



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:14 PM UTC

PDB ID : 5VZU / pdb_00005vzu
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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

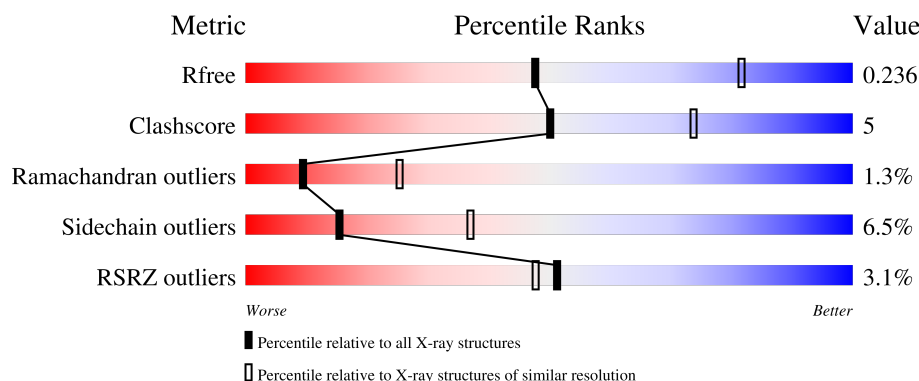
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	8% 83% 14% ..
1	C	149	8% 81% 13% ..
2	B	488	2% 68% 16% • 14%
2	D	488	2% 71% 12% • 15%
3	E	17	12% 29% 24% 47%

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Mol	Chain	Length	Quality of chain
3	F	17	18%29%6%65%

2 Entry composition

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
1	A	145	Total	C	N	O	S	0	0	0
			1149	729	186	228	6			
1	C	143	Total	C	N	O	S	0	0	0
			1137	722	184	225	6			

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
2	B	418	Total	C	N	O	S	0	6	0
			3437	2186	619	611	21			
2	D	417	Total	C	N	O	S	0	2	0
			3402	2168	611	602	21			

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

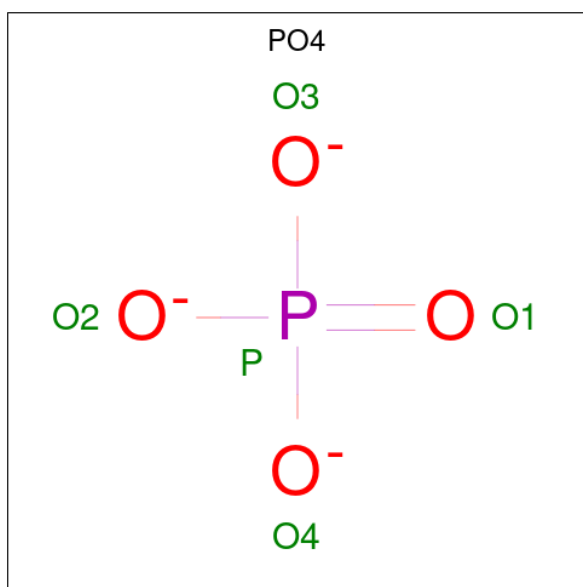
- Molecule 3 is a protein called Cyclin D1.

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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 6 is water.

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

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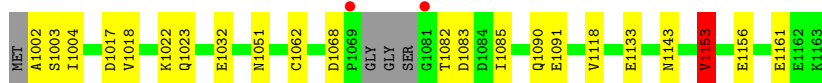
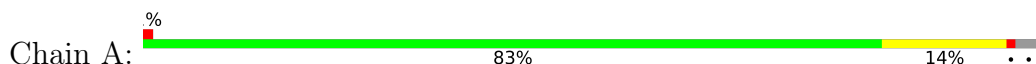
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	12	Total	O	0	0
			12	12		

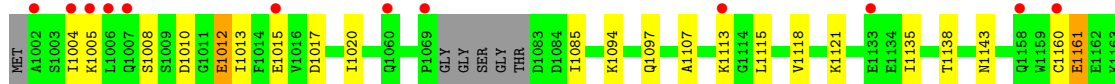
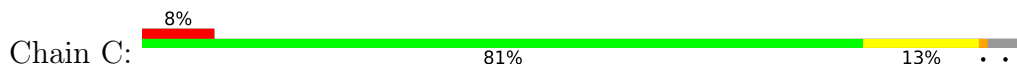
3 Residue-property plots

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.

