Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2016 – 11:00 PM EDT

PDB ID	:	5HL1
Title	:	Crystal structure of glutaminase C in complex with inhibitor CB-839
Authors	:	Huang, Q.; Cerione, R.A.
Deposited on	:	2016-01-14
Resolution	:	2.40 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

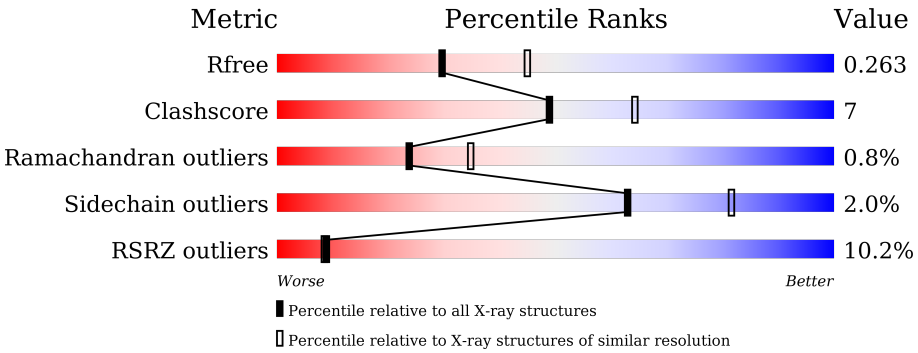
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	539	7% 62% 12% · 25%
1	B	539	9% 65% 10% · 24%
1	C	539	8% 66% 8% · 25%
1	D	539	7% 64% 9% · 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13120 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 Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	1	0	0
			3148	2003	533	584	28			
1	B	410	Total	C	N	O	S	1	0	0
			3197	2037	540	592	28			
1	C	404	Total	C	N	O	S	1	0	0
			3145	2002	533	582	28			
1	D	402	Total	C	N	O	S	1	0	0
			3128	1988	530	582	28			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	initiating methionine	UNP O94925
A	61	ARG	-	expression tag	UNP O94925
A	62	GLY	-	expression tag	UNP O94925
A	63	SER	-	expression tag	UNP O94925
A	64	HIS	-	expression tag	UNP O94925
A	65	HIS	-	expression tag	UNP O94925
A	66	HIS	-	expression tag	UNP O94925
A	67	HIS	-	expression tag	UNP O94925
A	68	HIS	-	expression tag	UNP O94925
A	69	HIS	-	expression tag	UNP O94925
A	70	GLY	-	expression tag	UNP O94925
A	71	SER	-	expression tag	UNP O94925
B	60	MET	-	initiating methionine	UNP O94925
B	61	ARG	-	expression tag	UNP O94925
B	62	GLY	-	expression tag	UNP O94925
B	63	SER	-	expression tag	UNP O94925
B	64	HIS	-	expression tag	UNP O94925
B	65	HIS	-	expression tag	UNP O94925
B	66	HIS	-	expression tag	UNP O94925
B	67	HIS	-	expression tag	UNP O94925
B	68	HIS	-	expression tag	UNP O94925

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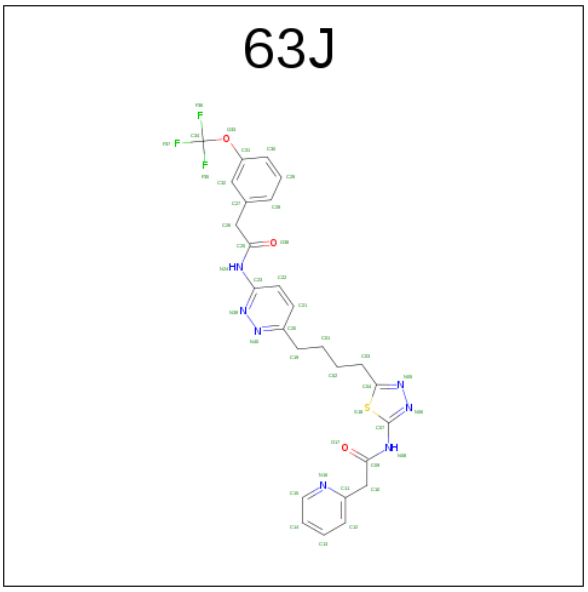
Chain	Residue	Modelled	Actual	Comment	Reference
B	69	HIS	-	expression tag	UNP O94925
B	70	GLY	-	expression tag	UNP O94925
B	71	SER	-	expression tag	UNP O94925
C	60	MET	-	initiating methionine	UNP O94925
C	61	ARG	-	expression tag	UNP O94925
C	62	GLY	-	expression tag	UNP O94925
C	63	SER	-	expression tag	UNP O94925
C	64	HIS	-	expression tag	UNP O94925
C	65	HIS	-	expression tag	UNP O94925
C	66	HIS	-	expression tag	UNP O94925
C	67	HIS	-	expression tag	UNP O94925
C	68	HIS	-	expression tag	UNP O94925
C	69	HIS	-	expression tag	UNP O94925
C	70	GLY	-	expression tag	UNP O94925
C	71	SER	-	expression tag	UNP O94925
D	60	MET	-	initiating methionine	UNP O94925
D	61	ARG	-	expression tag	UNP O94925
D	62	GLY	-	expression tag	UNP O94925
D	63	SER	-	expression tag	UNP O94925
D	64	HIS	-	expression tag	UNP O94925
D	65	HIS	-	expression tag	UNP O94925
D	66	HIS	-	expression tag	UNP O94925
D	67	HIS	-	expression tag	UNP O94925
D	68	HIS	-	expression tag	UNP O94925
D	69	HIS	-	expression tag	UNP O94925
D	70	GLY	-	expression tag	UNP O94925
D	71	SER	-	expression tag	UNP O94925

- Molecule 2 is 2-(pyridin-2-yl)-N-(5-{4-[6-({[3-(trifluoromethoxy)phenyl]acetyl}amino) pyridazin-3-yl]butyl}-1,3,4-thiadiazol-2-yl)acetamide (three-letter code: 63J) (formula: $C_{26}H_{24}F_3N_7O_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			40	26	3	7	3	1		
2	B	1	Total	C	F	N	O	S	0	0
			40	26	3	7	3	1		

- Molecule 3 is water.

