Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 11:18 AM EDT

PDB ID	:	5VZU
Title	:	Crystal structure of the Skp1-FBXO31-cyclin D1 complex
Authors	:	Li, Y.; Jin, K.; Hao, B.
Deposited on	:	2017-05-29
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

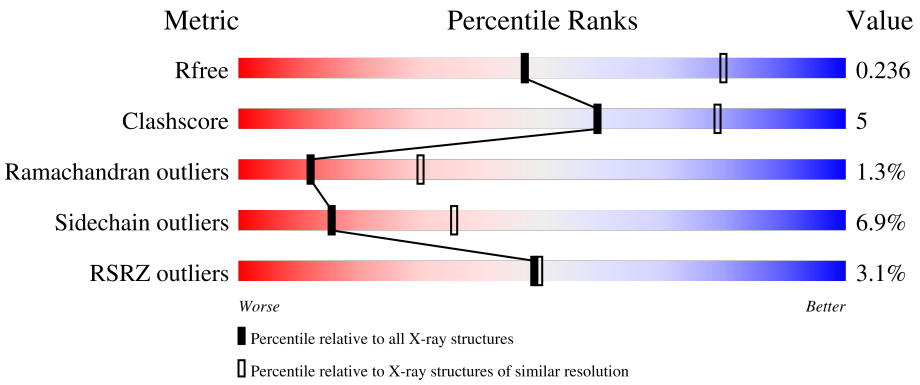
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	149	84% 12% • •
1	C	149	10% 82% 13% • •
2	B	488	% 68% 15% • 14%
2	D	488	3% 74% 10% • 15%
3	E	17	6% 35% 12% 6% 47%

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Mol	Chain	Length	Quality of chain
3	F	17	6% 29% 6% 65%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9361 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 S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	145	1149	729	186	228	6	0	0	0
			Total	C	N	O	S			
1	C	143	1137	722	184	225	6	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1002	ALA	PRO	engineered mutation	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	GLU	deletion	UNP P63208
A	?	-	GLY	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	PRO	deletion	UNP P63208
A	?	-	PRO	deletion	UNP P63208
A	?	-	PRO	deletion	UNP P63208
A	?	-	GLU	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	GLU	deletion	UNP P63208
A	?	-	ASN	deletion	UNP P63208
A	1078	GLY	LYS	see remark 999	UNP P63208
A	1079	GLY	GLU	see remark 999	UNP P63208
A	1080	SER	LYS	see remark 999	UNP P63208
A	1081	GLY	ARG	see remark 999	UNP P63208
C	1002	ALA	PRO	engineered mutation	UNP P63208
C	?	-	ASP	deletion	UNP P63208
C	?	-	GLU	deletion	UNP P63208
C	?	-	GLY	deletion	UNP P63208
C	?	-	ASP	deletion	UNP P63208
C	?	-	ASP	deletion	UNP P63208

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASP	deletion	UNP P63208
C	?	-	PRO	deletion	UNP P63208
C	?	-	PRO	deletion	UNP P63208
C	?	-	PRO	deletion	UNP P63208
C	?	-	GLU	deletion	UNP P63208
C	?	-	ASP	deletion	UNP P63208
C	?	-	ASP	deletion	UNP P63208
C	?	-	GLU	deletion	UNP P63208
C	?	-	ASN	deletion	UNP P63208
C	1078	GLY	LYS	see remark 999	UNP P63208
C	1079	GLY	GLU	see remark 999	UNP P63208
C	1080	SER	LYS	see remark 999	UNP P63208
C	1081	GLY	ARG	see remark 999	UNP P63208

