Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 12:12 PM EST

PDB ID	:	6ULT
Title	:	BRD2-BD2 in complex with the cyclic peptide 4.2_3
Authors	:	Patel, K.; Walshe, J.L.; Walport, L.J.; Mackay, J.P.
Deposited on	:	2019-10-08
Resolution	:	2.80 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

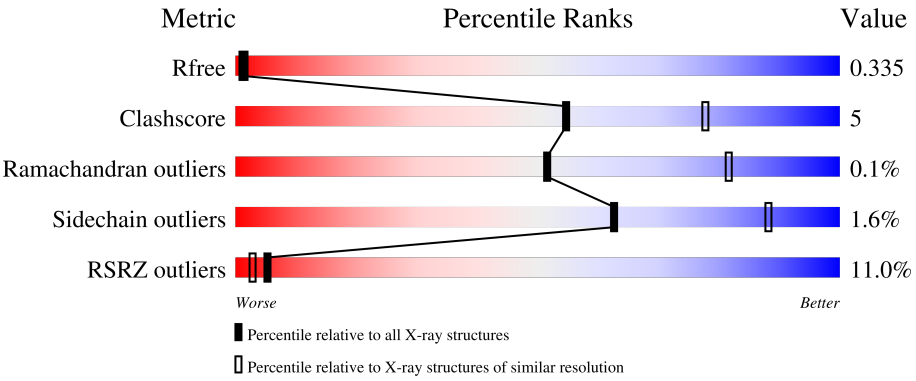
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	109	6% 82% 13% • 5%
1	B	109	9% 85% 14% •
1	C	109	13% 83% 10% 7%
1	D	109	16% 81% 17% ••
1	E	109	2% 88% 12%

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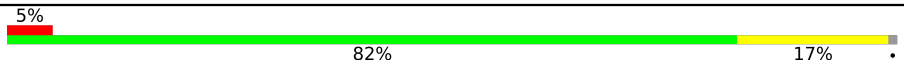
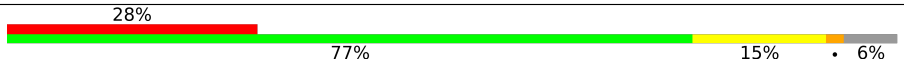
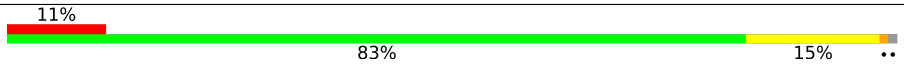
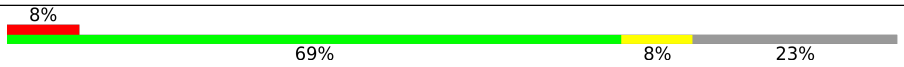
Mol	Chain	Length	Quality of chain
1	F	109	
1	G	109	
1	H	109	
2	I	13	
2	J	13	
2	K	13	
2	L	13	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7526 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 Bromodomain-containing protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			862	553	152	150	7			
1	B	108	Total	C	N	O	S	0	1	0
			895	571	157	160	7			
1	C	101	Total	C	N	O	S	0	0	0
			838	537	148	147	6			
1	D	107	Total	C	N	O	S	0	0	0
			887	567	156	157	7			
1	E	109	Total	C	N	O	S	0	2	0
			906	578	158	163	7			
1	F	108	Total	C	N	O	S	0	1	0
			898	574	158	159	7			
1	G	102	Total	C	N	O	S	6	1	0
			845	542	147	149	7			
1	H	108	Total	C	N	O	S	0	1	0
			897	572	157	161	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	SER	-	expression tag	UNP P25440
B	346	SER	-	expression tag	UNP P25440
C	346	SER	-	expression tag	UNP P25440
D	346	SER	-	expression tag	UNP P25440
E	346	SER	-	expression tag	UNP P25440
F	346	SER	-	expression tag	UNP P25440
G	346	SER	-	expression tag	UNP P25440
H	346	SER	-	expression tag	UNP P25440

