Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2021 – 06:09 PM EDT

PDB ID	:	7JR2
Title	:	Crystal structure of the R64M mutant of Bauhinia Bauhinioides Kallikrein Inhibitor complexed with Bovine Trypsin
Authors	:	Li, M.; Wlodawer, A.; Gustchina, A.
Deposited on	:	2020-08-11
Resolution	:	1.85 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

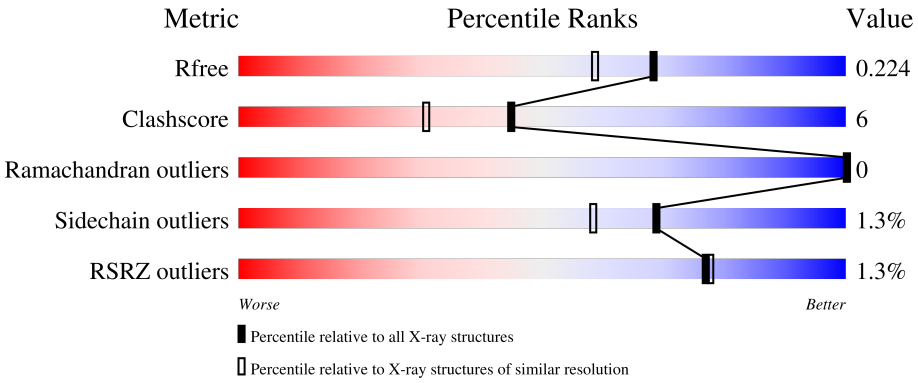
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 1.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	223	91% 9%
1	B	223	88% 12%
1	C	223	90% 10%
1	D	223	90% 10%
1	E	223	85% 15%

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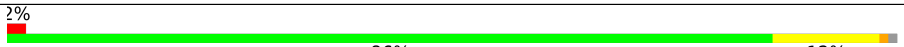
Mol	Chain	Length	Quality of chain
1	F	223	
2	G	164	
2	H	164	
2	I	164	
2	J	164	
2	K	164	
2	L	164	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18493 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 Cationic trypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	1	0
			1635	1016	280	325	14			
1	B	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	C	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	D	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	E	223	Total	C	N	O	S	0	2	0
			1641	1019	280	327	15			
1	F	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			

- Molecule 2 is a protein called Kunitz-type inihibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	163	Total	C	N	O	S	0	0	0
			1257	806	214	235	2			
2	H	163	Total	C	N	O	S	0	0	0
			1257	806	214	235	2			
2	I	163	Total	C	N	O	S	0	0	0
			1257	806	214	235	2			
2	J	163	Total	C	N	O	S	0	0	0
			1257	806	214	235	2			
2	K	163	Total	C	N	O	S	0	0	0
			1257	806	214	235	2			
2	L	163	Total	C	N	O	S	0	0	0
			1257	806	214	235	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	GLY	-	expression tag	UNP Q6VEQ7

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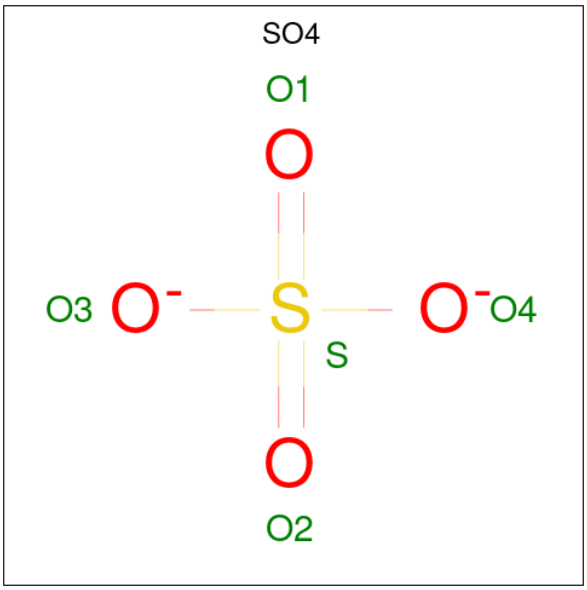
Chain	Residue	Modelled	Actual	Comment	Reference
G	64	MET	ARG	engineered mutation	UNP Q6VEQ7
H	0	GLY	-	expression tag	UNP Q6VEQ7
H	64	MET	ARG	engineered mutation	UNP Q6VEQ7
I	0	GLY	-	expression tag	UNP Q6VEQ7
I	64	MET	ARG	engineered mutation	UNP Q6VEQ7
J	0	GLY	-	expression tag	UNP Q6VEQ7
J	64	MET	ARG	engineered mutation	UNP Q6VEQ7
K	0	GLY	-	expression tag	UNP Q6VEQ7
K	64	MET	ARG	engineered mutation	UNP Q6VEQ7
L	0	GLY	-	expression tag	UNP Q6VEQ7
L	64	MET	ARG	engineered mutation	UNP Q6VEQ7

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	83	Total O 83 83	0	0
4	G	53	Total O 53 53	0	0
4	B	89	Total O 89 89	0	0

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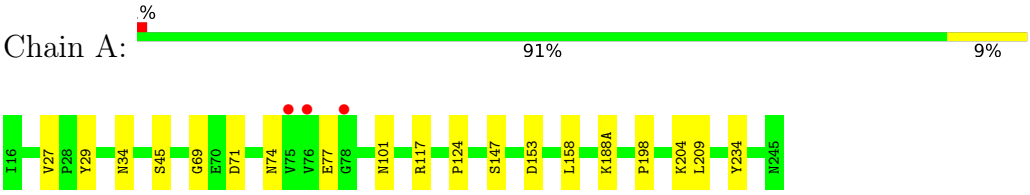
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	87	Total O 87 87	0	0
4	D	100	Total O 100 100	0	0
4	E	140	Total O 140 140	0	0
4	F	175	Total O 175 175	0	0
4	H	56	Total O 56 56	0	0
4	I	55	Total O 55 55	0	0
4	J	59	Total O 59 59	0	0
4	K	78	Total O 78 78	0	0
4	L	74	Total O 74 74	0	0