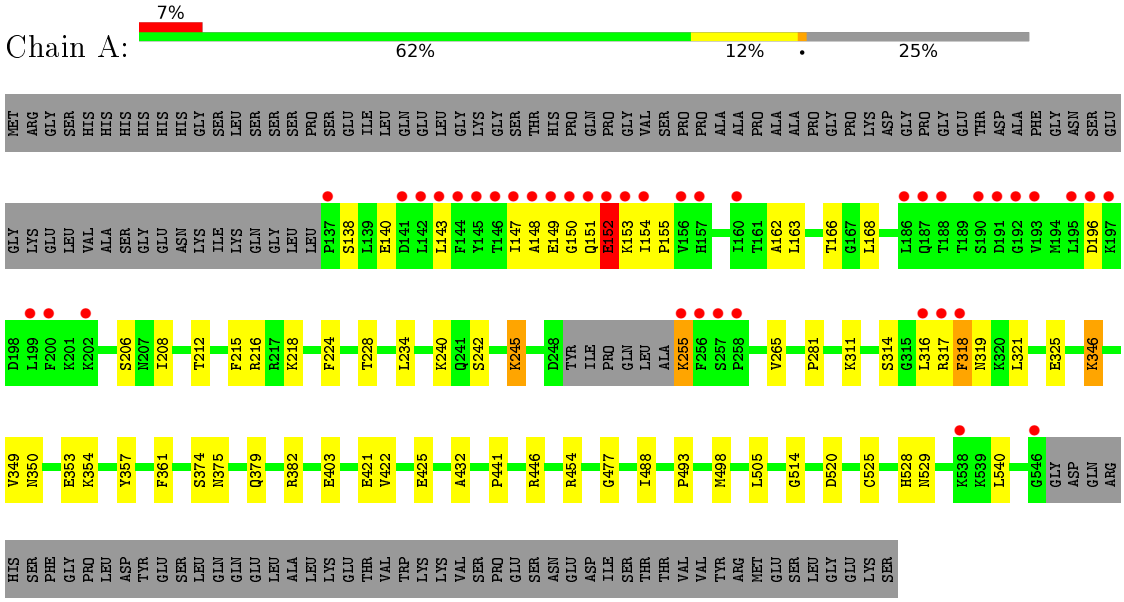
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	113	Total	O	0	0
			113	113		
3	B	91	Total	O	0	0
			91	91		
3	C	116	Total	O	0	0
			116	116		
3	D	102	Total	O	0	0
			102	102		

3 Residue-property plots (i)

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

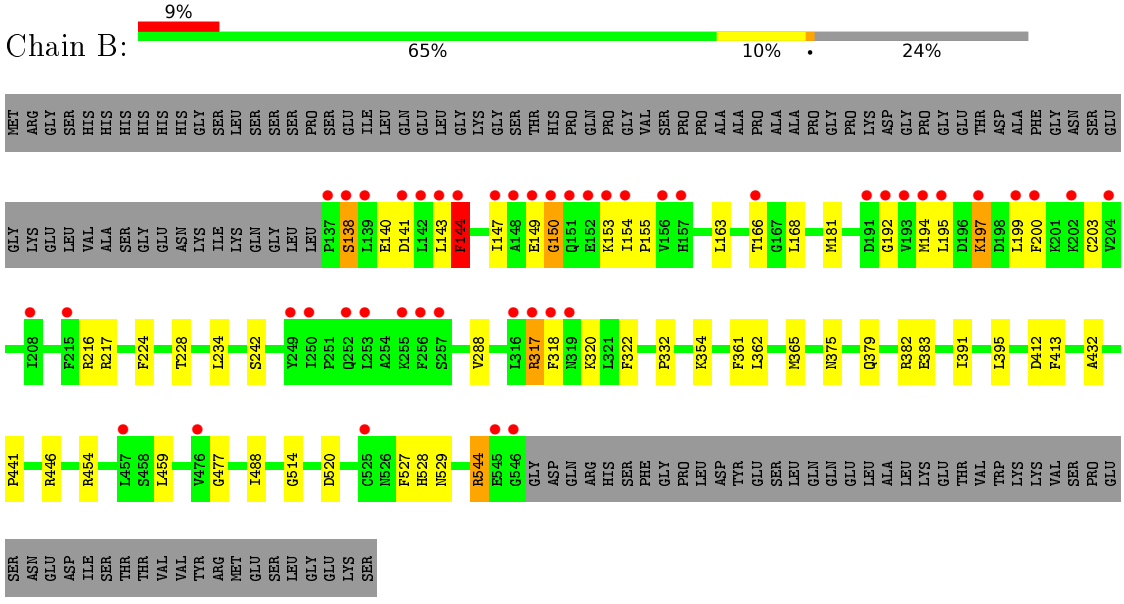
- Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain A:



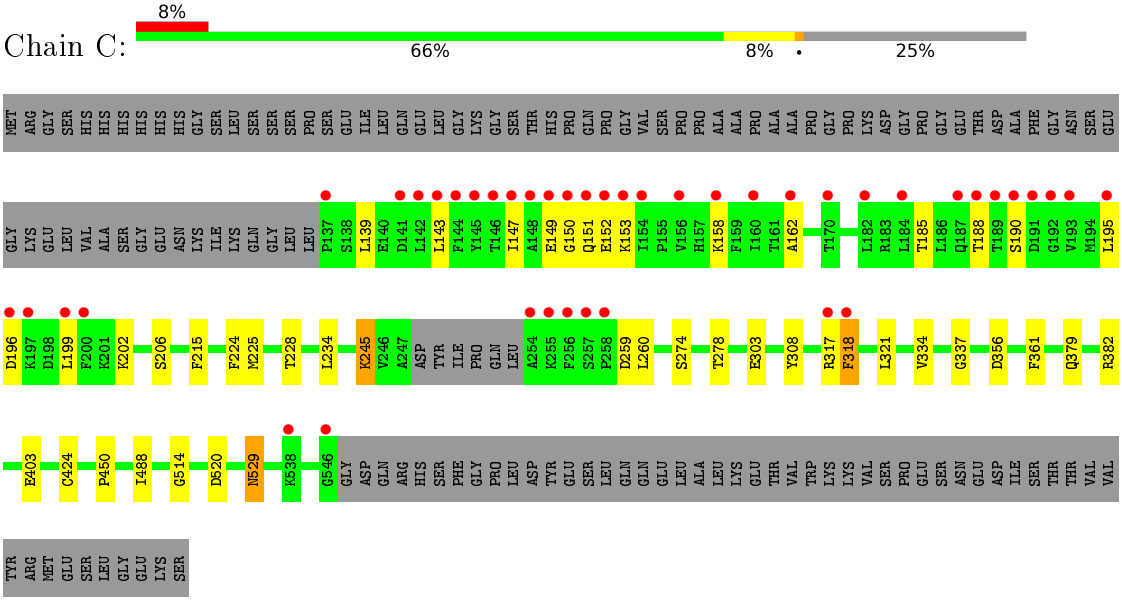
- Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain B:



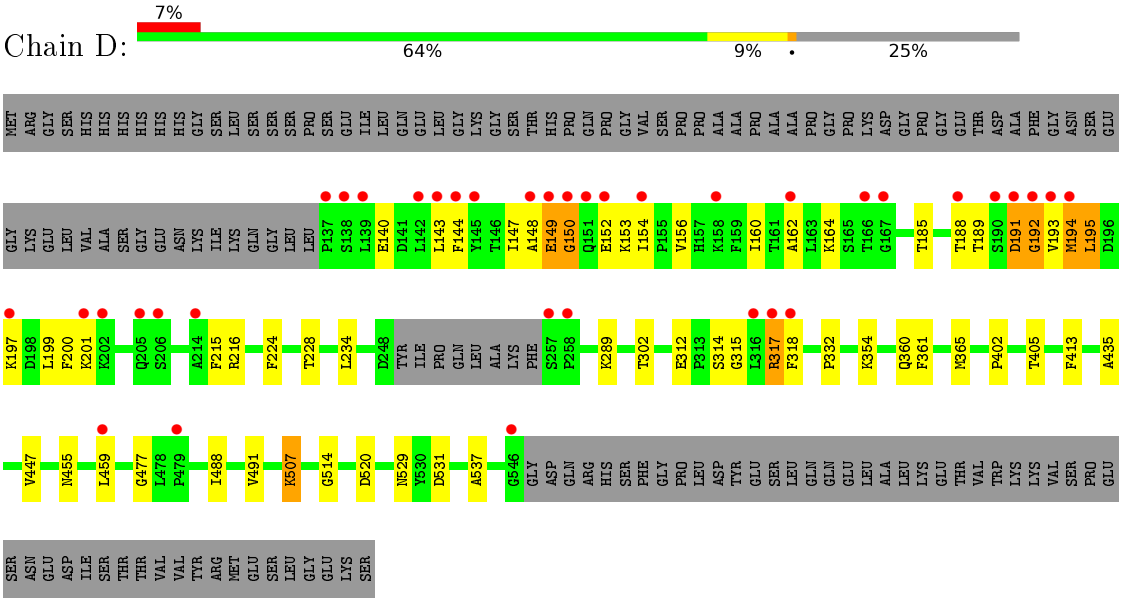
• Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain C:



• Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.53Å 139.38Å 177.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.48 – 2.40 47.93 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.48-2.40) 99.9 (47.93-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.225 , 0.264 0.222 , 0.263	Depositor DCC
R_{free} test set	1995 reflections (2.08%)	DCC
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13120	wwPDB-VP
Average B, all atoms (Å^2)	46.0	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 57.02 % 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 2.5157e-05.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: 63J

