WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 08:28 PM EST

PDB ID	:	4IGG
Title	:	Full-length human alpha-catenin crystal structure
Authors	:	Izard, T.; Rangarajan, E.S.
Deposited on	:	2012-12-17
Resolution	:	3.66 Å(reported)

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

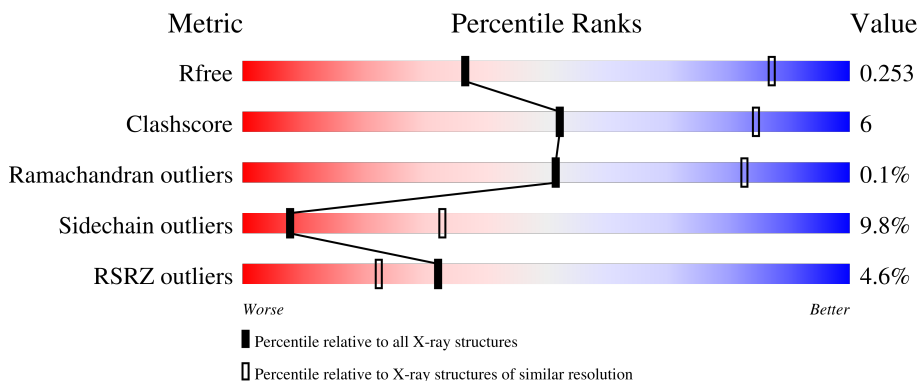|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.66 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		0.253
Clashscore		6
Ramachandran outliers		0.1%
Sidechain outliers		9.8%
RSRZ outliers		4.6%

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}	130704	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

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	832	4% — 72% — 17% — · — 10%
1	B	832	5% — 74% — 17% — · — 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	1001	-	-	-	X

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 11714 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.
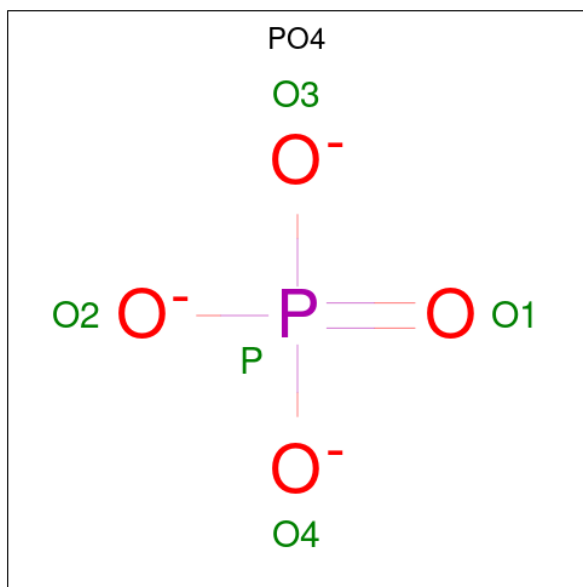
- Molecule 1 is a protein called Catenin alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	750	Total	C	N	O	S	0	0	0
			5766	3572	1027	1129	38			
1	B	771	Total	C	N	O	S	0	0	0
			5938	3679	1057	1164	38			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	907	PRO	-	expression tag	UNP P35221
A	908	HIS	-	expression tag	UNP P35221
A	909	HIS	-	expression tag	UNP P35221
A	910	HIS	-	expression tag	UNP P35221
A	911	HIS	-	expression tag	UNP P35221
A	912	HIS	-	expression tag	UNP P35221
A	913	HIS	-	expression tag	UNP P35221
B	907	PRO	-	expression tag	UNP P35221
B	908	HIS	-	expression tag	UNP P35221
B	909	HIS	-	expression tag	UNP P35221
B	910	HIS	-	expression tag	UNP P35221
B	911	HIS	-	expression tag	UNP P35221
B	912	HIS	-	expression tag	UNP P35221
B	913	HIS	-	expression tag	UNP P35221