- Molecule 2 is a protein called F-box only protein 31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	418	3437	2186	619	611	21	0	6	0
			Total	C	N	O	S			
2	D	417	3402	2168	611	602	21	0	2	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	52	MET	-	expression tag	UNP Q5XUX0
B	53	ALA	-	expression tag	UNP Q5XUX0
B	54	SER	-	expression tag	UNP Q5XUX0
B	55	TRP	-	expression tag	UNP Q5XUX0
B	56	SER	-	expression tag	UNP Q5XUX0
B	57	HIS	-	expression tag	UNP Q5XUX0
B	58	PRO	-	expression tag	UNP Q5XUX0
B	59	GLN	-	expression tag	UNP Q5XUX0
B	60	PHE	-	expression tag	UNP Q5XUX0
B	61	GLU	-	expression tag	UNP Q5XUX0
B	62	LYS	-	expression tag	UNP Q5XUX0
B	63	SER	-	expression tag	UNP Q5XUX0
B	64	GLY	-	expression tag	UNP Q5XUX0
B	65	ARG	-	expression tag	UNP Q5XUX0
D	52	MET	-	expression tag	UNP Q5XUX0
D	53	ALA	-	expression tag	UNP Q5XUX0
D	54	SER	-	expression tag	UNP Q5XUX0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	55	TRP	-	expression tag	UNP Q5XUX0
D	56	SER	-	expression tag	UNP Q5XUX0
D	57	HIS	-	expression tag	UNP Q5XUX0
D	58	PRO	-	expression tag	UNP Q5XUX0
D	59	GLN	-	expression tag	UNP Q5XUX0
D	60	PHE	-	expression tag	UNP Q5XUX0
D	61	GLU	-	expression tag	UNP Q5XUX0
D	62	LYS	-	expression tag	UNP Q5XUX0
D	63	SER	-	expression tag	UNP Q5XUX0
D	64	GLY	-	expression tag	UNP Q5XUX0
D	65	ARG	-	expression tag	UNP Q5XUX0

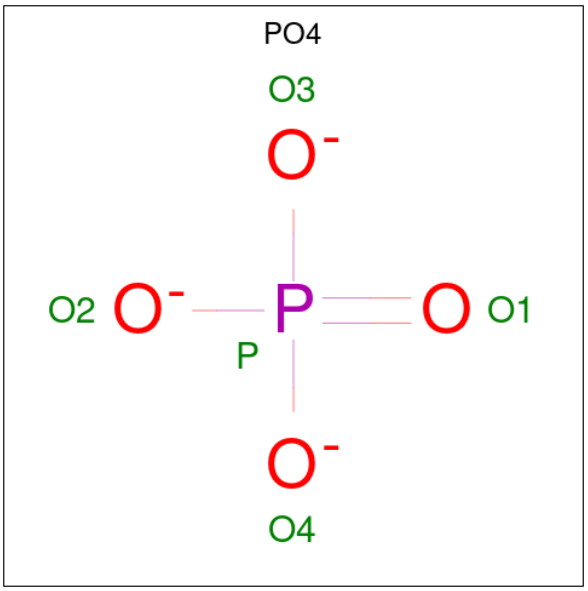
- Molecule 3 is a protein called Cyclin D1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	9	72	43	12	17	0	0	0
3	F	6	50	30	9	11	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	B	1	1	1	0	0
4	D	1	1	1	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O 8 8	0	0
6	B	42	Total O 42 42	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	D	12	12	12	0	0

3 Residue-property plots (i)

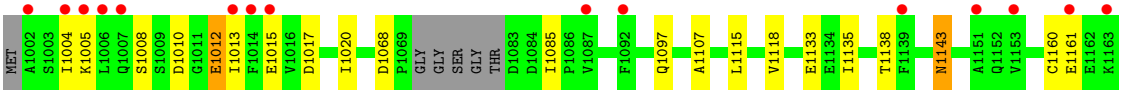
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: S-phase kinase-associated protein 1

Chain A:

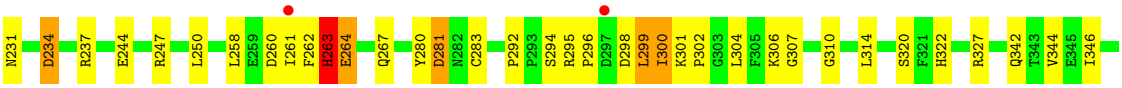
• Molecule 1: S-phase kinase-associated protein 1

Chain C:



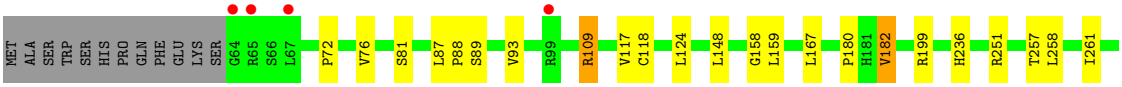
• Molecule 2: F-box only protein 31

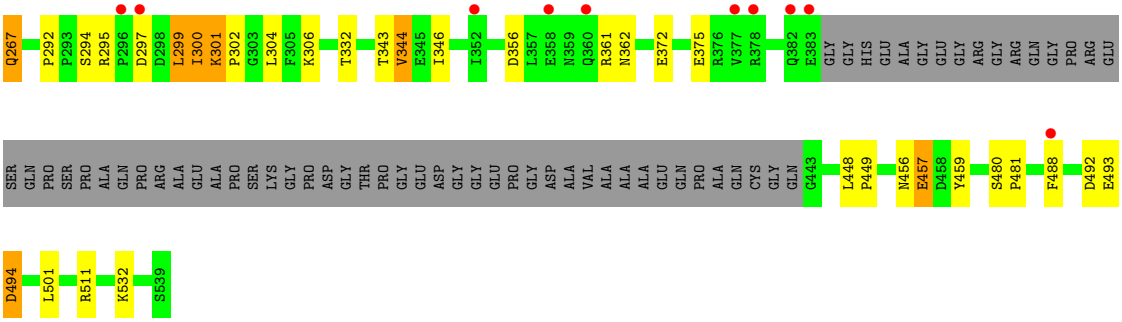
Chain B:



• Molecule 2: F-box only protein 31

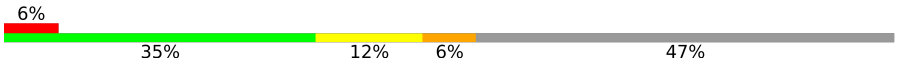
Chain D:

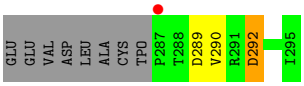




- Molecule 3: Cyclin D1

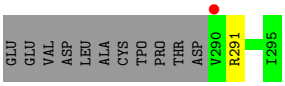
Chain E:





- Molecule 3: Cyclin D1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	87.68Å 156.24Å 155.52Å 90.00° 104.21° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 44.16 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.70) 99.0 (44.16-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.180 , 0.233 0.184 , 0.236	Depositor DCC
R_{free} test set	2674 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	70.2	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9361	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ZN

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	0.59	0/1167	0.73	0/1579
1	C	0.39	0/1155	0.56	0/1563
2	B	0.61	0/3529	0.82	2/4773 (0.0%)
2	D	0.50	0/3492	0.73	1/4724 (0.0%)
3	E	0.63	0/72	0.91	0/96
3	F	0.63	0/49	0.84	0/64
All	All	0.55	0/9464	0.75	3/12799 (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
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	511	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	D	109	ARG	NE-CZ-NH2	-5.50	117.55	120.30
2	B	237	ARG	NE-CZ-NH1	5.35	122.98	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	300	ILE	Peptide
2	D	300	ILE	Peptide