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	3/3217 (0.1%)	0.64	1/4338 (0.0%)
1	B	0.68	7/3269 (0.2%)	0.68	2/4412 (0.0%)
1	C	0.47	2/3214 (0.1%)	0.61	0/4334
1	D	0.46	0/3196	0.65	2/4311 (0.0%)
All	All	0.53	12/12896 (0.1%)	0.65	5/17395 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	317	ARG	CG-CD	-14.69	1.15	1.51
1	B	317	ARG	CZ-NH2	-13.76	1.15	1.33
1	B	197	LYS	CE-NZ	10.94	1.76	1.49
1	B	144	PHE	CB-CG	-9.96	1.34	1.51
1	B	317	ARG	CB-CG	-7.13	1.33	1.52
1	B	197	LYS	CD-CE	6.54	1.67	1.51
1	A	318	PHE	CB-CG	-6.37	1.40	1.51
1	A	152	GLU	CB-CG	6.37	1.64	1.52
1	C	318	PHE	CB-CG	-6.36	1.40	1.51
1	B	144	PHE	CE1-CZ	6.30	1.49	1.37
1	C	303	GLU	CD-OE1	-5.87	1.19	1.25
1	A	152	GLU	CD-OE2	-5.10	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	317	ARG	NE-CZ-NH1	-12.06	114.27	120.30
1	B	317	ARG	CG-CD-NE	-11.69	87.24	111.80
1	B	317	ARG	NE-CZ-NH2	10.10	125.35	120.30
1	A	152	GLU	CA-CB-CG	8.47	132.03	113.40
1	D	317	ARG	NE-CZ-NH2	5.32	122.96	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	544	ARG	Peptide
1	D	150	GLY	Mainchain

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	3148	0	3116	63	0
1	B	3197	0	3169	52	0
1	C	3145	0	3118	45	0
1	D	3128	0	3095	46	0
2	A	40	0	0	5	0
2	B	40	0	0	3	0
3	A	113	0	0	4	0
3	B	91	0	0	7	0
3	C	116	0	0	4	0
3	D	102	0	0	2	0
All	All	13120	0	12498	181	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 7.

