Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2017 – 11:02 AM EST

PDB ID	:	5LQF
Title	:	CDK1/CyclinB1/CKS2 in complex with NU6102
Authors	:	Coxon, C.R.; Anscombe, E.; Harnor, S.J.; Martin, M.P.; Carbain, B.J.; Hardcastle, I.R.; Harlow, L.K.; Korolchuk, S.; Matheson, C.J.; Noble, M.E.; Newell, D.R.; Turner, D.M.; Sivaprakasam, M.; Wang, L.Z.; Wong, C.; Golding, B.T.; Griffin, R.J.; Endicott, J.A.; Cano, C.
Deposited on	:	2016-08-17
Resolution	:	2.06 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:

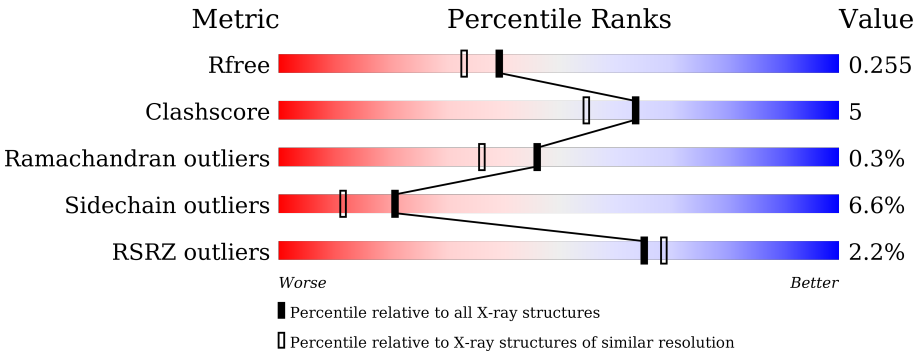
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance

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

The reported resolution of this entry is 2.06 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	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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	302	80% 14% • 5%
1	D	302	77% 15% • 6%
2	B	273	81% 14% • •
2	E	273	77% 17% • •
3	C	84	6% 74% 10% 5% 12%
3	F	84	14% 62% 20% 6% 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10580 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 Cyclin-dependent kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	1	0
			2319	1495	392	424	8			
1	D	285	Total	C	N	O	S	0	1	0
			2304	1485	391	420	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P06493
A	-3	PRO	-	expression tag	UNP P06493
A	-2	LEU	-	expression tag	UNP P06493
A	-1	GLY	-	expression tag	UNP P06493
A	0	SER	-	expression tag	UNP P06493
D	-4	GLY	-	expression tag	UNP P06493
D	-3	PRO	-	expression tag	UNP P06493
D	-2	LEU	-	expression tag	UNP P06493
D	-1	GLY	-	expression tag	UNP P06493
D	0	SER	-	expression tag	UNP P06493

- Molecule 2 is a protein called G2/mitotic-specific cyclin-B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	264	Total	C	N	O	S	0	1	0
			2144	1382	360	386	16			
2	E	264	Total	C	N	O	S	0	1	0
			2144	1382	360	386	16			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	161	GLY	-	expression tag	UNP P14635
B	162	SER	-	expression tag	UNP P14635

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	163	HIS	-	expression tag	UNP P14635
B	164	MET	-	expression tag	UNP P14635
B	167	SER	CYS	conflict	UNP P14635
B	238	SER	CYS	conflict	UNP P14635
B	350	SER	CYS	conflict	UNP P14635
E	161	GLY	-	expression tag	UNP P14635
E	162	SER	-	expression tag	UNP P14635
E	163	HIS	-	expression tag	UNP P14635
E	164	MET	-	expression tag	UNP P14635
E	167	SER	CYS	conflict	UNP P14635
E	238	SER	CYS	conflict	UNP P14635
E	350	SER	CYS	conflict	UNP P14635