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	1149	0	1141	8	0
1	C	1137	0	1129	11	0
2	B	3437	0	3349	40	0
2	D	3402	0	3334	28	0
3	E	72	0	68	1	0
3	F	50	0	49	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	25	0	0	0	0
5	D	25	0	0	0	0
6	A	8	0	0	1	0
6	B	42	0	0	1	0
6	D	12	0	0	1	0
All	All	9361	0	9070	86	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 (86) 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:182:VAL:O	2:B:306:LYS:HE2	1.76	0.86
2:D:295:ARG:HB2	2:D:299:LEU:HD13	1.64	0.79
1:C:1097:GLN:NE2	1:C:1138:THR:O	2.23	0.72
2:D:258:LEU:HD22	2:D:267:GLN:HB2	1.76	0.68
2:B:295:ARG:HB2	2:B:299:LEU:HD13	1.77	0.67
2:B:295:ARG:N	2:B:299:LEU:HD22	2.12	0.63
2:B:147:GLY:HA2	2:B:518:ASN:HB2	1.80	0.63
2:B:182:VAL:O	2:B:306:LYS:CE	2.46	0.61
2:B:295:ARG:H	2:B:299:LEU:HD22	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1005:LYS:HZ3	1:C:1015:GLU:HG2	1.67	0.60
2:B:120:ASN:OD1	2:B:122:ARG:N	2.35	0.60
1:C:1135:ILE:HG21	2:D:93:VAL:HG21	1.84	0.59
2:D:295:ARG:N	2:D:299:LEU:HD22	2.18	0.59
1:C:1005:LYS:NZ	1:C:1015:GLU:HG2	2.19	0.57
1:A:1153:VAL:HG13	2:B:98:ARG:HD2	1.88	0.56
2:B:494:ASP:HB2	2:B:511:ARG:HB2	1.88	0.55
2:B:261:ILE:O	2:B:263:HIS:N	2.39	0.55
2:B:260:ASP:O	2:B:263:HIS:NE2	2.40	0.55
1:C:1160:CYS:SG	1:C:1161:GLU:N	2.80	0.55
2:D:295:ARG:H	2:D:299:LEU:HD22	1.72	0.54
2:B:310:GLY:HA2	2:B:455:ARG:HD2	1.90	0.54
2:D:494:ASP:HB3	2:D:511:ARG:HE	1.73	0.53
1:C:1143:ASN:C	1:C:1143:ASN:HD22	2.11	0.52
1:A:1082:THR:OG1	1:A:1083:ASP:N	2.43	0.52
2:D:306:LYS:NZ	6:D:701:HOH:O	2.42	0.52
1:A:1002:ALA:C	1:A:1018:VAL:HG23	2.29	0.52
6:A:1203:HOH:O	2:B:95:THR:HB	2.10	0.52
1:A:1023:GLN:NE2	1:A:1062:CYS:O	2.43	0.51
1:C:1107:ALA:HB2	1:C:1115:LEU:HD23	1.93	0.50
2:D:297:ASP:O	2:D:299:LEU:N	2.43	0.50
2:B:494:ASP:HB2	2:B:511:ARG:CB	2.40	0.49
1:C:1133:GLU:H	1:C:1133:GLU:CD	2.15	0.49
2:B:494:ASP:HB3	2:B:511:ARG:HE	1.79	0.48
1:A:1143:ASN:HD22	1:A:1143:ASN:C	2.17	0.48
2:B:173[B]:MET:HG2	2:B:189:LYS:O	2.13	0.48
2:B:110:ARG:NH2	6:B:701:HOH:O	2.32	0.47
2:D:361:ARG:HA	2:D:449:PRO:HA	1.96	0.47
1:A:1004:ILE:HD12	1:A:1004:ILE:C	2.35	0.47
2:B:217[B]:HIS:ND1	2:B:231:ASN:OD1	2.42	0.47
3:E:289:ASP:HA	3:E:292:ASP:OD2	2.15	0.46
2:B:263:HIS:HA	2:B:264:GLU:HB2	1.97	0.46
1:C:1017:ASP:HB3	1:C:1020:ILE:HD12	1.98	0.46