All (181) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LYS:CE	1:B:197:LYS:NZ	1.76	1.48
2:A:601:63J:C13	1:D:317:ARG:HH12	1.52	1.22
1:B:163:LEU:O	1:B:166:THR:HG22	1.64	0.97
2:A:601:63J:C13	1:D:317:ARG:NH1	2.28	0.96
1:A:163:LEU:O	1:A:166:THR:HG22	1.68	0.93
1:C:318:PHE:HE1	1:D:317:ARG:HB3	1.32	0.93
1:B:166:THR:HG23	1:B:168:LEU:H	1.33	0.91
1:A:166:THR:HG23	1:A:168:LEU:H	1.38	0.88
1:D:156:VAL:HG12	1:D:195:LEU:HD22	1.60	0.84
1:C:152:GLU:C	1:C:153:LYS:HE2	2.02	0.79
1:B:446:ARG:NH1	3:B:701:HOH:O	2.14	0.79
1:C:318:PHE:CE1	1:D:317:ARG:HB3	2.18	0.79
1:A:216:ARG:O	1:A:218:LYS:NZ	2.21	0.73
1:D:140:GLU:HG3	1:D:201:LYS:HG3	1.68	0.73
1:A:446:ARG:NH2	3:A:702:HOH:O	2.16	0.72
1:A:317:ARG:HB2	1:B:318:PHE:CZ	2.23	0.72
1:C:403:GLU:OE1	3:C:601:HOH:O	2.06	0.72
1:A:403:GLU:CD	1:A:403:GLU:H	1.94	0.71
1:A:234:LEU:HD22	1:A:520:ASP:HB3	1.72	0.71
1:C:318:PHE:CZ	1:D:317:ARG:HG2	2.27	0.69
1:C:234:LEU:HD22	1:C:520:ASP:HB3	1.74	0.69
1:C:151:GLN:N	1:C:151:GLN:OE1	2.25	0.69
1:C:308:TYR:OH	3:C:601:HOH:O	2.11	0.69
1:B:144:PHE:CZ	1:B:200:PHE:HB3	2.28	0.69
1:D:531:ASP:O	3:D:601:HOH:O	2.11	0.69
1:A:152:GLU:HG2	1:A:153:LYS:HG2	1.74	0.68
2:A:601:63J:N08	2:A:601:63J:N16	2.40	0.68
1:A:425:GLU:OE2	3:A:701:HOH:O	2.13	0.67
1:B:144:PHE:CE1	1:B:197:LYS:HA	2.29	0.67
2:B:601:63J:C30	1:D:317:ARG:HE	2.08	0.67
1:A:325:GLU:HG3	1:B:317:ARG:NH1	2.10	0.66
1:B:144:PHE:CE1	1:B:200:PHE:HB3	2.31	0.66
1:A:529:ASN:ND2	1:B:529:ASN:OD1	2.29	0.66
1:A:321:LEU:CD1	2:A:601:63J:C15	2.76	0.64
1:C:150:GLY:N	1:C:151:GLN:OE1	2.31	0.64
1:D:488:ILE:HD12	1:D:514:GLY:HA3	1.80	0.64
1:D:332:PRO:HD2	1:D:459:LEU:HD13	1.80	0.63
1:D:365:MET:HG3	1:D:447:VAL:HG11	1.80	0.63
1:A:255:LYS:N	3:A:706:HOH:O	2.31	0.62
1:B:544:ARG:NH1	3:B:706:HOH:O	2.32	0.62
1:A:321:LEU:HD13	2:A:601:63J:C15	2.28	0.62
1:C:153:LYS:HD3	1:C:196:ASP:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:THR:OG1	1:D:191:ASP:OD2	2.10	0.62
1:A:153:LYS:HD2	1:A:196:ASP:HB3	1.82	0.62
1:B:153:LYS:HD2	1:B:194:MET:SD	2.40	0.62
1:A:316:LEU:O	1:A:319:ASN:ND2	2.33	0.61
1:A:317:ARG:HB2	1:B:318:PHE:CE2	2.35	0.61
1:C:317:ARG:HG3	1:D:318:PHE:CZ	2.36	0.61
1:C:245:LYS:O	1:C:245:LYS:HD2	2.01	0.60
1:C:143:LEU:O	1:C:147:ILE:HG12	2.02	0.60
1:C:152:GLU:HG2	1:C:153:LYS:HG2	1.83	0.59
1:B:197:LYS:NZ	1:B:197:LYS:CD	2.65	0.59
1:C:356:ASP:OD1	3:C:602:HOH:O	2.16	0.59
1:C:152:GLU:O	1:C:153:LYS:HE2	2.02	0.59
1:B:320:LYS:NZ	2:B:601:63J:F36	2.17	0.59
1:A:148:ALA:O	1:A:150:GLY:N	2.36	0.59
1:C:245:LYS:HD2	1:C:245:LYS:C	2.22	0.59
1:A:520:ASP:OD2	3:A:703:HOH:O	2.17	0.58
1:A:529:ASN:HD21	1:B:529:ASN:CG	2.05	0.58
1:A:153:LYS:CD	1:A:196:ASP:HA	2.33	0.58
1:A:208:ILE:O	1:A:212:THR:HG23	2.03	0.58
1:A:140:GLU:N	1:A:140:GLU:OE1	2.37	0.58
1:D:234:LEU:HD22	1:D:520:ASP:HB3	1.86	0.57
1:B:143:LEU:O	1:B:147:ILE:HD12	2.05	0.57
1:A:153:LYS:HD2	1:A:196:ASP:HA	1.85	0.57
1:D:289:LYS:NZ	3:D:609:HOH:O	2.37	0.57
1:B:322:PHE:O	3:B:702:HOH:O	2.17	0.56
1:A:153:LYS:HD2	1:A:196:ASP:CB	2.35	0.56
1:D:152:GLU:O	1:D:197:LYS:HE3	2.06	0.56
1:A:317:ARG:HB2	1:B:318:PHE:HZ	1.69	0.56
1:D:192:GLY:HA3	1:D:194:MET:H	1.68	0.56
1:B:234:LEU:HD22	1:B:520:ASP:HB3	1.88	0.56
1:A:148:ALA:HB2	1:A:154:ILE:HG12	1.87	0.55
1:B:362:LEU:HD23	1:B:365:MET:CE	2.36	0.55
1:A:350:ASN:ND2	1:A:353:GLU:OE1	2.38	0.54
1:C:139:LEU:H	1:C:139:LEU:HD12	1.72	0.54
1:A:477:GLY:O	1:A:529:ASN:HB2	2.08	0.54
1:B:379:GLN:O	1:B:383:GLU:HG3	2.07	0.54
1:D:195:LEU:HA	1:D:199:LEU:HD23	1.89	0.54
1:B:195:LEU:HA	1:B:199:LEU:HD23	1.90	0.53
1:C:153:LYS:CD	1:C:196:ASP:HA	2.39	0.53
1:D:144:PHE:CE2	1:D:197:LYS:HD2	2.44	0.52
1:B:332:PRO:HD2	1:B:459:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ASN:HD21	1:B:529:ASN:ND2	2.08	0.52
1:D:148:ALA:O	1:D:150:GLY:N	2.41	0.52
1:A:153:LYS:HD2	1:A:196:ASP:CA	2.39	0.52
1:C:403:GLU:H	1:C:403:GLU:CD	2.14	0.52
1:C:149:GLU:HB2	1:C:151:GLN:OE1	2.10	0.51
1:A:311:LYS:HE2	3:B:773:HOH:O	2.10	0.51
1:C:317:ARG:HB3	1:D:318:PHE:CE2	2.46	0.51
1:B:477:GLY:O	1:B:529:ASN:HB2	2.09	0.51
1:D:154:ILE:O	1:D:195:LEU:HB3	2.11	0.51
1:A:318:PHE:CZ	1:B:318:PHE:CE1	3.00	0.50
1:A:529:ASN:ND2	1:B:529:ASN:HD21	2.10	0.50
