A]	-	-	0/4/4/4	0/0/0/0
4	SO4	1-B	1105[A]	-	-	0/0/0/0	0/0/0/0
6	ACT	1-B	1106[A]	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	2-A	1105[C]	-	-	0/0/0/0	0/0/0/0
4	SO4	2-A	1106[C]	-	-	0/0/0/0	0/0/0/0
5	GOL	2-A	1107[C]	-	-	0/4/4/4	0/0/0/0
5	GOL	2-A	1108[C]	-	-	0/4/4/4	0/0/0/0
4	SO4	2-B	1105[C]	-	-	0/0/0/0	0/0/0/0
6	ACT	2-B	1106[C]	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1-A	1107[A]	GOL	O2-C2-C3	2.28	119.43	108.47
5	2-A	1107[C]	GOL	O2-C2-C3	2.28	119.43	108.47
5	2-A	1108[C]	GOL	O2-C2-C1	2.58	120.84	108.47
5	1-A	1108[A]	GOL	O2-C2-C1	2.58	120.84	108.47
5	2-A	1108[C]	GOL	O2-C2-C3	2.59	120.89	108.47
5	1-A	1108[A]	GOL	O2-C2-C3	2.59	120.89	108.47
4	2-B	1105[C]	SO4	O2-S-O1	2.60	118.29	109.59
4	1-B	1105[A]	SO4	O2-S-O1	2.60	118.29	109.59
5	1-A	1107[A]	GOL	O2-C2-C1	2.72	121.55	108.47
5	2-A	1107[C]	GOL	O2-C2-C1	2.72	121.55	108.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1-A	1108[A]	GOL	1	0
5	2-A	1108[C]	GOL	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1-A	94/99 (94%)	-0.34	1 (1%) 82 75	6, 10, 21, 23	94 (100%)
1	2-A	94/99 (94%)	-0.34	1 (1%) 82 75	6, 10, 21, 23	94 (100%)
2	1-B	94/99 (94%)	-0.10	2 (2%) 67 57	6, 11, 31, 41	94 (100%)
2	2-B	94/99 (94%)	-0.10	2 (2%) 67 57	6, 11, 31, 41	94 (100%)
3	1-C	4/7 (57%)	0.24	0 100 100	8, 9, 12, 18	4 (100%)
3	2-C	4/7 (57%)	0.24	0 100 100	8, 9, 12, 18	4 (100%)
All	All	384/410 (93%)	-0.21	6 (1%) 71 65	6, 11, 26, 41	384 (100%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	1-B	35[A]	GLU	3.6
2	2-B	35[C]	GLU	3.6
2	1-B	18[A]	ASN	3.2
2	2-B	18[C]	ASN	3.2
1	1-A	37[A]	ASN	2.0
1	2-A	37[C]	ASN	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
1	NLE	2-A	46[C]	8/9	0.99	0.07	-	6,8,11,11	8

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	ABA	1-A	67[A]	6/7	0.97	0.08	-	10,13,16,19	6
2	ABA	1-B	67[A]	6/7	0.97	0.05	-	12,15,16,21	6
3	JG3	1-C	4[A]	19/20	0.97	0.07	-	5,6,9,9	19
3	VME	1-C	6[A]	9/9	0.96	0.10	-	6,11,15,16	9
1	NLE	1-A	36[A]	8/9	0.94	0.08	-	13,17,21,28	8
2	NLE	2-B	46[C]	8/9	0.98	0.04	-	8,11,14,17	8
1	ABA	1-A	67[B]	3/7	0.97	0.08	-	12,12,13,16	3
2	ABA	1-B	95[A]	6/7	0.99	0.04	-	8,8,10,10	6
1	SLZ	1-A	41[A]	9/10	0.95	0.16	-	16,18,82,82	9
1	ABA	2-A	95[C]	6/7	0.98	0.07	-	7,7,8,8	6
2	SLZ	2-B	41[C]	9/10	0.94	0.18	-	14,17,83,89	9
1	NLE	2-A	36[C]	8/9	0.94	0.08	-	13,17,21,28	8
3	VME	2-C	6[C]	9/9	0.96	0.10	-	7,10,15,18	9
2	NLE	1-B	46[A]	8/9	0.98	0.04	-	8,11,14,17	8
2	ABA	2-B	95[C]	6/7	0.99	0.04	-	8,8,10,10	6
1	NLE	1-A	46[A]	8/9	0.99	0.07	-	6,8,11,11	8
2	SLZ	1-B	41[A]	9/10	0.94	0.18	-	14,17,83,89	9
2	NLE	2-B	36[C]	8/9	0.85	0.20	-	13,16,17,21	8
1	ABA	1-A	95[A]	6/7	0.98	0.07	-	7,7,8,8	6
2	NLE	1-B	36[A]	8/9	0.85	0.20	-	13,16,17,21	8
1	ABA	2-A	67[D]	3/7	0.97	0.08	-	12,12,13,16	3
1	SLZ	2-A	41[C]	9/10	0.95	0.16	-	16,18,82,82	9
3	JG3	2-C	4[C]	19/20	0.97	0.07	-	7,8,10,11	19
1	ABA	2-A	67[C]	6/7	0.97	0.08	-	10,13,16,19	6
2	ABA	2-B	67[C]	6/7	0.97	0.05	-	12,15,16,21	6

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. 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
5	GOL	2-A	1108[C]	6/6	0.82	0.15	6.32	30,36,42,47	6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	1-A	1108[A]	6/6	0.82	0.15	6.32	30,36,42,47	6
4	SO4	2-B	1105[C]	5/5	0.97	0.14	4.76	21,26,37,40	5
4	SO4	1-B	1105[A]	5/5	0.97	0.14	4.76	21,26,37,40	5
5	GOL	1-A	1107[A]	6/6	0.93	0.13	4.63	16,19,21,22	6
5	GOL	2-A	1107[C]	6/6	0.93	0.13	4.63	16,19,21,22	6
6	ACT	1-B	1106[A]	4/4	0.59	0.18	4.48	33,33,37,42	4
6	ACT	2-B	1106[C]	4/4	0.59	0.18	4.48	33,33,37,42	4
4	SO4	1-A	1106[A]	5/5	0.97	0.15	0.85	19,21,24,24	5
4	SO4	2-A	1106[C]	5/5	0.97	0.15	0.85	19,21,24,24	5
4	SO4	2-A	1105[C]	5/5	0.94	0.18	-	29,31,41,42	5
4	SO4	1-A	1105[A]	5/5	0.94	0.18	-	29,31,41,42	5

6.5 Other polymers ⓘ

There are no such residues in this entry.