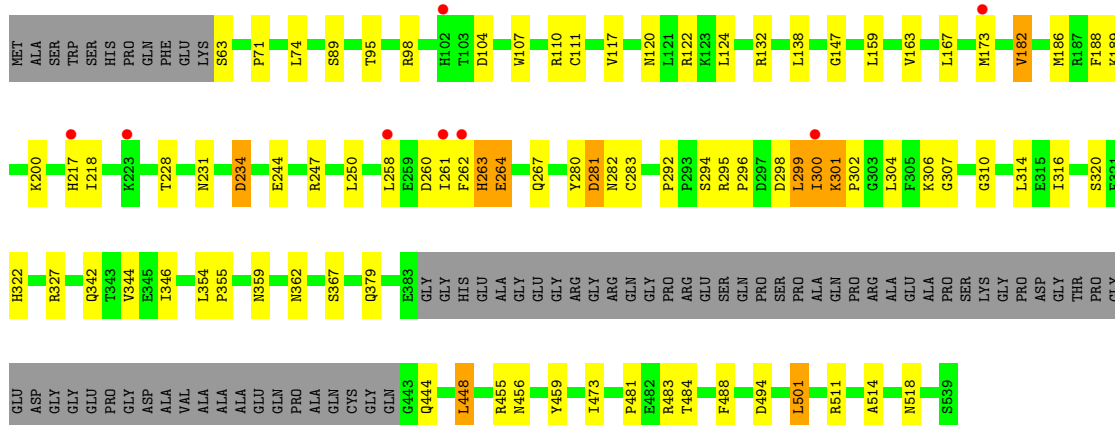
- Molecule 1: S-phase kinase-associated protein 1



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

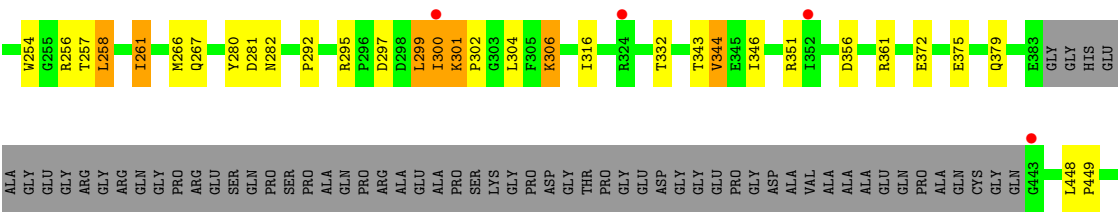


- Molecule 2: F-box only protein 31

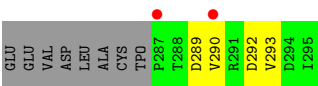
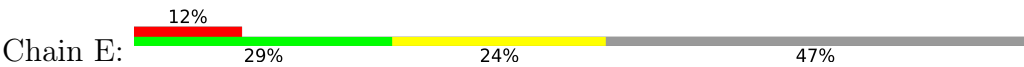


- Molecule 2: F-box only protein 31

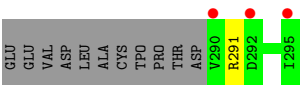




● Molecule 3: Cyclin D1



● Molecule 3: Cyclin D1



4 Data and refinement statistics

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 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.70) 99.0 (50.00-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.81%)	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)	0.27 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	0.87	0/1167	0.98	2/1579 (0.1%)
1	C	0.56	0/1155	0.85	0/1563
2	B	0.84	1/3529 (0.0%)	0.96	4/4773 (0.1%)
2	D	0.68	0/3492	0.90	3/4724 (0.1%)
3	E	0.81	0/72	1.12	0/96
3	F	0.79	0/49	0.86	0/64
All	All	0.76	1/9464 (0.0%)	0.93	9/12799 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	LYS	CA-C	5.75	1.60	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	LYS	N-CA-C	6.24	123.61	109.81
1	A	1153	VAL	CB-CA-C	-5.91	104.17	112.14
2	D	282	ASN	N-CA-C	5.77	119.63	112.47
1	A	1153	VAL	N-CA-CB	5.69	118.27	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	456	ASN	N-CA-C	5.68	117.28	111.14
2	D	261	ILE	N-CA-CB	5.33	116.34	110.53
2	D	306	LYS	N-CA-C	-5.23	101.17	109.96
2	B	71	PRO	CA-C-N	5.22	124.67	119.24
2	B	71	PRO	C-N-CA	5.22	124.67	119.24