1:D:477:GLY:O	1:D:529:ASN:HB2	2.12	0.50
1:C:529:ASN:ND2	1:D:529:ASN:OD1	2.45	0.49
1:B:153:LYS:HD2	1:B:194:MET:CG	2.42	0.49
1:D:185:THR:HA	1:D:188:THR:HB	1.95	0.49
1:A:525:CYS:HA	1:A:540:LEU:O	2.13	0.49
1:C:196:ASP:OD1	1:C:199:LEU:HB2	2.13	0.49
1:A:143:LEU:O	1:A:147:ILE:HG13	2.13	0.49
1:C:152:GLU:CD	1:C:153:LYS:H	2.17	0.48
1:D:162:ALA:HB1	1:D:215:PHE:HE1	1.77	0.48
1:C:158:LYS:HA	1:C:158:LYS:HD2	1.61	0.48
1:A:245:LYS:HE3	1:A:505:LEU:HB2	1.95	0.48
1:A:318:PHE:CE2	1:B:317:ARG:HG3	2.49	0.48
1:D:224:PHE:O	1:D:228:THR:HG23	2.14	0.48
1:C:224:PHE:O	1:C:228:THR:HG23	2.14	0.47
1:C:450:PRO:HG2	1:D:537:ALA:HB2	1.96	0.47
1:A:143:LEU:HD13	1:A:212:THR:HG22	1.95	0.47
1:B:379:GLN:O	1:B:382:ARG:HG2	2.13	0.47
1:A:325:GLU:HG3	1:B:317:ARG:CZ	2.45	0.47
1:A:379:GLN:O	1:A:382:ARG:HG2	2.14	0.47
1:A:493:PRO:HB3	3:B:787:HOH:O	2.14	0.46
1:A:432:ALA:HB1	1:A:441:PRO:HG3	1.97	0.46
1:B:527:PHE:O	3:B:703:HOH:O	2.21	0.46
1:D:148:ALA:O	1:D:149:GLU:HG2	2.15	0.46
1:B:362:LEU:HD23	1:B:365:MET:HE3	1.96	0.46
1:C:379:GLN:O	1:C:382:ARG:HG2	2.16	0.46
1:A:403:GLU:CD	1:A:403:GLU:N	2.65	0.46
1:B:318:PHE:CD1	1:B:318:PHE:N	2.81	0.46
1:A:375:ASN:O	1:A:379:GLN:HG2	2.16	0.46
1:C:162:ALA:HB1	1:C:215:PHE:HE1	1.80	0.46
1:C:334:VAL:HG23	1:C:337:GLY:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:THR:O	1:C:188:THR:HG22	2.16	0.45
1:A:162:ALA:HB1	1:A:215:PHE:HE1	1.82	0.45
1:A:528:HIS:CD2	1:B:454:ARG:HD2	2.52	0.45
1:B:354:LYS:HB3	1:B:413:PHE:CZ	2.51	0.45
1:D:144:PHE:HD1	1:D:200:PHE:CG	2.35	0.45
1:C:202:LYS:NZ	3:C:616:HOH:O	2.50	0.45
1:C:318:PHE:HZ	1:D:317:ARG:HG2	1.77	0.45
1:B:138:SER:O	1:B:141:ASP:HB2	2.17	0.45
1:C:318:PHE:CZ	1:D:318:PHE:CZ	3.04	0.45
1:B:149:GLU:HG3	1:B:150:GLY:N	2.32	0.44
1:A:281:PRO:HA	1:A:422:VAL:O	2.17	0.44
1:A:265:VAL:HG22	1:A:498:MET:HG2	2.00	0.44
1:B:144:PHE:HE1	1:B:197:LYS:O	1.99	0.44
1:C:152:GLU:OE2	1:C:152:GLU:N	2.51	0.44
1:C:149:GLU:HB2	1:C:151:GLN:NE2	2.32	0.44
1:C:488:ILE:HD12	1:C:514:GLY:HA3	1.98	0.44
1:A:154:ILE:HG22	1:A:155:PRO:O	2.17	0.44
1:C:317:ARG:HD2	1:C:317:ARG:O	2.18	0.44
1:A:349:VAL:O	1:A:354:LYS:HE3	2.17	0.43
1:B:154:ILE:HG22	1:B:155:PRO:O	2.18	0.43
1:B:181:MET:HG2	1:B:203:CYS:HA	2.01	0.43
1:D:354:LYS:HB3	1:D:413:PHE:CZ	2.53	0.43
1:B:224:PHE:O	1:B:228:THR:HG23	2.19	0.43
1:D:302:THR:OG1	1:D:455:ASN:ND2	2.47	0.43
1:B:432:ALA:HB1	1:B:441:PRO:HG3	2.00	0.42
1:B:140:GLU:O	1:B:144:PHE:HB2	2.19	0.42
1:B:216:ARG:HE	1:B:216:ARG:HA	1.83	0.42
1:C:318:PHE:CE1	1:D:317:ARG:CB	2.96	0.42
1:D:192:GLY:HA3	1:D:194:MET:N	2.33	0.42
1:A:454:ARG:HD2	1:B:528:HIS:CG	2.54	0.42
1:A:346:LYS:HG3	1:A:357:TYR:CD2	2.54	0.42
1:A:143:LEU:HA	1:A:143:LEU:HD12	1.91	0.42
1:A:488:ILE:HD12	1:A:514:GLY:HA3	2.01	0.42
1:B:375:ASN:OD1	3:B:704:HOH:O	2.21	0.42
1:C:149:GLU:HB2	1:C:151:GLN:HE22	1.84	0.42
1:D:197:LYS:HD3	1:D:197:LYS:N	2.35	0.42
1:A:245:LYS:C	1:A:245:LYS:HD2	2.41	0.41
1:C:318:PHE:CE1	1:D:317:ARG:HG2	2.54	0.41
1:A:153:LYS:HD3	1:A:196:ASP:HA	2.03	0.41
1:C:195:LEU:HA	1:C:199:LEU:HD23	2.02	0.41
1:D:192:GLY:HA3	1:D:193:VAL:HA	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:507:LYS:HE2	1:D:507:LYS:HA	2.01	0.41
1:C:278:THR:HA	1:C:424:CYS:HB2	2.02	0.41
1:D:160:ILE:HG22	1:D:164:LYS:HD2	2.02	0.41
1:B:488:ILE:HD12	1:B:514:GLY:HA3	2.02	0.41
1:A:314:SER:HB2	1:A:318:PHE:HB2	2.02	0.41
2:B:601:63J:N39	1:C:321:LEU:HB3	2.35	0.41
1:A:224:PHE:O	1:A:228:THR:HG23	2.21	0.41
1:A:529:ASN:ND2	1:B:529:ASN:ND2	2.68	0.41
1:D:143:LEU:HD11	1:D:147:ILE:HD11	2.03	0.40
1:D:402:PRO:O	1:D:405:THR:OG1	2.34	0.40
1:D:189:THR:HG23	1:D:189:THR:O	2.21	0.40
1:D:435:ALA:HB2	1:D:491:VAL:HG13	2.03	0.40
1:A:151:GLN:OE1	1:A:152:GLU:N	2.54	0.40
1:A:318:PHE:CZ	1:B:318:PHE:CZ	3.09	0.40
1:B:391:ILE:O	1:B:395:LEU:HG	2.21	0.40
1:A:374:SER:HB2	1:A:421:GLU:OE2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/539 (74%)	387 (97%)	10 (2%)	3 (1%)	24	35
1	B	408/539 (76%)	394 (97%)	11 (3%)	3 (1%)	26	38
1	C	400/539 (74%)	384 (96%)	15 (4%)	1 (0%)	46	63
1	D	398/539 (74%)	375 (94%)	17 (4%)	6 (2%)	13	17
All	All	1606/2156 (74%)	1540 (96%)	53 (3%)	13 (1%)	24	35