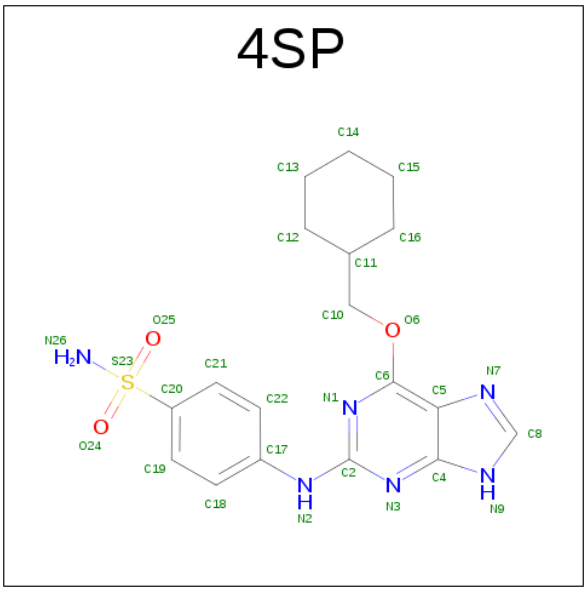
- Molecule 3 is a protein called Cyclin-dependent kinases regulatory subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	74	Total	C	N	O	S	0	1	0
			661	428	117	112	4			
3	F	74	Total	C	N	O	S	0	1	0
			661	428	117	112	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP P33552
C	-3	PRO	-	expression tag	UNP P33552
C	-2	LEU	-	expression tag	UNP P33552
C	-1	GLY	-	expression tag	UNP P33552
C	0	SER	-	expression tag	UNP P33552
F	-4	GLY	-	expression tag	UNP P33552
F	-3	PRO	-	expression tag	UNP P33552
F	-2	LEU	-	expression tag	UNP P33552
F	-1	GLY	-	expression tag	UNP P33552
F	0	SER	-	expression tag	UNP P33552

- Molecule 4 is O6-CYCLOHEXYLMETHOXY-2-(4'-SULPHAMOYLANILINO) PURINE (three-letter code: 4SP) (formula: $C_{18}H_{22}N_6O_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 28 18 6 3 1	0	0
4	D	1	Total C N O S 28 18 6 3 1	0	0

- Molecule 5 is water.

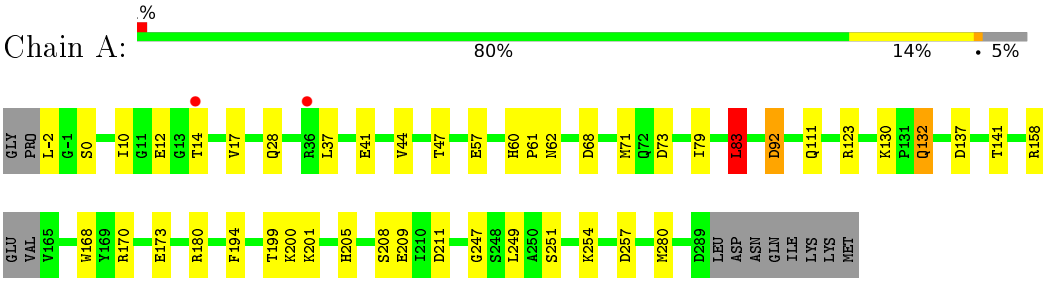
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	54	Total O 54 54	0	0
5	B	72	Total O 72 72	0	0
5	C	22	Total O 22 22	0	0
5	D	53	Total O 53 53	0	0
5	E	79	Total O 79 79	0	0
5	F	11	Total O 11 11	0	0

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.

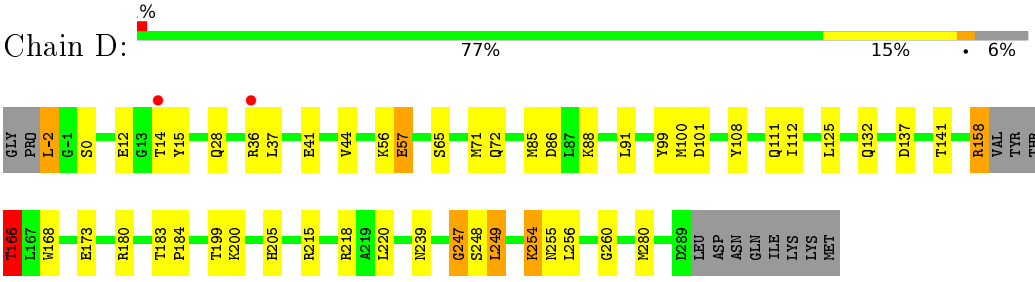
- Molecule 1: Cyclin-dependent kinase 1

Chain A:



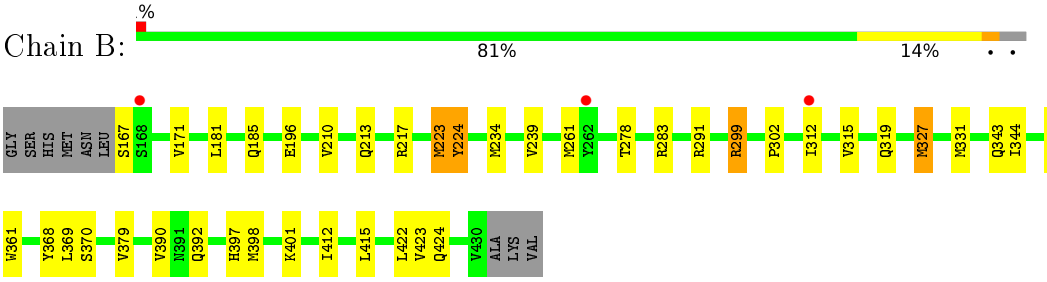
- Molecule 1: Cyclin-dependent kinase 1

Chain D:



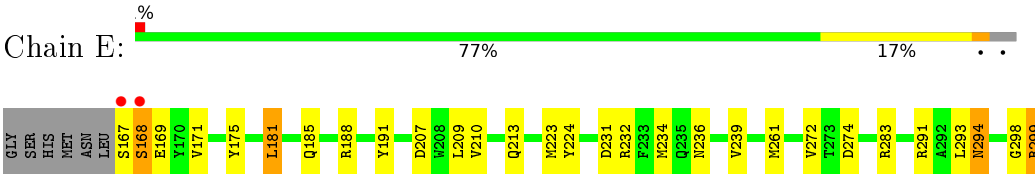
- Molecule 2: G2/mitotic-specific cyclin-B1

Chain B:

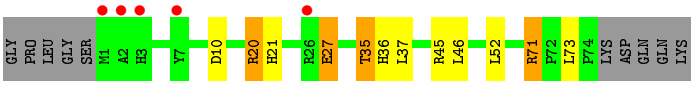


- Molecule 2: G2/mitotic-specific cyclin-B1

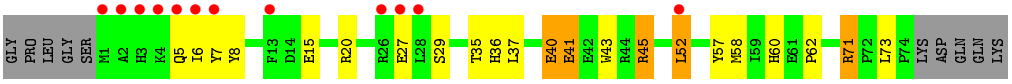
Chain E:



• Molecule 3: Cyclin-dependent kinases regulatory subunit 2



• Molecule 3: Cyclin-dependent kinases regulatory subunit 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	65.04Å 67.75Å 85.06Å 103.88° 90.89° 90.42°	Depositor
Resolution (Å)	65.70 – 2.06 65.77 – 2.06	Depositor EDS
% Data completeness (in resolution range)	97.3 (65.70-2.06) 89.7 (65.77-2.06)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.198 , 0.254 0.203 , 0.255	Depositor DCC
R_{free} test set	4136 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10580	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: 4SP

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	1.06	1/2371 (0.0%)	1.15	8/3204 (0.2%)
1	D	1.05	1/2359 (0.0%)	1.10	6/3186 (0.2%)
2	B	1.16	2/2189 (0.1%)	1.13	11/2960 (0.4%)
2	E	1.12	2/2189 (0.1%)	1.17	13/2960 (0.4%)
3	C	1.05	0/685	1.17	3/926 (0.3%)
3	F	0.95	1/685 (0.1%)	1.06	4/926 (0.4%)
All	All	1.09	7/10478 (0.1%)	1.14	45/14162 (0.3%)