2:B:320:SER:OG	2:B:322:HIS:HE1	1.98	0.46
2:B:473:ILE:O	2:B:481:PRO:HA	2.15	0.46
2:D:299:LEU:HD21	2:D:302:PRO:HD3	1.96	0.46
2:B:354:LEU:HD23	2:B:444:GLN:CG	2.45	0.46
2:B:448:LEU:HD22	2:B:459:TYR:CZ	2.51	0.46
2:D:158:GLY:HA2	2:D:332:THR:HG22	1.97	0.46
2:D:356:ASP:OD1	2:D:356:ASP:C	2.55	0.45
2:B:107:TRP:CE2	2:B:132:ARG:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:346:ILE:HD12	2:D:488:PHE:HB2	1.99	0.45
2:B:298:ASP:O	2:B:299:LEU:HD12	2.17	0.45
2:B:292:PRO:HG2	2:B:302:PRO:HB2	1.98	0.45
2:B:346:ILE:HD12	2:B:488:PHE:HB2	1.99	0.45
2:B:247:ARG:HG2	2:B:258:LEU:HD11	1.99	0.45
2:D:343:THR:HG23	2:D:344:VAL:HB	1.99	0.44
2:B:173[B]:MET:O	2:B:173[B]:MET:HG3	2.17	0.44
2:B:355:PRO:HB2	2:B:359:ASN:HB2	2.00	0.43
2:B:120:ASN:OD1	2:B:120:ASN:C	2.55	0.43
2:B:280:TYR:O	2:B:281:ASP:C	2.56	0.43
2:B:228:THR:O	2:B:283:CYS:HA	2.18	0.43
2:B:298:ASP:O	2:B:299:LEU:CD1	2.66	0.43
2:B:367:SER:HA	2:B:501:LEU:HD11	2.01	0.43
1:A:1002:ALA:O	1:A:1017:ASP:HA	2.19	0.42
2:B:327:ARG:HG3	2:B:342:GLN:HG3	2.01	0.42
1:A:1085:ILE:HG22	1:A:1090:GLN:HG3	2.02	0.42
2:B:307:GLY:O	2:B:314:LEU:HA	2.20	0.42
2:D:72:PRO:O	2:D:76:VAL:HG23	2.19	0.42
2:D:494:ASP:HB3	2:D:511:ARG:NE	2.33	0.42
2:B:111:CYS:HB3	2:B:117:VAL:HG13	2.02	0.42
2:D:148:LEU:HD12	2:D:148:LEU:HA	1.94	0.42
2:D:182:VAL:O	2:D:306:LYS:HE3	2.19	0.42
2:B:188:PHE:CD2	2:B:188:PHE:O	2.72	0.41
2:D:456:ASN:O	2:D:457:GLU:HB2	2.20	0.41
1:C:1004:ILE:O	1:C:1004:ILE:HD12	2.20	0.41
2:B:110:ARG:NE	2:B:110:ARG:HA	2.35	0.41
2:D:292:PRO:HG2	2:D:302:PRO:HB2	2.02	0.41
2:D:448:LEU:HB2	2:D:459:TYR:OH	2.20	0.41
1:C:1008:SER:OG	1:C:1012:GLU:HB2	2.20	0.41
2:D:301:LYS:HB3	2:D:493:GLU:OE1	2.20	0.41
2:D:87:LEU:N	2:D:88:PRO:CD	2.83	0.41
2:D:180:PRO:O	2:D:182:VAL:N	2.53	0.41
2:D:494:ASP:HB2	2:D:511:ARG:CB	2.51	0.41
2:D:236:HIS:CD2	2:D:236:HIS:N	2.89	0.40
2:D:480:SER:N	2:D:481:PRO:CD	2.83	0.40
2:D:372:GLU:O	2:D:375:GLU:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	141/149 (95%)	134 (95%)	6 (4%)	1 (1%)	22 46
1	C	139/149 (93%)	125 (90%)	11 (8%)	3 (2%)	6 17
2	B	420/488 (86%)	395 (94%)	17 (4%)	8 (2%)	8 20
2	D	415/488 (85%)	384 (92%)	29 (7%)	2 (0%)	29 54
3	E	7/17 (41%)	4 (57%)	2 (29%)	1 (14%)	0 0
3	F	4/17 (24%)	3 (75%)	1 (25%)	0	100 100
All	All	1126/1308 (86%)	1045 (93%)	66 (6%)	15 (1%)	12 30