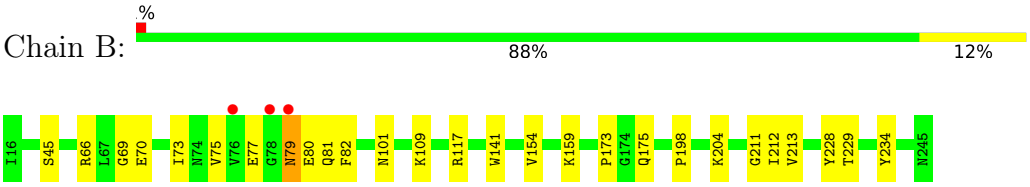
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

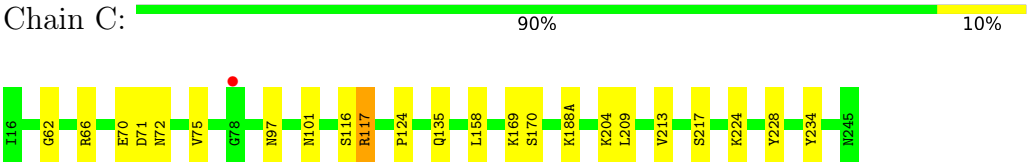
• Molecule 1: Cationic trypsin



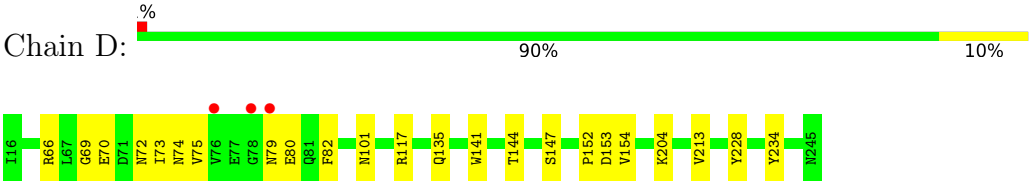
• Molecule 1: Cationic trypsin



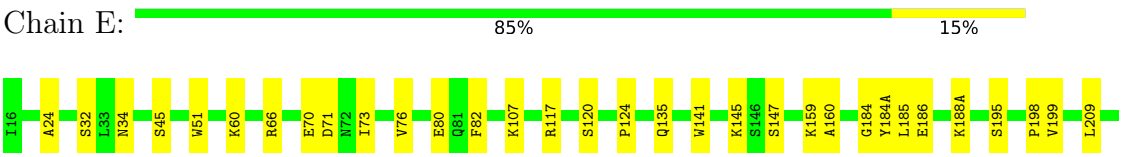
• Molecule 1: Cationic trypsin



• Molecule 1: Cationic trypsin

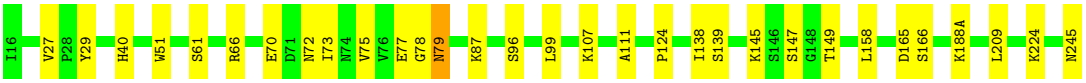


• Molecule 1: Cationic trypsin



• Molecule 1: Cationic trypsin

Chain F:

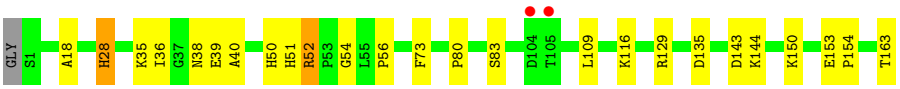


• Molecule 2: Kunitz-type inihibitor

Chain G:

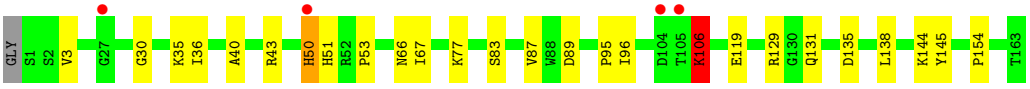
• Molecule 2: Kunitz-type inihibitor

Chain H:



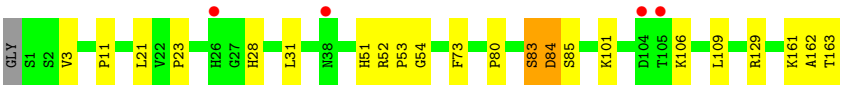
• Molecule 2: Kunitz-type inihibitor

Chain I:



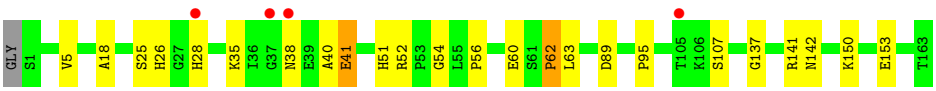
• Molecule 2: Kunitz-type inihibitor

Chain J:



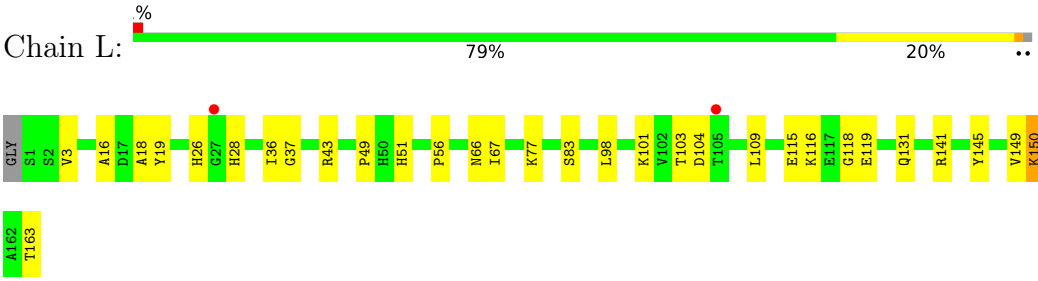
• Molecule 2: Kunitz-type inihibitor

Chain K:



• Molecule 2: Kunitz-type inihibitor

Chain L:


%
79%
20%
GLY S1 S2 V3 A16 D17 A18 Y19 H26 G27 H28 I36 G37 R43 P49 H50 H51 P56 N66 I67 K77 S83 L98 K101 V102 T103 D104 T105 L109 E115 K116 E117 G118 E119 Q131 R141 Y145 V149 K150 E153 K161
A162 T163

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	207.70Å 207.70Å 107.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.26 – 1.85 37.26 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.0 (37.26-1.85) 97.4 (37.26-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8	Depositor
R, R_{free}	0.165 , 0.221 0.169 , 0.224	Depositor DCC
R_{free} test set	2105 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 34.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.490 for k,h,-l	Depositor
Outliers	1 of 216994 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	18493	wwPDB-VP
Average B, all atoms (Å^2)	24.0	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 66.47 % 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 6.0151e-06. 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, 0.333 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: SO4

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	0.42	0/1669	0.59	0/2262
1	B	0.41	0/1660	0.60	0/2250
1	C	0.44	0/1660	0.59	0/2250
1	D	0.42	0/1660	0.62	1/2250 (0.0%)
1	E	0.43	0/1675	0.62	0/2270
1	F	0.44	0/1660	0.64	0/2250
2	G	0.43	0/1288	0.64	1/1750 (0.1%)
2	H	0.39	0/1288	0.66	2/1750 (0.1%)
2	I	0.41	0/1288	0.68	2/1750 (0.1%)
2	J	0.40	0/1288	0.63	0/1750
2	K	0.66	2/1288 (0.2%)	0.76	3/1750 (0.2%)
2	L	0.43	0/1288	0.64	0/1750
All	All	0.44	2/17712 (0.0%)	0.64	9/24032 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	62	PRO	N-CA	12.51	1.68	1.47
2	K	41	GLU	C-N	7.86	1.49	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	26	HIS	CB-CA-C	7.24	124.88	110.40
2	H	28	HIS	CB-CA-C	6.46	123.31	110.40
2	I	50	HIS	CB-CA-C	-6.21	97.99	110.40
2	K	41	GLU	CB-CA-C	-6.19	98.02	110.40
2	I	106	LYS	CB-CG-CD	-5.89	96.30	111.60
2	H	40	ALA	C-N-CA	5.77	136.12	121.70
2	K	38	ASN	CB-CA-C	-5.75	98.90	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	26	HIS	CB-CA-C	5.70	121.79	110.40
1	D	80	GLU	CB-CA-C	-5.16	100.08	110.40

There are no chirality outliers.

There are no planarity outliers.

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	1635	0	1596	11	0
1	B	1629	0	1588	20	0
1	C	1629	0	1588	19	0
1	D	1629	0	1588	13	0
1	E	1641	0	1597	23	0
1	F	1629	0	1588	24	0
2	G	1257	0	1261	11	1
2	H	1257	0	1261	24	0
2	I	1257	0	1261	21	1
2	J	1257	0	1261	22	0
2	K	1257	0	1261	23	0
2	L	1257	0	1261	25	1
3	A	10	0	0	0	0
3	B	10	0	0	1	0
3	C	15	0	0	0	0
3	D	15	0	0	1	0
3	E	15	0	0	0	0
3	F	15	0	0	1	0
3	G	5	0	0	0	0
3	I	5	0	0	1	0
3	J	5	0	0	0	0
3	K	5	0	0	1	0
3	L	10	0	0	1	0
4	A	83	0	0	2	1
4	B	89	0	0	1	0
4	C	87	0	0	6	0
4	D	100	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	140	0	0	9	0
4	F	175	0	0	11	2
4	G	53	0	0	1	1
4	H	56	0	0	5	0
4	I	55	0	0	2	0
4	J	59	0	0	4	1
4	K	78	0	0	3	1
4	L	74	0	0	4	0
All	All	18493	0	17111	224	6

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 6.