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	A	0	1
1	D	0	3
3	F	0	1
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	GLU	CD-OE1	9.19	1.35	1.25
2	B	224	TYR	CD2-CE2	7.45	1.50	1.39
3	F	40	GLU	CD-OE2	6.37	1.32	1.25
2	E	316	ASP	CA-CB	6.05	1.67	1.53
2	B	196	GLU	CD-OE2	5.79	1.32	1.25
2	E	373	GLU	CD-OE2	5.55	1.31	1.25
1	D	57	GLU	CG-CD	5.15	1.59	1.51

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	316	ASP	CB-CG-OD2	10.96	128.16	118.30
2	E	316	ASP	CB-CG-OD1	-10.25	109.08	118.30
2	E	331	MET	CG-SD-CE	-9.00	85.80	100.20
2	B	291	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	A	247	GLY	N-CA-C	-8.30	92.35	113.10
2	B	398	MET	CG-SD-CE	-8.21	87.07	100.20
2	B	217	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	D	215	ARG	NE-CZ-NH2	-7.95	116.32	120.30
2	E	299	ARG	NE-CZ-NH1	7.82	124.21	120.30
3	C	10	ASP	CB-CG-OD1	7.34	124.91	118.30
2	E	327	MET	CG-SD-CE	-7.27	88.57	100.20
2	E	335	ASP	CB-CG-OD1	6.88	124.49	118.30
3	F	20	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	123	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	257	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	194	PHE	CB-CG-CD1	6.21	125.14	120.80
1	D	247	GLY	N-CA-C	-6.21	97.58	113.10
2	B	291	ARG	NE-CZ-NH1	6.17	123.38	120.30
2	E	181	LEU	CA-CB-CG	6.12	129.39	115.30
1	A	92	ASP	CB-CG-OD2	-5.85	113.04	118.30
3	C	71	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	B	299	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	B	415	LEU	CB-CG-CD1	-5.58	101.51	111.00
2	B	291	ARG	CG-CD-NE	-5.58	100.08	111.80
1	D	-2	LEU	CA-CB-CG	5.58	128.14	115.30
2	E	398	MET	CG-SD-CE	-5.55	91.32	100.20
2	B	327	MET	CG-SD-CE	-5.53	91.35	100.20
3	F	45	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	218	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	83	LEU	CA-CB-CG	-5.45	102.78	115.30
3	F	52	LEU	CA-CB-CG	5.42	127.76	115.30
2	E	291	ARG	NE-CZ-NH2	-5.37	117.61	120.30
3	C	45	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	D	85	MET	CG-SD-CE	5.35	108.75	100.20
2	E	353	LEU	CA-CB-CG	5.34	127.58	115.30
1	D	86	ASP	CB-CG-OD2	-5.33	113.50	118.30
2	B	223	MET	CG-SD-CE	-5.27	91.77	100.20
1	A	173	GLU	CB-CA-C	-5.27	99.87	110.40
1	A	211	ASP	CB-CG-OD2	-5.22	113.60	118.30
2	B	415	LEU	CB-CG-CD2	5.18	119.81	111.00
2	E	299	ARG	NE-CZ-NH2	-5.11	117.75	120.30
3	F	71	ARG	NE-CZ-NH1	5.10	122.85	120.30
2	E	299	ARG	CD-NE-CZ	5.09	130.73	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	232	ARG	NE-CZ-NH2	-5.05	117.77	120.30
2	B	217	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	GLU	Peptide
1	D	12	GLU	Peptide
1	D	166	THR	Peptide
1	D	247	GLY	Peptide
3	F	5	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2319	0	2358	13	0
1	D	2304	0	2346	20	0
2	B	2144	0	2191	31	0
2	E	2144	0	2191	36	0
3	C	661	0	639	5	0
3	F	661	0	639	6	0
4	A	28	0	22	0	0
4	D	28	0	22	0	0
5	A	54	0	0	0	0
5	B	72	0	0	1	0
5	C	22	0	0	0	2
5	D	53	0	0	4	1
5	E	79	0	0	4	2
5	F	11	0	0	0	1
All	All	10580	0	10408	108	3