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 ⓘ

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	11	0
1	C	1137	0	1129	10	0
2	B	3437	0	3349	44	0
2	D	3402	0	3334	34	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	98	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 (98) 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:B:186:MET:HE1	2:B:316:ILE:HD11	1.73	0.70
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
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:A:1002:ALA:C	1:A:1018:VAL:HG23	2.29	0.58
1:C:1005:LYS:NZ	1:C:1015:GLU:HG2	2.19	0.57
2:D:186:MET:HE1	2:D:316:ILE:HD11	1.86	0.57
1:C:1143:ASN:C	1:C:1143:ASN:HD22	2.11	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
2:D:351:ARG:NH2	2:D:465:MET:HE2	2.23	0.53
1:A:1143:ASN:HD22	1:A:1143:ASN:C	2.17	0.53
1:A:1082:THR:OG1	1:A:1083:ASP:N	2.43	0.52
2:D:173[B]:MET:HE2	2:D:175:LEU:HD21	1.90	0.52
1:A:1004:ILE:HD12	1:A:1004:ILE:C	2.35	0.52
2:D:306:LYS:NZ	6:D:701:HOH:O	2.42	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:D:356:ASP:OD1	2:D:356:ASP:C	2.55	0.50
2:B:494:ASP:HB2	2:B:511:ARG:CB	2.40	0.49
1:C:1005:LYS:HZ3	1:C:1015:GLU:HG2	1.77	0.48
2:B:494:ASP:HB3	2:B:511:ARG:HE	1.79	0.48
2:B:173[B]:MET:HG2	2:B:189:LYS:O	2.13	0.48
2:B:120:ASN:OD1	2:B:120:ASN:C	2.55	0.48
2:B:280:TYR:O	2:B:281:ASP:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:107:TRP:CE2	2:B:132:ARG:HG3	2.51	0.45
2:B:186:MET:HE1	2:B:316:ILE:CD1	2.45	0.45
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:D:254:TRP:CZ3	2:D:266:MET:HE3	2.51	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
1:A:1051:ASN:OD1	1:A:1051:ASN:C	2.61	0.44
2:B:282:ASN:O	2:B:282:ASN:CG	2.61	0.44
2:B:355:PRO:HB2	2:B:359:ASN:HB2	2.00	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
2:D:142:TYR:O	2:D:143:ARG:C	2.60	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
1:A:1022:LYS:NZ	1:A:1032:GLU:OE1	2.47	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:280:TYR:O	2:D:281:ASP:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:488:PHE:CD2	2:B:488:PHE:C	2.99	0.40
1:A:1133:GLU:CD	1:A:1133:GLU:H	2.30	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%)	18	41
1	C	139/149 (93%)	125 (90%)	11 (8%)	3 (2%)	5	14
2	B	420/488 (86%)	395 (94%)	17 (4%)	8 (2%)	6	17
2	D	415/488 (85%)	384 (92%)	29 (7%)	2 (0%)	24	48
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%)	9	25

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 ⓘ

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%)	123 (95%)	6 (5%)	23	51
1	C	128/133 (96%)	122 (95%)	6 (5%)	23	51
2	B	370/421 (88%)	343 (93%)	27 (7%)	13	32
2	D	367/421 (87%)	342 (93%)	25 (7%)	14	35
3	E	9/15 (60%)	8 (89%)	1 (11%)	6	15
3	F	6/15 (40%)	5 (83%)	1 (17%)	2	6
All	All	1009/1138 (89%)	943 (94%)	66 (6%)	15	37

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1003	SER
1	A	1068	ASP
1	A	1091	GLU
1	A	1118	VAL

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Mol	Chain	Res	Type
1	A	1153	VAL
1	A	1161	GLU
2	B	63	SER
2	B	74	LEU
2	B	89	SER
2	B	104	ASP
2	B	124	LEU
2	B	138	LEU
2	B	159	LEU
2	B	163	VAL
2	B	167	LEU
2	B	182	VAL
2	B	200	LYS
2	B	218	ILE
2	B	234	ASP
2	B	244	GLU
2	B	250	LEU
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	362	ASN
2	B	379	GLN
2	B	448	LEU
2	B	483	ARG
2	B	484	THR
2	B	501	LEU
1	C	1012	GLU
1	C	1094	LYS
1	C	1113	LYS
1	C	1118	VAL
1	C	1121	LYS
1	C	1161	GLU
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

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Mol	Chain	Res	Type
2	D	138	LEU
2	D	159	LEU
2	D	163	VAL
2	D	167	LEU
2	D	182	VAL
2	D	251	ARG
2	D	256	ARG
2	D	257	THR
2	D	258	LEU
2	D	261	ILE
2	D	299	LEU
2	D	300	ILE
2	D	304	LEU
2	D	344	VAL
2	D	379	GLN
2	D	492	ASP
2	D	494	ASP
2	D	501	LEU
3	E	293	VAL
3	F	291	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1060	GLN
1	A	1064	HIS
1	A	1090	GLN
1	A	1108	ASN
1	A	1143	ASN
1	A	1158	GLN
2	B	140	HIS
2	B	181	HIS
2	B	195	HIS
2	B	232	GLN
2	B	279	GLN
2	B	322	HIS
2	B	360	GLN
2	B	362	ASN
2	B	476	HIS
2	B	513	GLN
1	C	1049	ASN
1	C	1090	GLN

