Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:55 PM GMT

PDB ID : 5C1V
Title : CRYSTAL STRUCTURE ANALYSIS OF CATALYTIC SUBUNIT OF HU-
MAN CALCINEURIN
Authors : Guasch, A.; Fita, I.; Perez-Luque, R.; Aparicio, D.; Aranguren-Ibanez, A.;
Perez-Riba, M.
Deposited on : 2015-06-15
Resolution : 3.35 Å(reported)

The following versions of software and data (see references ⓘ) 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-20026982
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-20026982
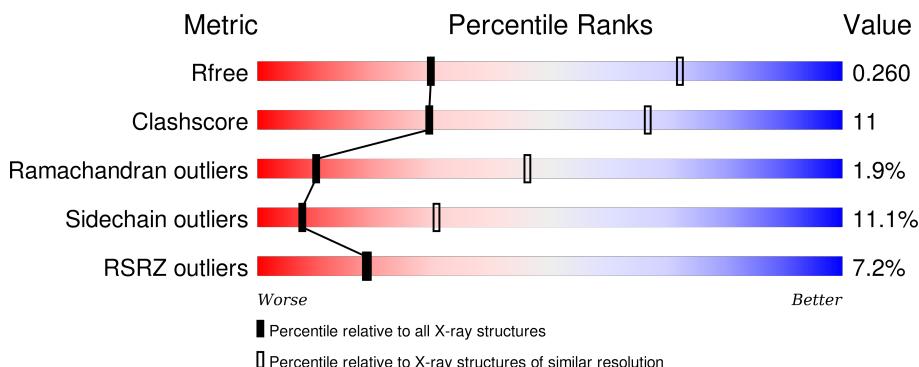
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
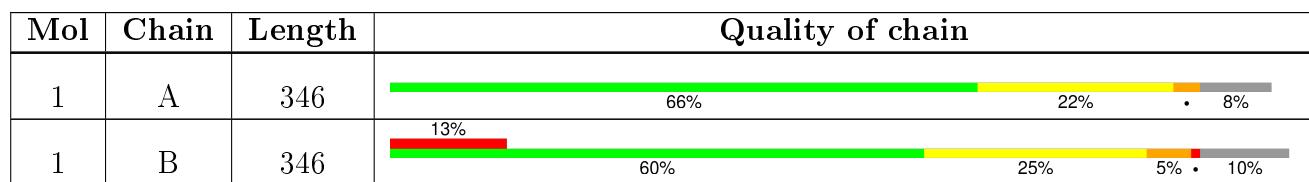
The reported resolution of this entry is 3.35 Å.

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	Percentile Ranks	Value
Rfree		0.260
Clashscore		11
Ramachandran outliers		1.9%
Sidechain outliers		11.1%
RSRZ outliers		7.2%

Worse ← → *Better*

▮ Percentile relative to all X-ray structures
⫿ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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	346	66%　22%　•　8%
1	B	346	13%　60%　25%　5% •　10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5077 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 Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total 2568	C 1644	N 436	O 470	S 18	0	0	0
1	B	311	Total 2495	C 1604	N 418	O 457	S 16	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	341	SER	TYR	conflict	UNP Q08209
A	343	ALA	LEU	conflict	UNP Q08209
A	347	ASP	-	expression tag	UNP Q08209
B	341	SER	TYR	conflict	UNP Q08209
B	343	ALA	LEU	conflict	UNP Q08209
B	347	ASP	-	expression tag	UNP Q08209
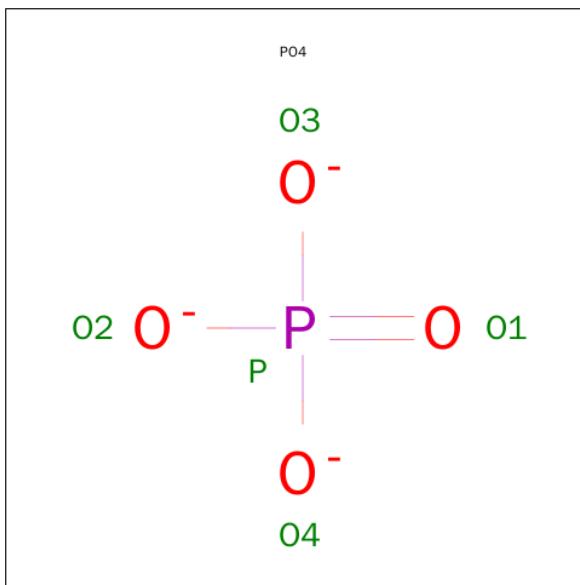
- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Fe 1	0	0
2	A	1	Total 1	Fe 1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Zn 1	0	0
3	A	1	Total 1	Zn 1	0	0

• Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
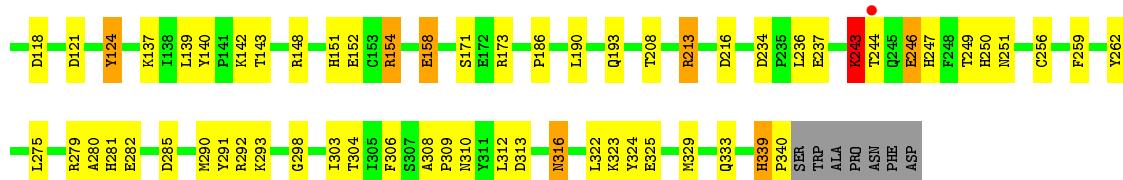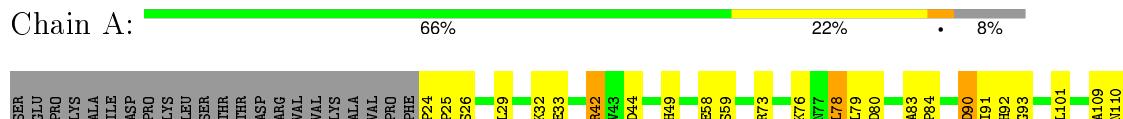
| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
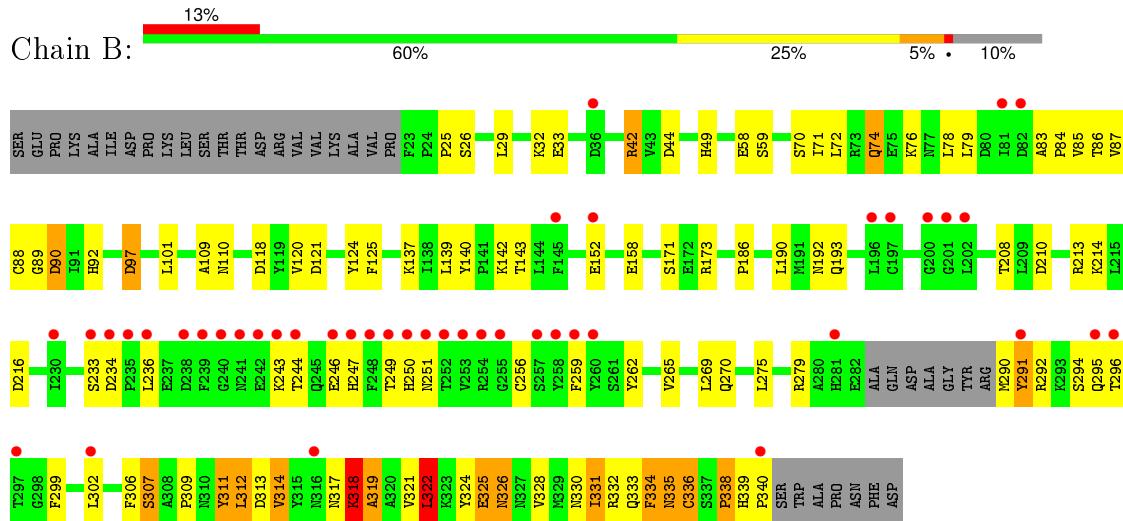
3 Residue-property plots ⓘ

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: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	185.01Å 185.01Å 106.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.80 – 3.35 47.76 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.80-3.35) 100.0 (47.76-3.35)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.49 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.216 , 0.249 0.229 , 0.260	Depositor DCC
R_{free} test set	822 reflections (5.42%)	DCC
Wilson B-factor (Å^2)	79.2	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 74.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning [2]	$<|L|> = 0.45$, $<L^2> = 0.28$	Xtriage
Outliers	0 of 15975 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5077	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, PO4, FE