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 (108) 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:B:210:VAL:HA	2:B:223:MET:HE1	1.47	0.96
1:D:41:GLU:O	2:E:283:ARG:NH1	2.03	0.91
2:E:327:MET:HE3	2:E:344:ILE:HG22	1.55	0.87
2:E:234:MET:CE	2:E:239:VAL:HB	2.14	0.78
3:C:27[B]:GLU:O	3:C:27[B]:GLU:HG2	1.85	0.75
2:B:213:GLN:HB2	2:B:223:MET:HE2	1.71	0.72
1:D:57:GLU:OE1	5:D:401:HOH:O	2.08	0.71
2:B:210:VAL:HA	2:B:223:MET:CE	2.20	0.71
2:B:213:GLN:CB	2:B:223:MET:HE2	2.22	0.69
2:B:234:MET:HE2	2:B:239:VAL:HB	1.74	0.69
2:E:213:GLN:HB2	2:E:223:MET:HE2	1.74	0.69
2:B:224:TYR:CE1	2:B:331:MET:HE3	2.28	0.68
2:B:234:MET:CE	2:B:239:VAL:HB	2.24	0.67
2:E:224:TYR:CD1	2:E:331:MET:HE2	2.29	0.66
2:E:224:TYR:CD1	2:E:331:MET:CE	2.79	0.66
2:B:302:PRO:HB3	2:B:327:MET:CE	2.26	0.66
2:B:302:PRO:HB3	2:B:327:MET:HE2	1.78	0.64
1:D:44:VAL:HG22	1:D:71:MET:HE1	1.79	0.64
2:B:343:GLN:HG2	2:B:379:VAL:HG21	1.80	0.64
2:B:392:GLN:HE22	2:B:424:GLN:HE22	1.46	0.62
1:A:111:GLN:HE22	1:A:141:THR:HA	1.64	0.61
2:E:213:GLN:HB2	2:E:223:MET:CE	2.31	0.60
2:E:392:GLN:HE22	2:E:424:GLN:HE22	1.48	0.60
2:B:224:TYR:CD1	2:B:331:MET:CE	2.86	0.58
2:E:234:MET:HE2	2:E:239:VAL:HB	1.85	0.57
2:E:314:GLU:HG2	5:E:575:HOH:O	2.03	0.57
3:C:36:HIS:HD2	3:C:37:LEU:O	1.88	0.56
3:F:40:GLU:HG3	3:F:43:TRP:CZ2	2.40	0.56
2:B:327:MET:HE3	2:B:344:ILE:HG22	1.87	0.56
1:D:166:THR:HG22	5:D:404:HOH:O	2.05	0.56
1:D:220:LEU:HD21	1:D:249:LEU:HD11	1.89	0.55
1:A:62:ASN:HD21	1:A:111:GLN:HE21	1.55	0.54
2:E:310:SER:O	2:E:313:GLY:O	2.26	0.54
2:B:224:TYR:CD1	2:B:331:MET:HE3	2.44	0.53
2:E:224:TYR:CE1	2:E:331:MET:HE3	2.44	0.53
3:F:41:GLU:OE1	3:F:45:ARG:NH1	2.37	0.53
2:E:224:TYR:CE1	2:E:331:MET:CE	2.92	0.53
2:B:185:GLN:HE22	2:B:299:ARG:H	1.57	0.53
2:B:210:VAL:HG22	2:B:223:MET:HE3	1.90	0.52
1:D:111:GLN:HE22	1:D:141:THR:HA	1.74	0.52
1:D:168:TRP:CD1	1:D:205:HIS:HA	2.45	0.52
1:D:256:LEU:HD22	1:D:260:GLY:HA3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:TYR:CD1	2:B:331:MET:HE2	2.45	0.52
3:C:35:THR:HG22	3:C:36:HIS:ND1	2.24	0.52
2:E:343:GLN:HG2	2:E:379:VAL:HG21	1.92	0.52
5:D:401:HOH:O	2:E:299:ARG:NH2	2.44	0.51
2:B:355:ILE:HD11	2:B:423:VAL:CG2	2.40	0.51
2:B:312:ILE:HD13	2:B:368:TYR:HB3	1.94	0.49
1:A:130:LYS:NZ	1:A:132[A]:GLN:HE21	2.11	0.49
2:B:397:HIS:HD2	5:B:561:HOH:O	1.95	0.49
2:B:210:VAL:CA	2:B:223:MET:HE1	2.30	0.49
2:E:391:ASN:HD22	2:E:419:ASN:ND2	2.10	0.49