- Molecule 2 is a protein called Cyclic peptide 4.2_3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	13	Total	C	N	O	S	0	0	0
			118	78	22	17	1			
2	J	11	Total	C	N	O	S	0	0	0
			101	67	19	14	1			
2	K	12	Total	C	N	O	S	0	0	0
			109	73	20	15	1			
2	L	10	Total	C	N	O	S	0	0	0
			90	61	15	13	1			

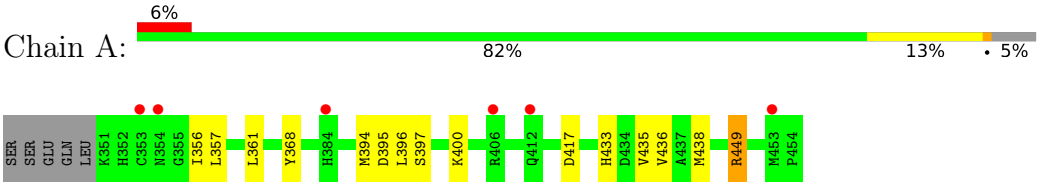
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	12	Total	O	0	0
			12	12		
3	C	7	Total	O	0	0
			7	7		
3	D	3	Total	O	0	0
			3	3		
3	E	12	Total	O	0	0
			12	12		
3	F	10	Total	O	0	0
			10	10		
3	G	12	Total	O	0	0
			12	12		
3	H	8	Total	O	0	0
			8	8		
3	J	1	Total	O	0	0
			1	1		
3	K	3	Total	O	0	0
			3	3		
3	L	1	Total	O	0	0
			1	1		

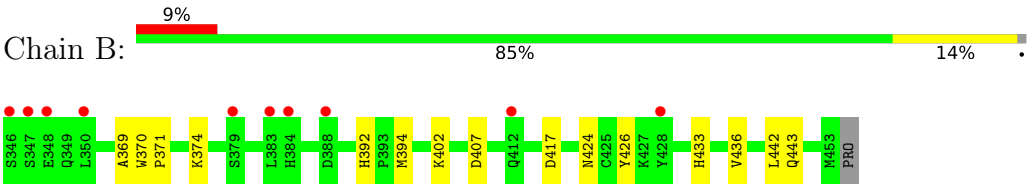
3 Residue-property plots (i)

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.

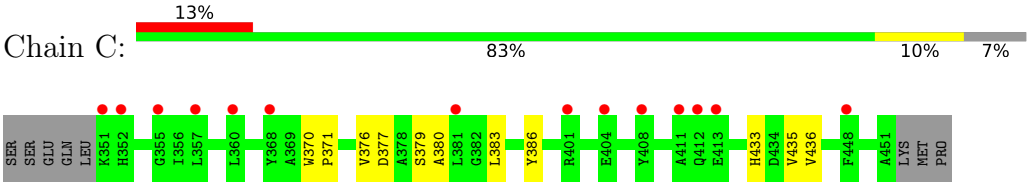
• Molecule 1: Bromodomain-containing protein 2



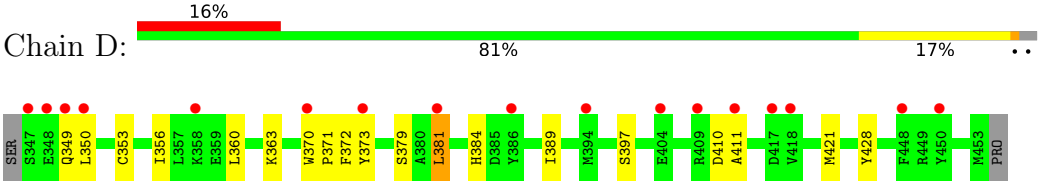
• Molecule 1: Bromodomain-containing protein 2