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	0.88	0/2634	1.05	5/3567 (0.1%)
1	B	0.85	3/2558 (0.1%)	1.00	4/3465 (0.1%)
All	All	0.86	3/5192 (0.1%)	1.02	9/7032 (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
1	A	0	1
1	B	0	3
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	SER	CB-OG	8.69	1.53	1.42
1	B	158	GLU	CB-CG	-6.55	1.39	1.52
1	B	97	ASP	CB-CG	5.61	1.63	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	LEU	CA-CB-CG	7.33	132.15	115.30
1	B	340	PRO	N-CA-CB	6.25	110.80	103.30
1	B	97	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	338	PRO	N-CA-CB	5.80	110.26	103.30
1	A	154	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	73	ARG	NE-CZ-NH2	-5.42	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	PRO	N-CA-CB	5.27	109.62	103.30
1	A	303	ILE	CB-CA-C	-5.26	101.08	111.60
1	A	148	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	339	HIS	Peptide
1	B	192	ASN	Peptide
1	B	317	ASN	Peptide
1	B	319	ALA	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	2568	0	2502	47	0
1	B	2495	0	2407	68	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
All	All	5077	0	4909	113	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 11.

All (113) 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:333:GLN:C	1:B:334:PHE:HD2	1.45	1.19
1:B:86:THR:CG2	1:B:311:TYR:CD2	2.29	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:GLN:O	1:B:334:PHE:CD2	2.01	1.13
1:B:312:LEU:HB2	1:B:322:LEU:HD13	1.37	1.06
1:B:86:THR:HG23	1:B:311:TYR:HD2	1.22	1.04
1:B:86:THR:HG23	1:B:311:TYR:CD2	1.93	1.04
1:B:333:GLN:C	1:B:334:PHE:CD2	2.34	1.00
1:A:124:TYR:O	1:A:124:TYR:HD1	1.51	0.94
1:B:322:LEU:HG	1:B:324:TYR:OH	1.74	0.88
1:B:86:THR:CG2	1:B:311:TYR:HD2	1.73	0.87
1:B:312:LEU:HB2	1:B:322:LEU:CD1	2.05	0.86
1:B:333:GLN:O	1:B:334:PHE:HD2	1.45	0.85
1:B:86:THR:HG21	1:B:311:TYR:CD2	2.22	0.73
1:B:324:TYR:O	1:B:325:GLU:CG	2.38	0.72
1:A:124:TYR:CD1	1:A:124:TYR:O	2.42	0.71
1:B:324:TYR:O	1:B:325:GLU:HG2	1.94	0.67
1:A:333:GLN:OE1	1:B:325:GLU:HA	1.95	0.67
1:A:310:ASN:HD22	1:A:316:ASN:HA	1.61	0.65
1:A:236:LEU:HD23	1:A:259:PHE:HB3	1.81	0.62