2:E:397:HIS:HD2	5:E:569:HOH:O	1.94	0.49
1:A:199:THR:O	1:A:200:LYS:HB2	2.13	0.48
1:A:41:GLU:O	2:B:283:ARG:HD3	2.13	0.48
1:D:91:LEU:HD21	1:D:100:MET:CE	2.44	0.48
1:A:168:TRP:CD1	1:A:205:HIS:HA	2.49	0.47
1:A:180:ARG:HG3	1:A:180:ARG:O	2.14	0.47
2:B:315:VAL:HG11	2:B:319:GLN:HG2	1.96	0.47
2:E:188:ARG:HH12	2:E:236:ASN:ND2	2.12	0.47
2:E:391:ASN:HD22	2:E:419:ASN:HD21	1.62	0.47
1:A:62:ASN:ND2	1:A:111:GLN:HE21	2.12	0.46
1:D:125:LEU:CD2	1:D:183:THR:HA	2.45	0.46
2:E:210:VAL:HA	2:E:223:MET:HE3	1.98	0.46
2:B:390:VAL:HB	2:B:401:LYS:HD2	1.97	0.46
2:E:185:GLN:HE22	2:E:299:ARG:H	1.64	0.46
2:E:175[B]:TYR:OH	5:E:501:HOH:O	2.21	0.46
1:D:108:TYR:O	1:D:112:ILE:HG13	2.17	0.45
2:E:234:MET:HE3	2:E:239:VAL:HB	1.93	0.45
2:E:401:LYS:HE2	5:E:523:HOH:O	2.16	0.45
1:D:125:LEU:HD21	1:D:183:THR:HA	1.99	0.44
1:D:199:THR:O	1:D:200:LYS:HB2	2.17	0.44
2:E:213:GLN:CB	2:E:223:MET:HE2	2.44	0.44
2:E:327:MET:CE	2:E:344:ILE:HG22	2.37	0.44
3:F:6:ILE:HG22	3:F:8:TYR:CE1	2.53	0.44
2:B:412:ILE:HD12	2:B:412:ILE:HA	1.90	0.43
1:D:183:THR:N	1:D:184:PRO:CD	2.81	0.43
1:A:47:THR:HG21	1:A:158:ARG:NH1	2.33	0.43
1:D:91:LEU:HA	1:D:91:LEU:HD23	1.82	0.43
1:D:15:TYR:CZ	1:D:158:ARG:HD3	2.52	0.43
3:F:57:TYR:CE2	3:F:58:MET:HG2	2.54	0.43
2:B:312:ILE:HD13	2:B:368:TYR:CB	2.47	0.43
1:D:56:LYS:HE2	2:E:294:ASN:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:MET:HE3	2:B:344:ILE:CG2	2.48	0.43
2:E:188:ARG:HH12	2:E:236:ASN:HD21	1.67	0.43
1:D:137:ASP:OD1	1:D:137:ASP:C	2.57	0.43
3:F:60:HIS:CD2	3:F:62:PRO:HD2	2.53	0.43
1:D:99:TYR:OH	1:D:254:LYS:NZ	2.51	0.43
3:C:37:LEU:HD23	3:C:37:LEU:HA	1.79	0.42
1:A:83:LEU:HD23	1:A:137:ASP:HB3	2.02	0.42
2:B:302:PRO:HB3	2:B:327:MET:HE1	2.01	0.42
2:E:209:LEU:O	2:E:223:MET:HE1	2.19	0.42
3:C:20:ARG:HG3	3:C:21:HIS:N	2.34	0.42
2:B:223:MET:HG3	2:B:331:MET:HE1	2.02	0.42
3:F:36:HIS:HD2	3:F:37:LEU:O	2.02	0.42
1:A:68:ASP:HB3	1:A:79:ILE:HB	2.02	0.42
1:A:44:VAL:HG22	1:A:71:MET:HE1	2.02	0.42
1:D:91:LEU:HD21	1:D:100:MET:HE3	2.01	0.42
2:B:361:TRP:CH2	2:B:369:LEU:HD12	2.55	0.41
2:E:185:GLN:NE2	2:E:298:GLY:HA3	2.35	0.41
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.55	0.41
2:E:207:ASP:HB2	2:E:332:LEU:HD21	2.03	0.41
2:E:213:GLN:CB	2:E:223:MET:CE	2.99	0.41
2:E:224:TYR:CE1	2:E:331:MET:HE2	2.55	0.41
2:B:234:MET:HE3	2:B:239:VAL:HB	2.03	0.40
2:E:168:SER:O	2:E:171:VAL:HG23	2.22	0.40
2:E:191:TYR:OH	2:E:231:ASP:OD1	2.34	0.40
5:D:401:HOH:O	2:E:299:ARG:NE	2.53	0.40