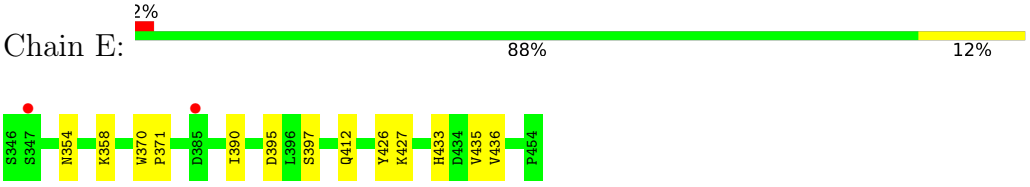
• Molecule 1: Bromodomain-containing protein 2



• Molecule 1: Bromodomain-containing protein 2

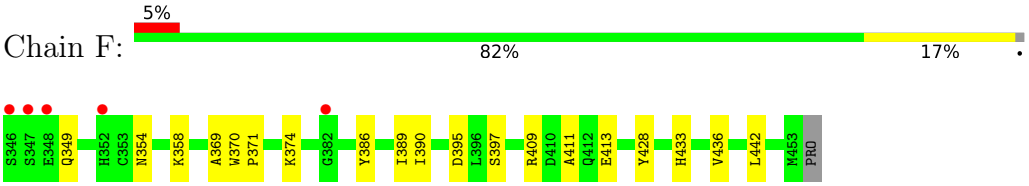


• Molecule 1: Bromodomain-containing protein 2



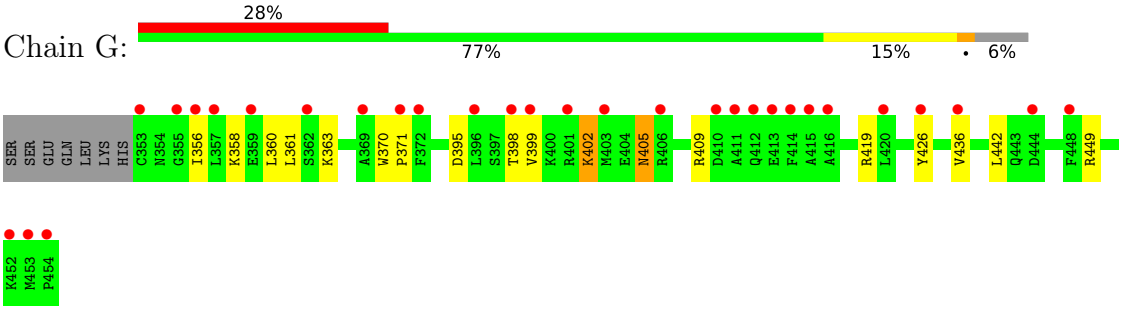
• Molecule 1: Bromodomain-containing protein 2

Chain F:



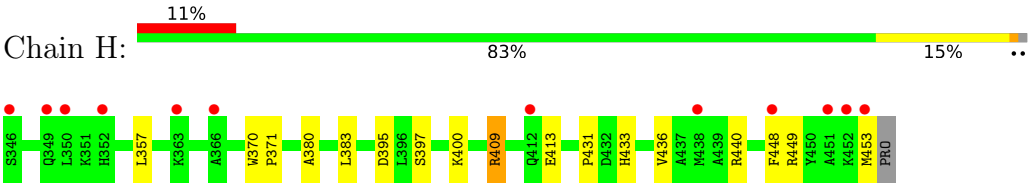
• Molecule 1: Bromodomain-containing protein 2

Chain G:



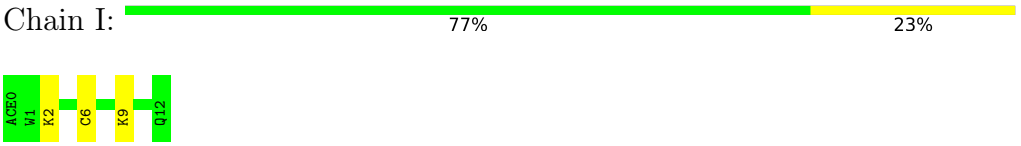
• Molecule 1: Bromodomain-containing protein 2

Chain H:



• Molecule 2: Cyclic peptide 4.2_3

Chain I:

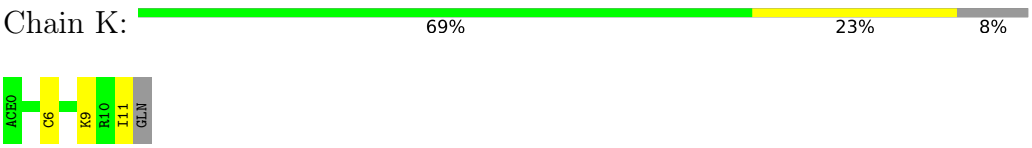


• Molecule 2: Cyclic peptide 4.2_3

Chain J:

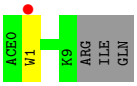
• Molecule 2: Cyclic peptide 4.2_3

Chain K:



• Molecule 2: Cyclic peptide 4.2_3

Chain L:


ACE0
W1
K9
ARG
ILE
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.08Å 63.63Å 120.34Å 90.00° 108.39° 90.00°	Depositor
Resolution (Å)	42.50 – 2.80 42.50 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (42.50-2.80) 98.2 (42.50-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.14_3260, PHENIX 1.14_3260	Depositor
R, R_{free}	0.284 , 0.335 0.284 , 0.335	Depositor DCC
R_{free} test set	1384 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 74.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	7526	wwPDB-VP
Average B, all atoms (Å^2)	57.0	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 45.74 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2657e-04. 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: ACE, ALY

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	0.25	0/887	0.40	0/1195
1	B	0.24	0/923	0.39	0/1242
1	C	0.25	0/862	0.39	0/1162
1	D	0.25	0/911	0.39	0/1226
1	E	0.26	0/939	0.40	0/1265
1	F	0.27	0/926	0.41	0/1246
1	G	0.26	0/873	0.43	0/1177
1	H	0.25	0/925	0.39	0/1245
2	I	0.26	0/92	0.46	0/120
2	J	0.24	0/75	0.39	0/97
2	K	0.21	0/83	0.39	0/108
2	L	0.23	0/65	0.45	0/86
All	All	0.25	0/7561	0.40	0/10169

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	862	0	844	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	895	0	873	10	0
1	C	838	0	815	7	0
1	D	887	0	867	13	0
1	E	906	0	880	8	0
1	F	898	0	881	10	0
1	G	845	0	825	11	0
1	H	897	0	872	10	0
2	I	118	0	122	2	0
2	J	101	0	103	1	0
2	K	109	0	115	2	0
2	L	90	0	91	0	0
3	A	11	0	0	0	0
3	B	12	0	0	0	0
3	C	7	0	0	0	0
3	D	3	0	0	0	0
3	E	12	0	0	0	0
3	F	10	0	0	0	0
3	G	12	0	0	2	0
3	H	8	0	0	0	0
3	J	1	0	0	0	0
3	K	3	0	0	0	0
3	L	1	0	0	0	0
All	All	7526	0	7288	77	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 5.