All (224) 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:K:62:PRO:N	2:K:62:PRO:CA	1.68	1.36
2:H:28:HIS:HB3	2:H:52:ARG:NH1	1.57	1.19
1:C:71:ASP:HB2	1:C:117:ARG:HH22	1.17	1.08
2:H:28:HIS:HB3	2:H:52:ARG:HH12	1.22	1.03
1:C:117:ARG:HH11	1:C:117:ARG:HB3	1.26	0.99
1:C:71:ASP:HB2	1:C:117:ARG:NH2	1.76	0.99
2:K:28:HIS:O	2:K:52:ARG:NE	1.97	0.96
2:J:28:HIS:HB3	2:J:52:ARG:NH1	1.83	0.93
2:J:28:HIS:HB3	2:J:52:ARG:HH11	1.31	0.91
1:C:117:ARG:HB3	1:C:117:ARG:NH1	1.88	0.86
2:H:28:HIS:CB	2:H:52:ARG:NH1	2.41	0.81
2:I:87:VAL:HG21	2:I:106:LYS:HB2	1.67	0.76
2:H:28:HIS:HA	2:H:52:ARG:HH11	1.50	0.75
4:A:407:HOH:O	2:G:66:ASN:HB2	1.85	0.74
1:A:69:GLY:O	1:A:117:ARG:NH1	2.20	0.74
1:F:87:LYS:NZ	1:F:245:ASN:O	2.21	0.74
1:B:79:ASN:O	1:B:79:ASN:ND2	2.22	0.73
2:G:92:GLN:NE2	4:G:301:HOH:O	2.21	0.72
1:B:204:LYS:HE2	1:C:204:LYS:HE2	1.73	0.71
1:F:138:ILE:HB	4:F:559:HOH:O	1.92	0.70
1:F:79:ASN:N	1:F:79:ASN:OD1	2.21	0.69
1:F:158:LEU:HB3	4:F:559:HOH:O	1.93	0.68
2:H:51:HIS:ND1	2:H:54:GLY:HA2	2.09	0.68
1:E:186[A]:GLU:OE1	4:E:401:HOH:O	2.12	0.68
1:C:117:ARG:HH11	1:C:117:ARG:CB	2.04	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:150:LYS:HG2	2:L:153:GLU:HB2	1.77	0.66
1:E:185:LEU:HD22	1:E:223:ASN:HA	1.78	0.66
1:E:71:ASP:OD2	4:E:404:HOH:O	2.15	0.65
2:H:150:LYS:NZ	2:H:153:GLU:OE1	2.30	0.65
1:E:73:ILE:HG21	4:E:423:HOH:O	1.96	0.65
2:H:28:HIS:C	2:H:52:ARG:HD2	2.17	0.65
1:E:24:ALA:O	4:E:402:HOH:O	2.14	0.64
2:J:51:HIS:ND1	2:J:54:GLY:HA2	2.12	0.64
2:K:25:SER:O	2:K:25:SER:OG	2.12	0.64
2:K:89:ASP:OD2	4:K:302:HOH:O	2.15	0.64
4:C:424:HOH:O	2:I:66:ASN:HB2	1.98	0.63
2:K:150:LYS:HG2	2:K:153:GLU:HB2	1.80	0.63
2:I:53:PRO:HD2	2:J:53:PRO:HD2	1.81	0.62
2:K:62:PRO:N	2:K:62:PRO:C	2.52	0.61
1:D:69:GLY:O	1:D:117:ARG:NH1	2.34	0.61
2:J:162:ALA:O	2:J:163:THR:HG22	2.01	0.60
2:K:5:VAL:HG22	4:K:341:HOH:O	2.01	0.60
1:F:99:LEU:HD11	2:L:109:LEU:HD11	1.85	0.59
1:B:77:GLU:HG2	1:B:80:GLU:HG3	1.85	0.59
2:G:26:HIS:CE1	2:G:138:LEU:CD1	2.86	0.58
2:K:51:HIS:ND1	2:K:54:GLY:HA2	2.17	0.58
1:B:77:GLU:O	1:B:77:GLU:HG3	2.03	0.58
1:A:74:ASN:ND2	1:A:153:ASP:OD1	2.36	0.58
1:F:96:SER:HB2	4:L:306:HOH:O	2.01	0.58
2:I:77:LYS:HE3	2:I:83:SER:O	2.04	0.58
2:L:141:ARG:NH2	4:L:303:HOH:O	2.24	0.58
2:K:28:HIS:HA	2:K:52:ARG:HD3	1.87	0.57
1:D:74:ASN:ND2	1:D:153:ASP:OD1	2.33	0.57
1:F:66:ARG:NE	1:F:70:GLU:OE1	2.38	0.57
1:A:34:ASN:HB3	4:A:449:HOH:O	2.05	0.57
2:G:28:HIS:O	2:G:49:PRO:HA	2.05	0.57
1:E:120:SER:HB3	4:E:517:HOH:O	2.04	0.57
2:H:28:HIS:CA	2:H:52:ARG:HH11	2.17	0.56
1:E:73:ILE:HG23	1:E:141:TRP:CE2	2.41	0.56
2:J:129:ARG:NH1	4:J:303:HOH:O	2.35	0.56
2:L:28:HIS:O	2:L:49:PRO:HA	2.06	0.56
2:L:119:GLU:OE1	2:L:119:GLU:N	2.38	0.56
1:A:158:LEU:HD11	1:A:188(A):LYS:HB3	1.88	0.56
2:L:77:LYS:HE3	2:L:83:SER:O	2.06	0.56
2:K:141:ARG:NH1	2:K:142:ASN:HD21	2.04	0.56
2:G:135:ASP:HB3	2:G:154:PRO:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:21:LEU:HD12	2:J:31:LEU:HD11	1.88	0.55
2:I:89:ASP:HB3	4:I:343:HOH:O	2.06	0.55
2:L:103:THR:HG22	2:L:104:ASP:N	2.20	0.55
2:J:80:PRO:HD2	2:J:83:SER:HB3	1.88	0.55
1:E:135:GLN:HB3	1:E:159:LYS:HE2	1.88	0.55
2:L:115:GLU:HG2	4:L:305:HOH:O	2.06	0.55
2:K:18:ALA:HB1	2:K:56:PRO:HB2	1.89	0.55
1:A:71:ASP:HB2	1:A:117:ARG:HH21	1.70	0.55
1:F:145:LYS:HE2	1:F:147:SER:O	2.07	0.55
2:L:103:THR:HG22	2:L:104:ASP:H	1.71	0.55