All (3) 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)
5:C:116:HOH:O	5:F:108:HOH:O[1_654]	1.63	0.57
5:C:110:HOH:O	5:E:535:HOH:O[1_565]	2.01	0.19
5:D:443:HOH:O	5:E:557:HOH:O[1_455]	2.07	0.13

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	284/302 (94%)	270 (95%)	13 (5%)	1 (0%)	39 28
1	D	282/302 (93%)	268 (95%)	14 (5%)	0	100 100
2	B	263/273 (96%)	254 (97%)	8 (3%)	1 (0%)	39 28
2	E	263/273 (96%)	255 (97%)	7 (3%)	1 (0%)	39 28
3	C	73/84 (87%)	67 (92%)	6 (8%)	0	100 100
3	F	73/84 (87%)	67 (92%)	5 (7%)	1 (1%)	14 4
All	All	1238/1318 (94%)	1181 (95%)	53 (4%)	4 (0%)	46 36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	358	ASN
3	F	15	GLU
2	B	358	ASN
1	A	208	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	257/270 (95%)	238 (93%)	19 (7%)	17 8
1	D	255/270 (94%)	234 (92%)	21 (8%)	14 6
2	B	236/242 (98%)	228 (97%)	8 (3%)	44 37
2	E	236/242 (98%)	224 (95%)	12 (5%)	29 19
3	C	72/79 (91%)	64 (89%)	8 (11%)	8 2
3	F	72/79 (91%)	63 (88%)	9 (12%)	6 1
All	All	1128/1182 (95%)	1051 (93%)	77 (7%)	21 11