All (77) 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:433:HIS:HB3	1:B:436:VAL:HG23	1.73	0.70
1:H:380:ALA:HB3	1:H:383:LEU:HD12	1.76	0.68
1:G:356:ILE:HG12	1:G:449:ARG:HG3	1.79	0.64
1:A:356:ILE:HG12	1:A:449:ARG:HD2	1.82	0.62
1:A:357:LEU:HD21	1:A:400:LYS:HA	1.82	0.61
1:H:383:LEU:HD21	2:I:2:ALY:HB3	1.82	0.61
1:H:448:PHE:HD2	1:H:449:ARG:HD2	1.68	0.59
1:B:374:LYS:HB2	1:D:381:LEU:HA	1.87	0.57
1:B:392:HIS:O	1:B:424:ASN:ND2	2.38	0.56
1:D:372:PHE:HB3	1:D:421:MET:CE	2.35	0.56
1:H:357:LEU:HD21	1:H:400:LYS:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:433:HIS:HB3	1:F:436:VAL:HG23	1.88	0.55
1:G:360:LEU:HD22	1:G:442:LEU:HD11	1.89	0.55
1:A:433:HIS:HB3	1:A:436:VAL:HG23	1.89	0.55
1:C:433:HIS:ND1	1:C:435:VAL:HG12	2.23	0.54
1:C:376:VAL:HG21	1:C:386:TYR:CZ	2.44	0.52
1:D:350:LEU:HA	1:D:353:CYS:HB2	1.92	0.52
1:H:370:TRP:CG	1:H:371:PRO:HD3	2.46	0.50
1:C:376:VAL:HG21	1:C:386:TYR:CE1	2.48	0.49
1:G:405:ASN:O	1:G:405:ASN:ND2	2.31	0.48
1:B:369:ALA:HB2	1:B:442:LEU:HD13	1.95	0.48
1:G:409:ARG:NH2	3:G:504:HOH:O	2.47	0.48
1:G:395:ASP:O	1:G:399:VAL:HG23	2.13	0.48
2:I:9:ALY:HB2	2:I:9:ALY:HE2	1.69	0.48
1:G:370:TRP:CG	1:G:371:PRO:HD3	2.49	0.48
1:F:369:ALA:HB2	1:F:442:LEU:HD13	1.95	0.47
1:C:377:ASP:OD1	1:C:379:SER:OG	2.24	0.47
1:E:371:PRO:HB3	2:J:9:ALY:HE3	1.96	0.47
1:C:380:ALA:HB3	1:C:383:LEU:HD12	1.95	0.47
1:D:370:TRP:CG	1:D:371:PRO:HD3	2.49	0.47
1:D:372:PHE:HB3	1:D:421:MET:HE1	1.97	0.47
1:C:433:HIS:O	1:C:436:VAL:HG22	2.13	0.47
1:H:395:ASP:OD2	1:H:397:SER:OG	2.21	0.47
1:E:354:ASN:O	1:E:358:LYS:HG2	2.15	0.47
1:E:433:HIS:HB3	1:E:436:VAL:HG23	1.96	0.46
1:A:394:MET:HG2	1:A:417:ASP:O	2.16	0.46
1:E:433:HIS:CE1	1:E:435:VAL:HG23	2.51	0.46
1:A:395:ASP:OD2	1:A:397:SER:OG	2.19	0.46
1:A:433:HIS:CE1	1:A:435:VAL:HG23	2.49	0.46
1:G:426:TYR:HD1	1:G:436:VAL:HG13	1.81	0.46
1:D:389:ILE:HD12	1:D:428:TYR:CE1	2.51	0.46
1:D:363:LYS:HB2	1:D:363:LYS:HE3	1.78	0.46
1:H:409:ARG:HG2	1:H:413:GLU:OE1	2.16	0.46
1:C:370:TRP:CG	1:C:371:PRO:HD3	2.52	0.45
1:B:370:TRP:HB2	1:D:384:HIS:NE2	2.31	0.45