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	263	HIS
2	B	296	PRO
2	B	301	LYS
1	C	1010	ASP
2	D	301	LYS
2	D	457	GLU
2	B	262	PHE
2	B	264	GLU
2	B	514	ALA
1	A	1156	GLU
1	C	1013	ILE
2	B	234	ASP
1	C	1085	ILE
2	B	281	ASP
3	E	290	VAL

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	129/133 (97%)	120 (93%)	9 (7%)	15	35
1	C	128/133 (96%)	124 (97%)	4 (3%)	40	69
2	B	370/421 (88%)	340 (92%)	30 (8%)	11	27
2	D	367/421 (87%)	342 (93%)	25 (7%)	16	36
3	E	9/15 (60%)	8 (89%)	1 (11%)	6	14
3	F	6/15 (40%)	5 (83%)	1 (17%)	2	5
All	All	1009/1138 (89%)	939 (93%)	70 (7%)	15	35

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1003	SER
1	A	1057	LYS
1	A	1068	ASP
1	A	1084	ASP
1	A	1091	GLU
1	A	1118	VAL
1	A	1143	ASN
1	A	1153	VAL
1	A	1154	ARG
2	B	63	SER
2	B	74	LEU
2	B	89	SER
2	B	104	ASP
2	B	110	ARG
2	B	124	LEU
2	B	138	LEU
2	B	159	LEU
2	B	167	LEU
2	B	182	VAL
2	B	199	ARG
2	B	200	LYS
2	B	234	ASP

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Mol	Chain	Res	Type
2	B	244	GLU
2	B	250	LEU
2	B	263	HIS
2	B	267	GLN
2	B	294	SER
2	B	299	LEU
2	B	300	ILE
2	B	304	LEU
2	B	344	VAL
2	B	349	ARG
2	B	362	ASN
2	B	379	GLN
2	B	448	LEU
2	B	483	ARG
2	B	484	THR
2	B	492	ASP
2	B	501	LEU
1	C	1012	GLU
1	C	1068	ASP
1	C	1118	VAL
1	C	1143	ASN
2	D	81	SER
2	D	89	SER
2	D	109	ARG
2	D	117	VAL
2	D	118[A]	CYS
2	D	118[B]	CYS
2	D	124	LEU
2	D	159	LEU
2	D	167	LEU
2	D	182	VAL
2	D	199	ARG
2	D	251	ARG
2	D	257	THR
2	D	261	ILE
2	D	267	GLN
2	D	294	SER
2	D	299	LEU
2	D	300	ILE
2	D	304	LEU
2	D	344	VAL
2	D	362	ASN