1:F:73:ILE:HD11	4:F:413:HOH:O	2.08	0.54
2:J:84:ASP:C	2:J:84:ASP:OD1	2.45	0.54
2:H:28:HIS:O	2:H:52:ARG:HD2	2.08	0.54
1:E:135:GLN:NE2	1:E:159:LYS:HG2	2.22	0.54
2:H:116:LYS:NZ	4:H:201:HOH:O	2.08	0.54
2:I:36:ILE:HD11	2:I:95:PRO:HD2	1.90	0.53
2:K:28:HIS:HB3	2:K:52:ARG:CZ	2.39	0.53
2:G:119:GLU:OE2	2:G:119:GLU:N	2.39	0.52
1:D:147:SER:OG	4:D:401:HOH:O	2.19	0.52
1:F:158:LEU:HD11	1:F:188(A):LYS:HB3	1.91	0.52
1:C:62:GLY:O	4:C:401:HOH:O	2.18	0.52
1:B:73:ILE:HG23	1:B:141:TRP:CE2	2.45	0.51
2:I:50:HIS:CD2	2:J:52:ARG:NH2	2.78	0.51
1:C:217:SER:HB3	1:C:224:LYS:HD2	1.90	0.51
2:K:150:LYS:HE3	2:K:153:GLU:OE2	2.09	0.51
2:J:54:GLY:O	4:J:301:HOH:O	2.19	0.51
1:C:117:ARG:NH1	4:C:407:HOH:O	2.43	0.51
2:H:39:GLU:HG2	4:H:218:HOH:O	2.11	0.51
1:E:184(A):TYR:HB3	1:E:186[A]:GLU:HG2	1.94	0.50
2:K:28:HIS:O	2:K:52:ARG:CZ	2.57	0.50
1:E:32:SER:O	4:E:405:HOH:O	2.19	0.50
2:G:26:HIS:CE1	2:G:138:LEU:HD13	2.46	0.50
1:E:45:SER:OG	1:E:198:PRO:HB3	2.12	0.50
1:E:117:ARG:HD3	4:E:420:HOH:O	2.10	0.50
2:H:36:ILE:O	2:H:39:GLU:HG3	2.12	0.50
1:D:73:ILE:HG23	1:D:141:TRP:CE2	2.46	0.50
2:L:43:ARG:NH1	3:L:202:SO4:O1	2.32	0.50
1:B:70:GLU:HG2	1:B:73:ILE:HA	1.93	0.50
1:C:116:SER:HA	4:C:405:HOH:O	2.12	0.49
2:G:77:LYS:HE3	2:G:83:SER:O	2.12	0.49
4:F:420:HOH:O	2:L:66:ASN:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:144:LYS:NZ	4:H:205:HOH:O	2.45	0.49
2:L:116:LYS:NZ	2:L:118:GLY:O	2.45	0.49
2:G:138:LEU:HB3	2:G:145:TYR:HB3	1.95	0.49
2:I:119:GLU:OE2	2:I:119:GLU:N	2.32	0.49
2:J:28:HIS:CB	2:J:52:ARG:HH11	2.14	0.49
4:I:301:HOH:O	2:J:52:ARG:NE	2.30	0.48
2:L:18:ALA:HB1	2:L:56:PRO:HB2	1.93	0.48
1:D:135:GLN:HG2	4:D:450:HOH:O	2.12	0.47
1:F:111:ALA:HB2	4:F:475:HOH:O	2.14	0.47
2:K:52:ARG:HD2	2:L:51:HIS:CE1	2.48	0.47
1:E:76:VAL:HG13	4:E:479:HOH:O	2.12	0.47
2:K:40:ALA:N	3:K:201:SO4:O4	2.45	0.47
2:H:18:ALA:HB1	2:H:56:PRO:HB2	1.96	0.47
2:I:135:ASP:HB3	2:I:154:PRO:HB3	1.96	0.47
2:J:28:HIS:C	2:J:52:ARG:HD3	2.35	0.47
1:B:173:PRO:O	1:B:175:GLN:NE2	2.48	0.47
1:F:224:LYS:HG2	4:F:457:HOH:O	2.13	0.47
1:F:27:VAL:HG13	1:F:29:TYR:CZ	2.50	0.47
1:A:101:ASN:HA	1:A:234:TYR:OH	2.14	0.47
2:I:51:HIS:CD2	2:J:52:ARG:NH2	2.83	0.46
2:I:35:LYS:NZ	2:I:40:ALA:O	2.19	0.46
2:I:138:LEU:HB3	2:I:145:TYR:HB3	1.98	0.46
2:J:84:ASP:OD1	2:J:85:SER:N	2.48	0.46
1:D:154:VAL:HG22	3:D:303:SO4:O4	2.16	0.46
1:C:97:ASN:HB3	2:I:129:ARG:HB3	1.97	0.46
2:G:18:ALA:HB1	2:G:56:PRO:HB2	1.97	0.46
2:H:150:LYS:HG2	2:H:153:GLU:HB2	1.98	0.46
1:D:144:THR:HG23	1:D:152:PRO:HD3	1.97	0.45
1:D:70:GLU:HG2	1:D:73:ILE:HA	1.97	0.45
2:L:36:ILE:HD12	2:L:37:GLY:H	1.81	0.45
1:C:97:ASN:O	2:I:129:ARG:NE	2.48	0.45
1:B:70:GLU:OE2	1:B:73:ILE:HG22	2.16	0.45
1:D:72:ASN:HB3	1:D:75:VAL:HG22	1.98	0.45
1:F:51:TRP:CZ2	1:F:107:LYS:HD2	2.52	0.45
2:H:80:PRO:HD2	2:H:83:SER:HB2	1.97	0.45
2:K:28:HIS:C	2:K:52:ARG:HE	2.09	0.45
1:B:213:VAL:HA	1:B:228:TYR:CD1	2.51	0.45
1:E:51:TRP:CH2	1:E:107:LYS:HB2	2.52	0.45
1:E:70:GLU:HG2	1:E:80:GLU:CD	2.36	0.45
1:E:160:ALA:HB1	1:E:184:GLY:HA2	1.98	0.45
1:B:45:SER:OG	1:B:198:PRO:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:28:HIS:CA	2:H:52:ARG:NH1	2.79	0.45
1:C:158:LEU:HD11	1:C:188(A):LYS:HB3	1.99	0.44
1:F:72:ASN:O	1:F:75:VAL:HG22	2.17	0.44
1:F:73:ILE:O	1:F:73:ILE:HG13	2.17	0.44
2:J:3:VAL:HG11	2:J:11:PRO:HB3	1.99	0.44
2:K:62:PRO:N	2:K:63:LEU:N	2.65	0.44