1:G:398:THR:O	1:G:402:LYS:N	2.34	0.45
1:B:426:TYR:OH	1:B:443:GLN:OE1	2.18	0.45
1:D:373:TYR:O	1:D:397:SER:OG	2.27	0.44
1:H:409:ARG:HG2	1:H:409:ARG:H	1.54	0.44
1:F:349:GLN:HB3	1:F:411:ALA:HB2	1.98	0.44
2:K:9:ALY:HB2	2:K:9:ALY:HE2	1.73	0.44
1:F:386:TYR:CZ	1:F:390:ILE:HG13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:358:LYS:HD2	1:G:361:LEU:HD12	2.01	0.43
1:B:394:MET:HG2	1:B:417:ASP:O	2.18	0.43
1:F:354:ASN:O	1:F:358:LYS:HG2	2.18	0.43
1:F:370:TRP:CG	1:F:371:PRO:HD3	2.53	0.43
1:A:361:LEU:HD21	1:A:396:LEU:HB3	2.01	0.43
1:F:409:ARG:N	1:F:413:GLU:OE1	2.26	0.42
1:E:395:ASP:OD2	1:E:397:SER:OG	2.20	0.42
1:A:368:TYR:O	1:A:438:MET:HB3	2.20	0.42
1:H:431:PRO:O	1:H:440:ARG:NH2	2.52	0.42
1:D:349:GLN:HB3	1:D:411:ALA:HB2	2.02	0.42
1:G:426:TYR:CD1	1:G:436:VAL:HG13	2.55	0.41
1:B:370:TRP:CG	1:B:371:PRO:HD3	2.55	0.41
1:H:433:HIS:HB3	1:H:436:VAL:HG23	2.01	0.41
1:E:390:ILE:HD13	1:E:427:LYS:HD2	2.01	0.41
1:D:410:ASP:N	1:D:410:ASP:OD1	2.54	0.41
1:A:433:HIS:CD2	2:K:11:ILE:HG12	2.56	0.41
1:B:402:LYS:HB3	1:B:407:ASP:HB3	2.03	0.41
1:E:426:TYR:HD1	1:E:436:VAL:HG13	1.86	0.41
1:F:389:ILE:HD12	1:F:428:TYR:CE1	2.56	0.41
1:F:395:ASP:OD2	1:F:397:SER:OG	2.23	0.40
1:D:356:ILE:O	1:D:360:LEU:HG	2.21	0.40
1:E:370:TRP:CG	1:E:371:PRO:HD3	2.57	0.40
1:B:374:LYS:HG3	1:D:379:SER:O	2.22	0.40
1:G:419:ARG:NH2	3:G:505:HOH:O	2.53	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	102/109 (94%)	97 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	107/109 (98%)	103 (96%)	4 (4%)	0	100 100
1	C	99/109 (91%)	97 (98%)	2 (2%)	0	100 100
1	D	105/109 (96%)	100 (95%)	4 (4%)	1 (1%)	15 44
1	E	109/109 (100%)	103 (94%)	6 (6%)	0	100 100
1	F	107/109 (98%)	104 (97%)	3 (3%)	0	100 100
1	G	101/109 (93%)	97 (96%)	4 (4%)	0	100 100
1	H	107/109 (98%)	102 (95%)	5 (5%)	0	100 100
2	I	9/13 (69%)	9 (100%)	0	0	100 100
2	J	7/13 (54%)	7 (100%)	0	0	100 100
2	K	8/13 (62%)	8 (100%)	0	0	100 100
2	L	7/13 (54%)	7 (100%)	0	0	100 100
All	All	868/924 (94%)	834 (96%)	33 (4%)	1 (0%)	51 81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	381	LEU