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	A	149	GLU
1	B	150	GLY
1	B	192	GLY
1	D	149	GLU
1	D	192	GLY
1	D	194	MET
1	D	315	GLY
1	C	190	SER
1	D	314	SER
1	D	195	LEU
1	A	152	GLU
1	B	138	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/462 (76%)	342 (98%)	7 (2%)	63	81
1	B	354/462 (77%)	348 (98%)	6 (2%)	68	85
1	C	348/462 (75%)	340 (98%)	8 (2%)	58	78
1	D	347/462 (75%)	340 (98%)	7 (2%)	63	81
All	All	1398/1848 (76%)	1370 (98%)	28 (2%)	63	81

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	SER
1	A	240	LYS
1	A	242	SER
1	A	245	LYS
1	A	255	LYS
1	A	346	LYS
1	A	361	PHE
1	B	144	PHE
1	B	217	ARG

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Mol	Chain	Res	Type
1	B	242	SER
1	B	288	VAL
1	B	361	PHE
1	B	412	ASP
1	C	206	SER
1	C	225	MET
1	C	245	LYS
1	C	259	ASP
1	C	260	LEU
1	C	274	SER
1	C	361	PHE
1	C	529	ASN
1	D	153	LYS
1	D	191	ASP
1	D	216	ARG
1	D	312	GLU
1	D	360	GLN
1	D	361	PHE
1	D	507	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	HIS
1	A	455	ASN
1	A	529	ASN
1	B	529	ASN
1	C	241	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
2	63J	A	601	-	35,43,43	2.02	8 (22%)	37,58,58	4.08	12 (32%)
2	63J	B	601	-	35,43,43	1.37	4 (11%)	37,58,58	1.46	8 (21%)

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
2	63J	A	601	-	-	0/22/28/28	0/3/4/4
2	63J	B	601	-	-	0/22/28/28	0/3/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	63J	C09-N08	2.08	1.40	1.35
2	A	601	63J	C13-C12	2.55	1.43	1.38
2	A	601	63J	C25-N24	2.86	1.42	1.35
2	A	601	63J	C14-C13	2.93	1.45	1.38
2	B	601	63J	C09-N08	3.16	1.43	1.35
2	B	601	63J	C25-N24	3.23	1.43	1.35
2	A	601	63J	C10-C11	3.35	1.54	1.51
2	A	601	63J	C07-N08	3.75	1.42	1.36
2	B	601	63J	C07-N08	3.92	1.43	1.36
2	B	601	63J	C03-C04	4.70	1.52	1.49
2	A	601	63J	C11-N16	5.81	1.46	1.34
2	A	601	63J	C03-C04	6.28	1.53	1.49