2:I:50:HIS:HD2	2:J:52:ARG:NH2	2.15	0.44
1:B:79:ASN:HD22	1:B:79:ASN:C	2.20	0.44
1:C:66:ARG:NH2	1:C:70:GLU:OE2	2.51	0.44
1:C:124:PRO:HD3	1:C:209:LEU:O	2.18	0.44
1:C:135:GLN:NE2	4:C:413:HOH:O	2.51	0.44
1:D:213:VAL:HA	1:D:228:TYR:CD1	2.53	0.44
2:H:163:THR:N	4:H:206:HOH:O	2.48	0.44
2:K:35:LYS:HE2	2:K:40:ALA:O	2.18	0.44
1:D:101:ASN:HA	1:D:234:TYR:OH	2.17	0.44
1:F:139:SER:HB3	4:F:406:HOH:O	2.17	0.44
2:L:101:LYS:HE2	2:L:101:LYS:HB3	1.85	0.44
2:L:161:LYS:HG2	2:L:163:THR:H	1.83	0.44
1:F:149:THR:HG21	2:L:16:ALA:CB	2.48	0.43
1:E:188(A):LYS:NZ	4:E:403:HOH:O	2.14	0.43
1:F:70:GLU:HB3	4:F:555:HOH:O	2.17	0.43
2:H:28:HIS:CB	2:H:52:ARG:HH11	2.23	0.43
2:K:95:PRO:HG3	2:K:141:ARG:CZ	2.49	0.43
2:L:36:ILE:HD12	2:L:37:GLY:N	2.33	0.43
2:I:3:VAL:HG22	2:I:67:ILE:HD12	2.01	0.43
2:J:161:LYS:NZ	4:J:305:HOH:O	2.51	0.43
2:J:101:LYS:HE2	2:J:101:LYS:HB3	1.85	0.43
2:L:19:TYR:CD2	2:L:161:LYS:HA	2.54	0.43
1:B:154:VAL:HG22	3:B:302:SO4:O3	2.19	0.43
1:B:212:ILE:HB	1:B:229:THR:HB	2.01	0.43
1:C:72:ASN:O	1:C:75:VAL:HG12	2.19	0.43
2:H:73:PHE:HB2	2:H:109:LEU:HD22	2.00	0.43
2:H:135:ASP:HB3	2:H:154:PRO:HB3	2.00	0.43
1:E:124:PRO:HD3	1:E:209:LEU:O	2.19	0.42
2:L:26:HIS:CD2	2:L:145:TYR:CZ	3.07	0.42
1:A:204:LYS:HE2	1:D:204:LYS:HE2	2.01	0.42
1:B:159:LYS:HG3	4:C:405:HOH:O	2.18	0.42
2:I:43:ARG:NH1	3:I:201:SO4:O2	2.42	0.42
2:K:28:HIS:C	2:K:52:ARG:NE	2.68	0.42
2:J:106:LYS:NZ	4:J:307:HOH:O	2.52	0.42
2:J:73:PHE:HB2	2:J:109:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:161:LYS:NZ	4:L:309:HOH:O	2.46	0.42
1:D:66:ARG:HD3	1:D:82:PHE:CE1	2.55	0.42
2:H:35:LYS:HB2	2:H:35:LYS:HE3	1.77	0.42
1:E:66:ARG:HD3	1:E:82:PHE:CE1	2.54	0.42
2:I:36:ILE:CD1	2:I:95:PRO:HD2	2.49	0.42
2:I:144:LYS:HE2	2:I:144:LYS:HB3	1.83	0.42
1:C:213:VAL:HA	1:C:228:TYR:CD1	2.55	0.42
1:F:166:SER:HA	4:F:573:HOH:O	2.19	0.42
1:B:69:GLY:O	1:B:117:ARG:NH1	2.53	0.42
1:E:199:VAL:HG21	1:E:228:TYR:CD1	2.55	0.42
2:K:137:GLY:HA3	2:K:150:LYS:HB3	2.02	0.42
1:C:101:ASN:HA	1:C:234:TYR:OH	2.19	0.41
1:F:149:THR:HG21	2:L:16:ALA:HB1	2.02	0.41
2:L:3:VAL:HG22	2:L:67:ILE:HD13	2.03	0.41
2:G:52:ARG:HG2	2:H:50:HIS:O	2.20	0.41
1:B:66:ARG:HD3	1:B:82:PHE:CE1	2.56	0.41
1:B:101:ASN:HA	1:B:234:TYR:OH	2.21	0.41
1:A:124:PRO:HD3	1:A:209:LEU:O	2.20	0.41
2:L:98:LEU:HB2	2:L:149:VAL:HB	2.03	0.41
1:A:27:VAL:HG13	1:A:29:TYR:CZ	2.56	0.41
1:A:71:ASP:CB	1:A:117:ARG:HH21	2.34	0.41
1:E:145:LYS:HE2	1:E:147:SER:O	2.21	0.41
1:E:184(A):TYR:HB3	1:E:186[A]:GLU:CD	2.41	0.41
1:B:81:GLN:OE1	4:B:401:HOH:O	2.21	0.40
1:F:124:PRO:HD3	1:F:209:LEU:O	2.21	0.40
3:F:302:SO4:O2	4:F:401:HOH:O	2.19	0.40
2:H:129:ARG:NH1	4:H:207:HOH:O	2.50	0.40
1:A:45:SER:OG	1:A:198:PRO:HB3	2.21	0.40
1:F:40:HIS:CG	4:F:428:HOH:O	2.74	0.40
1:F:77:GLU:HG2	1:F:78:GLY:N	2.36	0.40
2:I:36:ILE:CD1	2:I:96:ILE:HG12	2.51	0.40
1:B:211:GLY:HA2	1:B:229:THR:O	2.21	0.40
2:I:30:GLY:HA3	2:I:51:HIS:O	2.20	0.40
2:K:60:GLU:HG3	4:K:310:HOH:O	2.20	0.40
1:B:73:ILE:HG23	1:B:141:TRP:NE1	2.37	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:96:ILE:O	2:I:131:GLN:NE2[4_655]	2.06	0.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:416:HOH:O	4:K:332:HOH:O[6_554]	2.09	0.11
4:A:477:HOH:O	4:J:347:HOH:O[3_664]	2.12	0.08
4:G:351:HOH:O	4:D:451:HOH:O[3_664]	2.13	0.07
2:G:96:ILE:O	2:L:131:GLN:NE2[4_665]	2.17	0.03
4:F:475:HOH:O	4:F:489:HOH:O[6_554]	2.19	0.01