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	LEU
1	A	0	SER
1	A	10	ILE
1	A	14	THR
1	A	17	VAL
1	A	28	GLN
1	A	37	LEU
1	A	57	GLU
1	A	73	ASP
1	A	83	LEU
1	A	92	ASP
1	A	132[A]	GLN
1	A	132[B]	GLN
1	A	170	ARG
1	A	201	LYS
1	A	249	LEU
1	A	251	SER
1	A	254	LYS
1	A	280	MET
2	B	167	SER
2	B	171	VAL
2	B	181	LEU
2	B	261	MET
2	B	278	THR
2	B	358	ASN
2	B	370	SER
2	B	422	LEU
3	C	20	ARG
3	C	27[A]	GLU
3	C	27[B]	GLU
3	C	35	THR
3	C	46	LEU
3	C	52	LEU
3	C	71	ARG
3	C	73	LEU
1	D	-2	LEU
1	D	0	SER
1	D	14	THR
1	D	28	GLN
1	D	36	ARG
1	D	37	LEU
1	D	65	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	72	GLN
1	D	88	LYS
1	D	101	ASP
1	D	132	GLN
1	D	158	ARG
1	D	166	THR
1	D	173	GLU
1	D	180	ARG
1	D	239	ASN
1	D	248	SER
1	D	249	LEU
1	D	254	LYS
1	D	255	ASN
1	D	280	MET
2	E	167	SER
2	E	168	SER
2	E	169	GLU
2	E	181	LEU
2	E	261	MET
2	E	272	VAL
2	E	274	ASP
2	E	293	LEU
2	E	294	ASN
2	E	311	LYS
2	E	396	LYS
2	E	422	LEU
3	F	7	TYR
3	F	27[A]	GLU
3	F	27[B]	GLU
3	F	29	SER
3	F	35	THR
3	F	41	GLU
3	F	52	LEU
3	F	71	ARG
3	F	73	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	111	GLN
1	A	255	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	185	GLN
2	B	200	ASN
2	B	236	ASN
2	B	304	HIS
2	B	397	HIS
2	B	419	ASN
2	B	424	GLN
3	C	36	HIS
3	C	49	GLN
1	D	67	GLN
1	D	111	GLN
2	E	185	GLN
2	E	211	GLN
2	E	236	ASN
2	E	392	GLN
2	E	397	HIS
2	E	419	ASN
3	F	36	HIS

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

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	$\#\|Z\| > 2$
4	4SP	A	301	-	28,31,31	0.62	1 (3%)	36,44,44	1.17	4 (11%)
4	4SP	D	301	-	28,31,31	0.47	0	36,44,44	1.12	4 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	4SP	A	301	-	-	0/15/23/23	0/4/4/4
4	4SP	D	301	-	-	0/15/23/23	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	4SP	O6-C6	-2.24	1.33	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	301	4SP	C5-C6-N1	-3.26	119.72	124.09
4	D	301	4SP	C5-C6-N1	-2.94	120.15	124.09
4	A	301	4SP	C5-C4-N9	-2.90	105.97	111.12
4	D	301	4SP	C5-C4-N9	-2.72	106.29	111.12
4	A	301	4SP	O25-S23-O24	2.41	122.11	118.87
4	D	301	4SP	O6-C6-C5	2.47	119.45	115.67
4	A	301	4SP	C2-N1-C6	2.95	119.39	115.25
4	D	301	4SP	C2-N1-C6	3.07	119.56	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	287/302 (95%)	-0.18	2 (0%) 89 90	30, 44, 64, 78	0
1	D	285/302 (94%)	-0.10	2 (0%) 89 90	32, 46, 70, 82	0
2	B	264/273 (96%)	-0.11	4 (1%) 76 79	30, 41, 60, 71	0
2	E	264/273 (96%)	-0.11	2 (0%) 87 89	29, 41, 63, 71	0
3	C	74/84 (88%)	0.37	5 (6%) 20 22	36, 52, 82, 108	0
3	F	74/84 (88%)	0.96	12 (16%) 3 2	41, 67, 106, 129	0
All	All	1248/1318 (94%)	-0.03	27 (2%) 65 69	29, 44, 70, 129	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	1	MET	13.4
3	C	2	ALA	12.2
3	F	3	HIS	12.1
3	F	2	ALA	11.0
3	C	3	HIS	8.8
3	C	1	MET	8.4
3	F	27[A]	GLU	5.8
1	D	14	THR	3.5
2	B	358	ASN	3.5
3	F	7	TYR	3.4
3	F	26	ARG	3.2
2	E	168	SER	3.0
3	F	4	LYS	2.9
1	D	36	ARG	2.9
2	B	168	SER	2.7
1	A	14	THR	2.6
2	E	167	SER	2.5
3	F	28	LEU	2.4
3	C	7	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	26	ARG	2.3
3	F	13	PHE	2.2
3	F	6	ILE	2.2
3	F	5	GLN	2.2
1	A	36	ARG	2.2
2	B	262	TYR	2.2
3	F	52	LEU	2.1
2	B	312	ILE	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
4	4SP	D	301	28/28	0.92	0.12	0.21	37,48,54,56	0
4	4SP	A	301	28/28	0.94	0.12	0.09	34,46,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.