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	63J	C13-C12-C11	-12.05	103.71	118.93
2	A	601	63J	C14-C15-N16	-10.86	104.89	123.42
2	A	601	63J	C10-C11-N16	-10.34	102.57	117.00
2	A	601	63J	O17-C09-N08	-4.37	116.11	123.77
2	A	601	63J	C01-C19-C20	-3.48	102.89	113.31
2	B	601	63J	C01-C19-C20	-2.32	106.37	113.31
2	B	601	63J	C30-C31-C32	-2.26	117.43	120.56
2	B	601	63J	C10-C11-C12	-2.24	119.10	122.06
2	B	601	63J	C23-N24-C25	-2.08	124.59	128.07
2	B	601	63J	C29-C30-C31	2.22	122.77	118.93
2	A	601	63J	C31-C32-C27	2.29	122.18	119.70
2	A	601	63J	C10-C09-N08	2.33	121.36	114.69
2	B	601	63J	C26-C25-N24	2.46	121.74	114.69
2	B	601	63J	C15-N16-C11	2.49	120.69	117.35
2	A	601	63J	C12-C11-N16	2.62	126.14	122.19
2	B	601	63J	C23-N39-N40	3.58	122.23	119.37
2	A	601	63J	C13-C14-C15	3.71	125.86	118.59
2	A	601	63J	C14-C13-C12	4.87	126.97	120.20
2	A	601	63J	C10-C11-C12	6.86	131.15	122.06
2	A	601	63J	C15-N16-C11	9.58	130.19	117.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	63J	5	0
2	B	601	63J	3	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	404/539 (74%)	0.62	40 (9%) 9 9	25, 39, 85, 128	0
1	B	410/539 (76%)	0.67	46 (11%) 7 7	27, 39, 90, 124	0
1	C	404/539 (74%)	0.60	43 (10%) 8 8	26, 39, 84, 126	0
1	D	402/539 (74%)	0.59	37 (9%) 11 11	27, 39, 85, 112	0
All	All	1620/2156 (75%)	0.62	166 (10%) 9 8	25, 39, 87, 128	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	PHE	9.1
1	A	317	ARG	8.0
1	B	318	PHE	7.9
1	A	256	PHE	7.6
1	B	144	PHE	7.1
1	B	149	GLU	7.0
1	C	145	TYR	6.9
1	B	546	GLY	6.7
1	B	138	SER	6.1
1	C	190	SER	5.9
1	A	148	ALA	5.9
1	C	317	ARG	5.9
1	B	191	ASP	5.9
1	A	192	GLY	5.8
1	B	317	ARG	5.8
1	A	200	PHE	5.7
1	A	258	PRO	5.7
1	A	156	VAL	5.7
1	A	193	VAL	5.7
1	C	318	PHE	5.7
1	B	192	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	192	GLY	5.7
1	A	150	GLY	5.6
1	D	318	PHE	5.6
1	B	194	MET	5.5
1	D	144	PHE	5.4
1	C	256	PHE	5.2
1	B	142	LEU	4.9
1	C	150	GLY	4.9
1	A	147	ILE	4.9
1	B	151	GLN	4.8
1	A	257	SER	4.8
1	A	144	PHE	4.8
1	C	149	GLU	4.7
1	D	192	GLY	4.7
1	B	252	GLN	4.7
1	A	151	GLN	4.7
1	D	149	GLU	4.6
1	B	200	PHE	4.6
1	B	253	LEU	4.6
1	D	138	SER	4.6
1	C	191	ASP	4.5
1	A	146	THR	4.5
1	D	151	GLN	4.4
1	A	145	TYR	4.4
1	C	146	THR	4.2
1	D	194	MET	4.2
1	D	258	PRO	4.2
1	D	150	GLY	4.1
1	C	255	LYS	4.1
1	B	193	VAL	4.1
1	B	204	VAL	4.1
1	A	153	LYS	4.1
1	B	150	GLY	4.1
1	A	195	LEU	4.1
1	D	190	SER	4.0
1	C	151	GLN	4.0
1	D	546	GLY	4.0
1	C	144	PHE	3.8
1	A	152	GLU	3.8
1	D	143	LEU	3.7
1	B	256	PHE	3.7
1	A	546	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	191	ASP	3.7
1	B	249	TYR	3.7
1	C	153	LYS	3.6
1	A	141	ASP	3.6
1	A	154	ILE	3.5
1	C	197	LYS	3.5
1	D	257	SER	3.5
1	D	139	LEU	3.5
1	C	148	ALA	3.5
1	A	197	LYS	3.5
1	C	147	ILE	3.4
1	A	142	LEU	3.4
1	A	191	ASP	3.4
1	B	257	SER	3.4
1	A	196	ASP	3.4
1	C	162	ALA	3.4
1	B	195	LEU	3.3
1	B	137	PRO	3.3
1	C	254	ALA	3.3
1	C	257	SER	3.3
1	B	143	LEU	3.3
1	C	158	LYS	3.3
1	A	137	PRO	3.2
1	D	145	TYR	3.2
1	A	316	LEU	3.2
1	A	149	GLU	3.2
1	B	139	LEU	3.2
1	C	152	GLU	3.1
1	D	193	VAL	3.1
1	A	143	LEU	3.1
1	D	197	LYS	3.0
1	C	156	VAL	2.9
1	A	157	HIS	2.9
1	D	152	GLU	2.9
1	C	200	PHE	2.9
1	C	137	PRO	2.9
1	B	255	LYS	2.9
1	C	142	LEU	2.9
1	C	193	VAL	2.8
1	B	152	GLU	2.8
1	C	160	ILE	2.8
1	D	316	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	188	THR	2.8
1	D	201	LYS	2.7
1	B	250	ILE	2.7
1	D	479	PRO	2.7
1	A	255	LYS	2.7
1	C	196	ASP	2.7
1	D	188	THR	2.6
1	D	162	ALA	2.6
1	D	142	LEU	2.6
1	C	184	LEU	2.6
1	B	215	PHE	2.6
1	C	195	LEU	2.6
1	C	538	LYS	2.5
1	A	190	SER	2.5
1	B	156	VAL	2.5
1	A	160	ILE	2.5
1	D	154	ILE	2.5
1	C	546	GLY	2.5
1	D	167	GLY	2.5
1	B	197	LYS	2.5
1	B	199	LEU	2.4
1	B	316	LEU	2.4
1	D	166	THR	2.4
1	A	187	GLN	2.4
1	D	214	ALA	2.4
1	C	141	ASP	2.4
1	C	182	LEU	2.4
1	D	317	ARG	2.4
1	A	186	LEU	2.4
1	A	538	LYS	2.3
1	B	153	LYS	2.3
1	B	141	ASP	2.3
1	A	199	LEU	2.3
1	C	154	ILE	2.3
1	C	143	LEU	2.3
1	B	202	LYS	2.3
1	C	170	THR	2.3
1	B	157	HIS	2.3
1	C	187	GLN	2.3
1	B	457	LEU	2.2
1	D	459	LEU	2.2
1	D	137	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	319	ASN	2.2
1	B	545	GLU	2.2
1	B	148	ALA	2.2
1	B	208	ILE	2.2
1	D	202	LYS	2.2
1	D	206	SER	2.2
1	D	158	LYS	2.2
1	B	476	VAL	2.2
1	B	166	THR	2.2
1	C	258	PRO	2.2
1	C	199	LEU	2.1
1	B	525	CYS	2.1
1	B	154	ILE	2.1
1	D	148	ALA	2.1
1	C	189	THR	2.1
1	B	147	ILE	2.1
1	A	188	THR	2.0
1	A	202	LYS	2.0
1	D	205	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	63J	A	601	40/40	0.76	0.29	0.14	38,72,112,115	0
2	63J	B	601	40/40	0.76	0.26	-0.14	39,60,140,146	0

6.5 Other polymers (i)

There are no such residues in this entry.