1:B:335:ASN:O	1:B:336:CYS:CB	2.48	0.61
1:B:236:LEU:HD23	1:B:259:PHE:HB3	1.83	0.60
1:A:151:HIS:NE2	4:A:503:PO4:O1	2.33	0.60
1:B:85:VAL:HG12	1:B:314:VAL:HG23	1.82	0.60
1:A:310:ASN:OD1	1:A:313:ASP:HA	2.01	0.59
1:B:290:MET:HG3	1:B:290:MET:O	2.01	0.59
1:B:97:ASP:HB3	1:B:309:PRO:HD3	1.83	0.58
1:B:306:PHE:O	1:B:307:SER:HB3	2.01	0.58
1:A:312:LEU:O	1:A:313:ASP:CG	2.40	0.58
1:B:90:ASP:OD2	1:B:92:HIS:NE2	2.36	0.58
1:B:311:TYR:CD1	1:B:311:TYR:N	2.73	0.57
1:A:84:PRO:HB3	1:A:325:GLU:HG3	1.86	0.57
1:A:79:LEU:HD21	1:A:186:PRO:CG	2.35	0.56
1:B:86:THR:HG22	1:B:311:TYR:CD2	2.36	0.56
1:A:90:ASP:OD2	1:A:92:HIS:NE2	2.40	0.55
1:A:152:GLU:OE1	1:A:152:GLU:N	2.40	0.55
1:B:92:HIS:CE1	1:B:118:ASP:HB3	2.42	0.55
1:B:334:PHE:N	1:B:334:PHE:CD2	2.75	0.54
1:B:334:PHE:N	1:B:334:PHE:HD2	2.04	0.54
1:A:322:LEU:HD23	1:A:322:LEU:C	2.28	0.54
1:B:190:LEU:HD21	1:B:193:GLN:HA	1.89	0.54
1:B:291:TYR:HB2	1:B:302:LEU:O	2.08	0.54
1:B:109:ALA:HA	1:B:140:TYR:CE1	2.44	0.53
1:A:109:ALA:HA	1:A:140:TYR:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:VAL:CG1	1:B:314:VAL:HG23	2.39	0.53
1:A:154:ARG:O	1:A:158:GLU:HB3	2.09	0.52
1:A:234:ASP:O	1:A:259:PHE:HA	2.10	0.52
1:B:79:LEU:HD21	1:B:186:PRO:CG	2.40	0.52
1:B:152:GLU:N	1:B:152:GLU:OE1	2.43	0.52
1:A:33:GLU:O	1:A:42:ARG:HD2	2.10	0.52
1:A:339:HIS:HB2	1:A:340:PRO:HD2	1.92	0.51
1:B:71:ILE:O	1:B:74:GLN:HG2	2.10	0.51
1:A:101:LEU:HD23	1:A:101:LEU:C	2.31	0.50
1:B:326:ASN:ND2	1:B:326:ASN:H	2.09	0.50
1:B:324:TYR:O	1:B:325:GLU:CB	2.59	0.49
1:B:58:GLU:OE1	1:B:171:SER:HB3	2.11	0.49
1:B:299:PHE:HE2	1:B:318:LYS:HE3	1.76	0.49
1:B:210:ASP:OD1	1:B:214:LYS:HD2	2.13	0.49
1:B:234:ASP:O	1:B:259:PHE:HA	2.12	0.49
1:B:325:GLU:OE1	1:B:326:ASN:ND2	2.45	0.49
1:A:92:HIS:CE1	1:A:118:ASP:HB3	2.47	0.49
1:B:88:CYS:SG	1:B:89:GLY:N	2.85	0.49
1:A:25:PRO:HG2	1:A:49:HIS:CE1	2.47	0.49
1:B:86:THR:CG2	1:B:311:TYR:CE2	2.91	0.49
1:A:324:TYR:HB2	1:A:329:MET:HE2	1.95	0.49
1:B:33:GLU:O	1:B:42:ARG:HD2	2.11	0.49
1:B:124:TYR:HB3	1:B:125:PHE:CD1	2.47	0.49
1:A:329:MET:HB3	1:B:321:VAL:HA	1.95	0.48
1:A:244:THR:OG1	1:A:246:GLU:HB2	2.13	0.47