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	222/223 (100%)	216 (97%)	6 (3%)	0	100	100
1	B	221/223 (99%)	217 (98%)	4 (2%)	0	100	100
1	C	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	D	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
1	E	223/223 (100%)	220 (99%)	3 (1%)	0	100	100
1	F	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
2	G	161/164 (98%)	157 (98%)	4 (2%)	0	100	100
2	H	161/164 (98%)	159 (99%)	2 (1%)	0	100	100
2	I	161/164 (98%)	157 (98%)	4 (2%)	0	100	100
2	J	161/164 (98%)	156 (97%)	5 (3%)	0	100	100
2	K	161/164 (98%)	156 (97%)	5 (3%)	0	100	100
2	L	161/164 (98%)	156 (97%)	5 (3%)	0	100	100
All	All	2295/2322 (99%)	2241 (98%)	54 (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	A	185/184 (100%)	183 (99%)	2 (1%)	73	65
1	B	184/184 (100%)	181 (98%)	3 (2%)	62	49
1	C	184/184 (100%)	181 (98%)	3 (2%)	62	49
1	D	184/184 (100%)	183 (100%)	1 (0%)	88	86
1	E	186/184 (101%)	183 (98%)	3 (2%)	62	49
1	F	184/184 (100%)	181 (98%)	3 (2%)	62	49
2	G	137/137 (100%)	137 (100%)	0	100	100
2	H	137/137 (100%)	134 (98%)	3 (2%)	52	36
2	I	137/137 (100%)	136 (99%)	1 (1%)	84	79
2	J	137/137 (100%)	134 (98%)	3 (2%)	52	36
2	K	137/137 (100%)	135 (98%)	2 (2%)	65	53
2	L	137/137 (100%)	136 (99%)	1 (1%)	84	79
All	All	1929/1926 (100%)	1904 (99%)	25 (1%)	69	58