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	91/96 (95%)	90 (99%)	1 (1%)	73 92
1	B	96/96 (100%)	96 (100%)	0	100 100
1	C	88/96 (92%)	88 (100%)	0	100 100
1	D	94/96 (98%)	94 (100%)	0	100 100
1	E	98/96 (102%)	97 (99%)	1 (1%)	76 93
1	F	96/96 (100%)	96 (100%)	0	100 100
1	G	90/96 (94%)	87 (97%)	3 (3%)	38 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	96/96 (100%)	94 (98%)	2 (2%)	53 84
2	I	9/9 (100%)	8 (89%)	1 (11%)	6 19
2	J	7/9 (78%)	5 (71%)	2 (29%)	0 1
2	K	8/9 (89%)	7 (88%)	1 (12%)	4 14
2	L	6/9 (67%)	5 (83%)	1 (17%)	2 6
All	All	779/804 (97%)	767 (98%)	12 (2%)	62 89

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	449	ARG
1	E	412	GLN
1	G	363	LYS
1	G	402	LYS
1	G	405	ASN
1	H	409	ARG
1	H	453	MET
2	I	6	CYS
2	J	1	TRP
2	J	8	ARG
2	K	6	CYS
2	L	1	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	429	ASN
1	H	349	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ALY	K	2	2	10,11,12	0.83	0	7,12,14	0.54	0
2	ALY	K	9	2	10,11,12	0.87	0	7,12,14	0.63	0
2	ALY	L	9	2	10,11,12	0.87	0	7,12,14	0.83	0
2	ALY	J	2	1,2	10,11,12	0.86	0	7,12,14	1.65	1 (14%)
2	ALY	I	2	2	10,11,12	0.87	0	7,12,14	0.77	0
2	ALY	L	2	2	10,11,12	0.86	0	7,12,14	0.99	0
2	ALY	I	9	2	10,11,12	0.86	0	7,12,14	0.70	0
2	ALY	J	9	2	10,11,12	0.83	0	7,12,14	0.92	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
2	ALY	K	2	2	-	1/9/10/12	-
2	ALY	K	9	2	-	1/9/10/12	-
2	ALY	L	9	2	-	2/9/10/12	-
2	ALY	J	2	1,2	-	4/9/10/12	-
2	ALY	I	2	2	-	4/9/10/12	-
2	ALY	L	2	2	-	5/9/10/12	-
2	ALY	I	9	2	-	1/9/10/12	-
2	ALY	J	9	2	-	6/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	2	ALY	CD-CG-CB	-3.90	99.83	113.62

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	2	ALY	N-CA-CB-CG
2	J	2	ALY	C-CA-CB-CG
2	L	2	ALY	N-CA-CB-CG
2	L	2	ALY	C-CA-CB-CG
2	L	2	ALY	O-C-CA-CB
2	J	9	ALY	N-CA-CB-CG
2	J	9	ALY	C-CA-CB-CG
2	J	9	ALY	O-C-CA-CB
2	I	2	ALY	OH-CH-NZ-CE
2	I	2	ALY	CH3-CH-NZ-CE
2	J	2	ALY	OH-CH-NZ-CE
2	J	2	ALY	CH3-CH-NZ-CE
2	L	2	ALY	OH-CH-NZ-CE
2	L	2	ALY	CH3-CH-NZ-CE
2	J	9	ALY	OH-CH-NZ-CE
2	J	9	ALY	CH3-CH-NZ-CE
2	L	9	ALY	OH-CH-NZ-CE
2	L	9	ALY	CH3-CH-NZ-CE
2	I	2	ALY	CG-CD-CE-NZ
2	K	9	ALY	CA-CB-CG-CD
2	I	9	ALY	CA-CB-CG-CD
2	J	9	ALY	CG-CD-CE-NZ
2	I	2	ALY	CE-CD-CG-CB
2	K	2	ALY	CE-CD-CG-CB