1:B:314:VAL:HG12	1:B:319:ALA:O	2.14	0.47
1:B:244:THR:OG1	1:B:246:GLU:HB2	2.14	0.47
1:A:58:GLU:OE1	1:A:171:SER:HB3	2.14	0.47
1:A:78:LEU:CD2	1:A:213:ARG:HE	2.27	0.47
1:A:293:LYS:HE2	1:A:298:GLY:O	2.15	0.46
1:B:87:VAL:HB	1:B:312:LEU:HD23	1.97	0.46
1:A:251:ASN:HB3	1:A:256:CYS:O	2.16	0.46
1:B:330:ASN:O	1:B:331:ILE:CB	2.64	0.46
1:B:251:ASN:HB3	1:B:256:CYS:O	2.16	0.45
1:A:262:TYR:CZ	1:A:292:ARG:HD3	2.52	0.45
1:B:120:VAL:O	1:B:121:ASP:HB2	2.17	0.45
1:A:190:LEU:HD21	1:A:193:GLN:HA	1.98	0.45
1:B:29:LEU:HG	1:B:49:HIS:CD2	2.52	0.45
1:A:121:ASP:OD2	1:A:151:HIS:ND1	2.50	0.44
1:B:83:ALA:HB1	1:B:84:PRO:HA	2.00	0.44
1:B:262:TYR:CZ	1:B:292:ARG:HD3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LEU:HD23	1:B:140:TYR:CE2	2.53	0.44
1:A:308:ALA:HA	1:A:309:PRO:HD2	1.91	0.43
1:B:294:SER:HB3	1:B:299:PHE:O	2.18	0.43
1:B:311:TYR:HD1	1:B:311:TYR:H	1.60	0.43
1:A:29:LEU:HG	1:A:49:HIS:CD2	2.53	0.43
1:A:90:ASP:HB2	1:A:306:PHE:CD1	2.53	0.43
1:A:243:LYS:HG3	1:A:243:LYS:H	1.64	0.42
1:B:58:GLU:OE2	1:B:173:ARG:NH1	2.52	0.42
1:A:280:ALA:O	1:A:281:HIS:HB3	2.20	0.42
1:B:216:ASP:C	1:B:216:ASP:OD1	2.58	0.42
1:B:101:LEU:HD23	1:B:101:LEU:C	2.40	0.42
1:B:86:THR:HG23	1:B:311:TYR:CE2	2.47	0.42
1:A:243:LYS:HE2	1:A:244:THR:H	1.84	0.42
1:B:70:SER:O	1:B:74:GLN:NE2	2.53	0.42
1:A:280:ALA:O	1:A:281:HIS:CB	2.68	0.41
1:B:265:VAL:HG12	1:B:269:LEU:CD1	2.50	0.41
1:A:316:ASN:HA	1:A:316:ASN:HD22	1.63	0.41
1:A:251:ASN:OD1	1:A:259:PHE:CZ	2.73	0.41
1:A:83:ALA:HB1	1:A:84:PRO:HA	2.03	0.41
1:B:318:LYS:HE2	1:B:319:ALA:HA	2.01	0.41
1:A:139:LEU:HD23	1:A:140:TYR:CE2	2.55	0.41
1:B:72:LEU:HA	1:B:72:LEU:HD23	1.94	0.41
1:A:216:ASP:OD1	1:A:216:ASP:C	2.59	0.41
1:A:234:ASP:OD1	1:A:282:GLU:HG3	2.22	0.40
1:B:251:ASN:OD1	1:B:259:PHE:CZ	2.75	0.40
1:A:322:LEU:HD23	1:A:323:LYS:N	2.36	0.40
1:B:86:THR:HG23	1:B:313:ASP:OD1	2.22	0.40
1:A:91:ILE:HG22	1:A:93:GLY:N	2.37	0.40
1:A:291:TYR:HE2	1:A:304:THR:HG1	1.69	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	315/346 (91%)	295 (94%)	19 (6%)	1 (0%)	46	82
1	B	307/346 (89%)	272 (89%)	24 (8%)	11 (4%)	4	31
All	All	622/692 (90%)	567 (91%)	43 (7%)	12 (2%)	10	46