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Mol	Chain	Res	Type
2	D	492	ASP
2	D	494	ASP
2	D	501	LEU
2	D	532	LYS
3	E	292	ASP
3	F	291	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1060	GLN
1	A	1090	GLN
1	A	1143	ASN
2	B	232	GLN
2	B	267	GLN
2	B	322	HIS
2	B	336	ASN
2	B	341	GLN
2	B	360	GLN
2	B	362	ASN
2	B	513	GLN
1	C	1090	GLN
1	C	1143	ASN
2	D	161	ASN
2	D	232	GLN
2	D	322	HIS
2	D	336	ASN
2	D	341	GLN
2	D	350	HIS
2	D	362	ASN
2	D	444	GLN
2	D	476	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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	$\#\|Z\| > 2$
5	PO4	D	605	-	4,4,4	1.01	0	6,6,6	0.77	0
5	PO4	B	602	-	4,4,4	0.66	0	6,6,6	1.14	0
5	PO4	D	602	-	4,4,4	0.76	0	6,6,6	0.78	0
5	PO4	B	603	-	4,4,4	0.67	0	6,6,6	0.73	0
5	PO4	B	605	-	4,4,4	0.72	0	6,6,6	1.23	1 (16%)
5	PO4	D	604	-	4,4,4	0.71	0	6,6,6	0.83	0
5	PO4	B	606	-	4,4,4	0.78	0	6,6,6	0.64	0
5	PO4	D	603	-	4,4,4	0.80	0	6,6,6	0.72	0
5	PO4	B	604	-	4,4,4	0.85	0	6,6,6	0.45	0
5	PO4	D	606	-	4,4,4	0.93	0	6,6,6	0.47	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	605	PO4	O4-P-O3	2.61	116.34	107.97

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	145/149 (97%)	-0.67	0 100 100	43, 63, 99, 155	0
1	C	143/149 (95%)	0.22	15 (10%) 6 4	67, 132, 166, 181	4 (2%)
2	B	418/488 (85%)	-0.38	4 (0%) 82 83	44, 65, 117, 171	6 (1%)
2	D	417/488 (85%)	-0.12	14 (3%) 45 45	48, 93, 180, 209	0
3	E	9/17 (52%)	0.94	1 (11%) 5 4	34, 112, 184, 219	0
3	F	6/17 (35%)	0.27	1 (16%) 1 1	54, 110, 153, 176	0
All	All	1138/1308 (87%)	-0.23	35 (3%) 49 49	34, 79, 162, 219	10 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	287	PRO	7.6
2	D	64	GLY	7.1
2	B	297	ASP	6.0
2	D	383	GLU	5.5
2	D	360	GLN	4.2
2	D	297	ASP	4.0
1	C	1005	LYS	3.9
1	C	1015	GLU	3.9
2	D	382	GLN	3.8
2	B	63	SER	3.7
2	D	378	ARG	3.7
2	D	488	PHE	3.5
2	D	352	ILE	3.4
1	C	1002	ALA	3.3
1	C	1014	PHE	3.3
2	D	358	GLU	3.2
2	B	261	ILE	3.1
1	C	1006	LEU	3.1
1	C	1004	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	1139	PHE	2.6
1	C	1163	LYS	2.6
1	C	1153	VAL	2.6
1	C	1007	GLN	2.3
1	C	1013	ILE	2.3
1	C	1092	PHE	2.3
2	D	377	VAL	2.3
2	D	65	ARG	2.2
1	C	1151	ALA	2.2
2	D	296	PRO	2.1
2	B	199	ARG	2.1
1	C	1087	VAL	2.1
1	C	1161	GLU	2.1
3	F	290	VAL	2.0
2	D	99	ARG	2.0
2	D	67	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PO4	D	605	5/5	0.65	0.26	83,92,127,157	0
5	PO4	B	606	5/5	0.86	0.37	91,110,169,212	0
5	PO4	B	602	5/5	0.86	0.19	76,88,124,132	0
5	PO4	D	604	5/5	0.88	0.14	76,109,129,161	0
5	PO4	B	604	5/5	0.89	0.18	72,94,139,142	0
5	PO4	D	602	5/5	0.90	0.21	66,95,126,136	0
5	PO4	B	605	5/5	0.91	0.25	84,116,136,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PO4	D	606	5/5	0.92	0.16	110,125,143,152	0
5	PO4	D	603	5/5	0.93	0.21	90,95,112,155	0
5	PO4	B	603	5/5	0.94	0.19	94,101,139,143	0
4	ZN	B	601	1/1	0.97	0.04	41,41,41,41	0
4	ZN	D	601	1/1	0.98	0.04	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.