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Mol	Chain	Res	Type
1	C	1125	ASN
1	C	1143	ASN
2	D	161	ASN
2	D	232	GLN
2	D	336	ASN
2	D	350	HIS
2	D	362	ASN
2	D	476	HIS
2	D	518	ASN

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 oligosaccharides 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	B	604	-	4,4,4	0.89	0	6,6,6	0.48	0
5	PO4	B	602	-	4,4,4	0.70	0	6,6,6	1.19	1 (16%)
5	PO4	D	603	-	4,4,4	0.84	0	6,6,6	0.76	0
5	PO4	B	605	-	4,4,4	0.75	0	6,6,6	1.29	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PO4	B	603	-	4,4,4	0.71	0	6,6,6	0.77	0
5	PO4	D	602	-	4,4,4	0.80	0	6,6,6	0.82	0
5	PO4	D	604	-	4,4,4	0.75	0	6,6,6	0.87	0
5	PO4	D	606	-	4,4,4	0.98	0	6,6,6	0.49	0
5	PO4	D	605	-	4,4,4	1.06	0	6,6,6	0.80	0
5	PO4	B	606	-	4,4,4	0.83	0	6,6,6	0.67	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	605	PO4	O4-P-O3	2.71	116.34	107.91
5	B	602	PO4	O3-P-O2	2.04	114.26	107.91

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

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, 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%)	-0.36	2 (1%) 73 72	43, 63, 99, 155	0
1	C	143/149 (95%)	0.43	12 (8%) 17 14	47, 132, 166, 181	4 (2%)
2	B	418/488 (85%)	-0.31	8 (1%) 66 63	29, 64, 112, 171	12 (2%)
2	D	417/488 (85%)	-0.02	8 (1%) 66 63	37, 93, 180, 209	2 (0%)
3	E	9/17 (52%)	2.14	2 (22%) 2 2	34, 112, 184, 219	0
3	F	6/17 (35%)	2.01	3 (50%) 0 0	54, 110, 153, 176	0
All	All	1138/1308 (87%)	-0.08	35 (3%) 51 48	29, 78, 162, 219	18 (1%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1160	CYS	7.1
3	E	290	VAL	5.4
1	C	1006	LEU	5.3
1	C	1060	GLN	5.2
1	C	1133	GLU	5.1
3	E	287	PRO	4.9
1	A	1081	GLY	3.9
2	B	300	ILE	3.8
2	B	217[A]	HIS	3.8
1	A	1069	PRO	3.7
2	B	262	PHE	3.5
1	C	1069	PRO	3.4
1	C	1158	GLN	3.4
1	C	1004	ILE	3.3
2	D	466	CYS	3.2
3	F	290	VAL	3.2
1	C	1005	LYS	2.9
2	B	223	LYS	2.8
2	B	102[A]	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	488	PHE	2.7
1	C	1002	ALA	2.6
2	D	300	ILE	2.6
1	C	1015	GLU	2.6
2	B	261	ILE	2.5
3	F	292	ASP	2.4
3	F	295	ILE	2.4
1	C	1007	GLN	2.3
2	D	464	ARG	2.2
2	B	173[A]	MET	2.1
2	D	443	GLY	2.1
2	D	324	ARG	2.1
2	D	352	ILE	2.1
2	B	258	LEU	2.1
2	D	537	LEU	2.1
1	C	1113	LYS	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 oligosaccharides 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	B	604	5/5	0.82	0.11	72,94,139,142	0
5	PO4	D	605	5/5	0.87	0.14	83,92,127,157	0
5	PO4	D	604	5/5	0.88	0.09	76,109,129,161	0
5	PO4	B	606	5/5	0.88	0.11	91,110,169,212	0
5	PO4	D	606	5/5	0.88	0.08	110,125,143,152	0
5	PO4	D	602	5/5	0.90	0.13	66,95,126,136	0
5	PO4	B	605	5/5	0.90	0.14	84,116,136,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PO4	B	602	5/5	0.93	0.14	76,88,124,132	0
5	PO4	D	603	5/5	0.94	0.10	90,95,112,155	0
5	PO4	B	603	5/5	0.94	0.07	94,101,139,143	0
4	ZN	D	601	1/1	0.98	0.11	38,38,38,38	0
4	ZN	B	601	1/1	0.99	0.10	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.