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	PRO
1	B	318	LYS
1	B	325	GLU
1	B	331	ILE
1	B	332	ARG
1	B	335	ASN
1	B	336	CYS
1	B	338	PRO
1	B	339	HIS
1	A	243	LYS
1	B	243	LYS
1	B	307	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	280/307 (91%)	251 (90%)	29 (10%)	9	34
1	B	268/307 (87%)	236 (88%)	32 (12%)	6	26
All	All	548/614 (89%)	487 (89%)	61 (11%)	8	30

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	32	LYS
1	A	42	ARG
1	A	44	ASP

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Mol	Chain	Res	Type
1	A	59	SER
1	A	76	LYS
1	A	78	LEU
1	A	80	ASP
1	A	90	ASP
1	A	110	ASN
1	A	124	TYR
1	A	137	LYS
1	A	142	LYS
1	A	143	THR
1	A	158	GLU
1	A	173	ARG
1	A	208	THR
1	A	213	ARG
1	A	237	GLU
1	A	243	LYS
1	A	246	GLU
1	A	247	HIS
1	A	249	THR
1	A	250	HIS
1	A	275	LEU
1	A	279	ARG
1	A	285	ASP
1	A	290	MET
1	A	316	ASN
1	B	26	SER
1	B	32	LYS
1	B	42	ARG
1	B	44	ASP
1	B	59	SER
1	B	74	GLN
1	B	76	LYS
1	B	78	LEU
1	B	90	ASP
1	B	110	ASN
1	B	137	LYS
1	B	142	LYS
1	B	143	THR
1	B	208	THR
1	B	213	ARG
1	B	247	HIS
1	B	249	THR

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Mol	Chain	Res	Type
1	B	250	HIS
1	B	270	GLN
1	B	275	LEU
1	B	279	ARG
1	B	291	TYR
1	B	295	GLN
1	B	296	THR
1	B	311	TYR
1	B	312	LEU
1	B	314	VAL
1	B	318	LYS
1	B	322	LEU
1	B	326	ASN
1	B	328	VAL
1	B	334	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	94	GLN
1	A	110	ASN
1	A	207	ASN
1	A	310	ASN
1	A	316	ASN
1	B	37	ASN
1	B	74	GLN
1	B	207	ASN
1	B	326	ASN
1	B	327	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\#|Z| > 2$
4	PO4	A	503	3,2	4,4,4	0.83	0	6,6,6	0.40	0
4	PO4	B	503	3,2	4,4,4	0.63	0	6,6,6	0.22	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
4	PO4	A	503	3,2	-	0/0/0/0	0/0/0/0
4	PO4	B	503	3,2	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	317/346 (91%)	0.06	1 (0%)	94 95	61, 94, 134, 171	0
1	B	311/346 (89%)	0.85	44 (14%)	4 3	79, 130, 193, 219	0
All	All	628/692 (90%)	0.45	45 (7%)	18 19	61, 111, 187, 219	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	340	PRO	5.7
1	B	250	HIS	5.5
1	B	252	THR	5.3
1	B	260	TYR	5.2
1	B	255	GLY	4.8
1	B	244	THR	4.6
1	B	251	ASN	4.5
1	B	236	LEU	4.5
1	B	201	GLY	4.4
1	B	238	ASP	4.4
1	B	202	LEU	4.3
1	B	243	LYS	4.0
1	B	239	PHE	3.9
1	B	235	PRO	3.8
1	B	291	TYR	3.7
1	B	197	CYS	3.6
1	B	249	THR	3.6
1	B	246	GLU	3.5
1	B	254	ARG	3.4
1	B	259	PHE	3.4
1	B	258	TYR	3.2
1	B	241	ASN	3.2
1	B	297	THR	3.0
1	B	296	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	247	HIS	2.9
1	B	295	GLN	2.9
1	B	257	SER	2.8
1	B	248	PHE	2.7
1	B	253	VAL	2.7
1	B	36	ASP	2.7
1	B	230	ILE	2.5
1	B	242	GLU	2.5
1	B	196	LEU	2.5
1	B	81	ILE	2.4
1	B	200	GLY	2.4
1	B	240	GLY	2.4
1	B	316	ASN	2.3
1	A	244	THR	2.3
1	B	82	ASP	2.2
1	B	281	HIS	2.2
1	B	233	SER	2.2
1	B	145	PHE	2.1
1	B	234	ASP	2.1
1	B	152	GLU	2.1
1	B	302	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 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, 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	LLDF	B-factors($Å^2$)	Q<0.9
3	ZN	A	502	1/1	0.98	0.21	0.16	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	PO4	A	503	5/5	0.98	0.22	0.13	77,78,88,92	0
4	PO4	B	503	5/5	0.95	0.14	-0.92	99,99,99,99	0
2	FE	A	501	1/1	0.99	0.15	-1.75	99,99,99,99	0
3	ZN	B	502	1/1	0.92	0.04	-1.78	99,99,99,99	0
2	FE	B	501	1/1	0.91	0.19	-	99,99,99,99	0

6.5 Other polymers (i)

There are no such residues in this entry.