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	9	ALY	1	0
2	I	2	ALY	1	0
2	I	9	ALY	1	0
2	J	9	ALY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	104/109 (95%)	0.68	6 (5%) 23 15	32, 57, 80, 99	0
1	B	108/109 (99%)	0.81	10 (9%) 8 4	52, 65, 75, 81	0
1	C	101/109 (92%)	0.78	14 (13%) 2 1	38, 56, 86, 95	0
1	D	107/109 (98%)	1.06	17 (15%) 1 1	55, 74, 90, 108	0
1	E	109/109 (100%)	0.32	2 (1%) 68 61	16, 39, 63, 82	0
1	F	108/109 (99%)	0.41	5 (4%) 32 22	19, 38, 67, 82	0
1	G	102/109 (93%)	1.47	30 (29%) 0 0	53, 72, 94, 103	2 (1%)
1	H	108/109 (99%)	0.75	12 (11%) 5 3	25, 47, 79, 90	0
2	I	10/13 (76%)	0.45	0 100 100	30, 35, 50, 62	0
2	J	8/13 (61%)	0.49	0 100 100	54, 56, 62, 63	0
2	K	9/13 (69%)	0.30	0 100 100	43, 49, 64, 65	0
2	L	7/13 (53%)	0.60	1 (14%) 2 1	54, 62, 70, 73	0
All	All	881/924 (95%)	0.77	97 (11%) 5 3	16, 59, 87, 108	2 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	399	VAL	4.4
1	G	357	LEU	4.3
1	G	401	ARG	4.2
1	G	412	GLN	4.0
1	G	452	LYS	3.9
1	G	353	CYS	3.9
1	G	444	ASP	3.8
1	F	347	SER	3.8
1	C	413	GLU	3.8
1	G	411	ALA	3.7
1	D	350	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	398	THR	3.7
1	A	353	CYS	3.6
1	A	354	ASN	3.6
1	D	418	VAL	3.6
1	G	453	MET	3.6
1	G	355	GLY	3.6
1	D	417	ASP	3.4
1	H	363	LYS	3.4
1	D	409	ARG	3.4
1	H	346	SER	3.4
1	G	420	LEU	3.4
1	E	347	SER	3.4
1	F	346	SER	3.3
1	B	388	ASP	3.3
1	H	412	GLN	3.2
1	A	384	HIS	3.2
1	G	356	ILE	3.2
1	G	371	PRO	3.2
1	B	348	GLU	3.1
1	C	355	GLY	3.1
1	D	358	LYS	3.1
1	G	359	GLU	3.1
1	G	369	ALA	3.1
1	H	350	LEU	3.1
1	C	404	GLU	3.1
1	F	352	HIS	3.0
1	D	448	PHE	3.0
1	D	349	GLN	3.0
1	B	346	SER	2.9
1	B	379[A]	SER	2.9
1	G	403	MET	2.9
1	C	408	TYR	2.9
1	C	412	GLN	2.9
1	D	394	MET	2.8
1	A	453	MET	2.8
1	H	352	HIS	2.8
1	D	404	GLU	2.8
1	G	396	LEU	2.8
1	C	411	ALA	2.8
1	G	413	GLU	2.8
1	G	426	TYR	2.8
1	C	381	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	416	ALA	2.7
1	C	368	TYR	2.7
1	D	386	TYR	2.7
1	F	382	GLY	2.7
1	G	414	PHE	2.7
1	G	436	VAL	2.6
1	D	381	LEU	2.6
1	G	415	ALA	2.6
1	D	370	TRP	2.6
1	H	453	MET	2.5
1	C	360	LEU	2.5
1	C	448	PHE	2.5
1	C	352	HIS	2.4
1	E	385	ASP	2.4
1	B	412	GLN	2.4
1	G	406	ARG	2.4
1	H	451	ALA	2.4
1	C	401	ARG	2.3
1	H	448	PHE	2.3
1	D	450	TYR	2.3
1	G	454	PRO	2.3
1	B	428	TYR	2.3
1	H	366	ALA	2.3
1	H	438	MET	2.3
1	B	350	LEU	2.3
1	F	348	GLU	2.3
1	A	406	ARG	2.2
1	H	452	LYS	2.2
1	D	411	ALA	2.2
1	C	357	LEU	2.2
1	D	347	SER	2.2
1	B	347	SER	2.1
1	G	410	ASP	2.1
1	D	373	TYR	2.1
1	G	372	PHE	2.1
1	D	348	GLU	2.1
1	G	362	SER	2.1
1	B	383	LEU	2.1
1	H	349	GLN	2.1
1	G	448	PHE	2.1
1	A	412	GLN	2.1
1	C	351	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	1	TRP	2.0
1	B	384	HIS	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. 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
2	ALY	J	2	12/13	0.80	0.29	50,56,67,80	0
2	ALY	L	2	12/13	0.84	0.26	54,57,64,75	0
2	ALY	L	9	12/13	0.86	0.30	15,36,59,63	0
2	ALY	J	9	12/13	0.87	0.27	51,53,55,66	0
2	ALY	I	2	12/13	0.90	0.23	23,37,54,62	0
2	ALY	K	9	12/13	0.91	0.21	39,47,54,58	0
2	ALY	K	2	12/13	0.92	0.28	37,39,63,79	0
2	ALY	I	9	12/13	0.94	0.17	23,24,44,58	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.