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLU
1	A	147	SER
1	B	75	VAL
1	B	79	ASN
1	B	109	LYS
1	C	117	ARG
1	C	169	LYS
1	C	170	SER
1	D	79	ASN
1	E	34	ASN
1	E	60	LYS
1	E	195	SER
1	F	61	SER
1	F	79	ASN

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Mol	Chain	Res	Type
1	F	165	ASP
2	H	38	ASN
2	H	52	ARG
2	H	143	ASP
2	I	106	LYS
2	J	23	PRO
2	J	83	SER
2	J	84	ASP
2	K	41	GLU
2	K	107	SER
2	L	150	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	26	HIS
1	B	79	ASN
1	C	74	ASN
2	H	38	ASN
2	I	50	HIS
2	I	51	HIS
2	J	26	HIS
2	J	38	ASN
2	K	142	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

22 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	$\#\|Z\| > 2$
3	SO4	F	302	-	4,4,4	0.16	0	6,6,6	0.53	0
3	SO4	D	303	-	4,4,4	0.17	0	6,6,6	0.20	0
3	SO4	E	302	-	4,4,4	0.21	0	6,6,6	0.31	0
3	SO4	B	301	-	4,4,4	0.16	0	6,6,6	0.31	0
3	SO4	D	302	-	4,4,4	0.17	0	6,6,6	0.18	0
3	SO4	E	303	-	4,4,4	0.13	0	6,6,6	0.44	0
3	SO4	A	301	-	4,4,4	0.19	0	6,6,6	0.31	0
3	SO4	F	301	-	4,4,4	0.19	0	6,6,6	0.44	0
3	SO4	C	301	-	4,4,4	0.16	0	6,6,6	0.31	0
3	SO4	K	201	-	4,4,4	0.17	0	6,6,6	0.16	0
3	SO4	B	302	-	4,4,4	0.16	0	6,6,6	0.32	0
3	SO4	C	302	-	4,4,4	0.24	0	6,6,6	0.46	0
3	SO4	C	303	-	4,4,4	0.12	0	6,6,6	0.24	0
3	SO4	A	302	-	4,4,4	0.25	0	6,6,6	0.46	0
3	SO4	E	301	-	4,4,4	0.17	0	6,6,6	0.18	0
3	SO4	L	201	-	4,4,4	0.16	0	6,6,6	0.30	0
3	SO4	F	303	-	4,4,4	0.32	0	6,6,6	0.10	0
3	SO4	L	202	-	4,4,4	0.15	0	6,6,6	0.20	0
3	SO4	I	201	-	4,4,4	0.12	0	6,6,6	0.12	0
3	SO4	G	201	-	4,4,4	0.14	0	6,6,6	0.20	0
3	SO4	D	301	-	4,4,4	0.15	0	6,6,6	0.40	0
3	SO4	J	201	-	4,4,4	0.12	0	6,6,6	0.05	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	302	SO4	1	0
3	D	303	SO4	1	0
3	K	201	SO4	1	0
3	B	302	SO4	1	0
3	L	202	SO4	1	0
3	I	201	SO4	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	223/223 (100%)	-0.64	3 (1%)	77	78	11, 21, 35, 66	0
1	B	223/223 (100%)	-0.63	3 (1%)	77	78	12, 23, 39, 72	0
1	C	223/223 (100%)	-0.64	1 (0%)	92	92	14, 22, 37, 62	0
1	D	223/223 (100%)	-0.64	3 (1%)	77	78	12, 22, 36, 66	0
1	E	223/223 (100%)	-0.62	0	100	100	9, 18, 30, 54	0
1	F	223/223 (100%)	-0.62	0	100	100	9, 19, 31, 53	0
2	G	163/164 (99%)	-0.46	4 (2%)	57	56	13, 24, 52, 80	0
2	H	163/164 (99%)	-0.41	2 (1%)	79	79	14, 26, 53, 72	0
2	I	163/164 (99%)	-0.43	4 (2%)	57	56	14, 25, 56, 78	0
2	J	163/164 (99%)	-0.46	4 (2%)	57	56	13, 24, 51, 68	0
2	K	163/164 (99%)	-0.43	4 (2%)	57	56	10, 24, 52, 68	0
2	L	163/164 (99%)	-0.48	2 (1%)	79	79	10, 23, 44, 68	0
All	All	2316/2322 (99%)	-0.55	30 (1%)	77	78	9, 22, 46, 80	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	27	GLY	7.5
2	G	105	THR	5.6
2	I	105	THR	5.5
1	D	78	GLY	4.7
2	I	27	GLY	4.7
2	J	105	THR	4.4
2	K	105	THR	4.2
1	C	78	GLY	4.1
2	H	105	THR	4.0
1	B	76	VAL	3.9
1	D	79	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
2	J	26	HIS	3.5
1	D	76	VAL	3.5
2	L	27	GLY	3.3
2	L	105	THR	3.0
1	B	78	GLY	2.8
2	K	38	ASN	2.7
2	I	50	HIS	2.7
1	A	78	GLY	2.6
2	J	104	ASP	2.6
1	B	79	ASN	2.5
2	I	104	ASP	2.5
2	K	28	HIS	2.4
2	H	104	ASP	2.4
2	G	26	HIS	2.3
2	G	25	SER	2.2
2	J	38	ASN	2.2
1	A	76	VAL	2.2
2	K	37	GLY	2.1
1	A	75	VAL	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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	301	5/5	0.95	0.09	41,41,45,45	5
3	SO4	F	302	5/5	0.95	0.17	36,40,46,49	5
3	SO4	E	303	5/5	0.96	0.17	39,40,40,43	5
3	SO4	G	201	5/5	0.96	0.07	57,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	K	201	5/5	0.96	0.11	47,48,50,52	5
3	SO4	C	303	5/5	0.97	0.16	39,39,44,48	0
3	SO4	A	301	5/5	0.97	0.10	25,32,36,42	5
3	SO4	D	302	5/5	0.98	0.07	27,35,37,43	5
3	SO4	B	302	5/5	0.98	0.11	41,46,47,53	0
3	SO4	C	302	5/5	0.98	0.13	23,24,30,30	5
3	SO4	F	303	5/5	0.98	0.09	31,31,34,34	0
3	SO4	J	201	5/5	0.98	0.13	47,47,49,51	5
3	SO4	A	302	5/5	0.98	0.11	32,33,41,41	0
3	SO4	F	301	5/5	0.99	0.09	21,24,28,34	0
3	SO4	C	301	5/5	0.99	0.08	20,25,26,32	5
3	SO4	D	303	5/5	0.99	0.10	39,40,41,46	0
3	SO4	I	201	5/5	0.99	0.05	47,48,49,51	0
3	SO4	E	302	5/5	0.99	0.08	28,29,33,33	0
3	SO4	D	301	5/5	0.99	0.14	20,22,27,28	5
3	SO4	L	201	5/5	0.99	0.07	24,27,29,35	5
3	SO4	L	202	5/5	0.99	0.03	45,45,48,50	0
3	SO4	E	301	5/5	1.00	0.06	22,23,28,33	5

6.5 Other polymers (i)

There are no such residues in this entry.