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O⁻

O2 O⁻ — P ═══ O O1

P

O⁻

O4

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

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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 geometr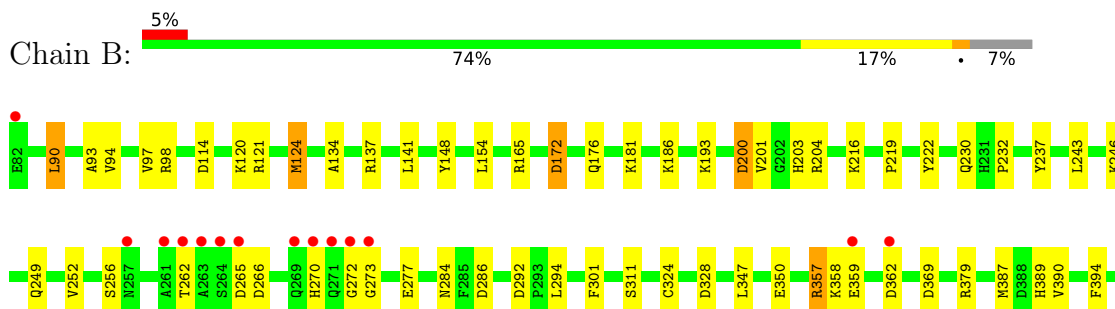ic quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Catenin alpha-1

- Molecule 1: Catenin alpha-1

L402 I405 N410 G411 N412 V416 K417 E418 L430 V433 L449 M452 A470 K474 S477 K478 N483 K493 V497 I508 I519 V527 Q531 V535 L538 D539 A550 R551 V552 I553 E559 M560 D561 E570 T576 K577

S580 N581 V591 L598 A603 E608 I612 I622 L630 M631 I632 R633 T634 P635 E636 E637 LEU ASP ASP SER ASP PHE GLU THR GLU ASP PHE ASP VAL ARG SER ARG THR SER VAL GLN THR GLU ASP ASP GLN LEU I664 S668 A669 R670 M673 L676 P677

Q680 K681 I684 A685 E686 K695 L698 D699 V702 S703 K704 S708 G709 N710 D711 I712 I713 M719 I722 M723 T727 T730 R731 L736 K737 D741 K748 I749 A750 M756 D757 D765 P768 K773 Q774 L777 L780 Q781 R782 C787 H788

Q789 L790 N791 V796 K797 A798 E799 V800 L803 G804 G805 E806 L807 V812 A815 M816 S817 L818 K845 S846 Q847 G848 M849 A850 S851 L852 N853 L854 P855 A856 V857 M861 P864 R872 Q875 T878 GLN THR LYS ILE LYS ARG ALA SER GLN LYS LYS HIS VAL ASN

PRO VAL GLN ALA LEU SER GLU PHE LYS ALA MET ASP SER ILE PRO HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	145.63Å 145.63Å 139.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.21 – 3.66 93.43 – 3.66	Depositor EDS
% Data completeness (in resolution range)	99.9 (23.21-3.66) 99.9 (93.43-3.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 3.67Å)	Xtriage
Refinement program	TNT, BUSTER 2.11.2	Depositor
R, R_{free}	0.217 , 0.241 0.228 , 0.253	Depositor DCC
R_{free} test set	1828 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	114.3	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 120.5	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l 0.039 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11714	wwPDB-VP
Average B, all atoms (Å^2)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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, 0.333 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

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	0.40	0/5825	0.57	0/7848
1	B	0.41	0/5999	0.59	0/8080
All	All	0.41	0/11824	0.58	0/15928

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	5766	0	5856	74	0
1	B	5938	0	6038	63	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
All	All	11714	0	11894	130	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 6.

All (130) 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:A:519:ILE:HG13	1:A:622:ILE:HD13	1.57	0.83
1:B:519:ILE:HG13	1:B:622:ILE:HD13	1.61	0.82
1:A:533:LYS:HB3	1:A:598:LEU:HD21	1.67	0.77
1:A:154:LEU:HD21	1:A:256:SER:HB2	1.73	0.69
1:A:216:LYS:O	1:A:219:PRO:HD2	1.94	0.67
1:B:577:LYS:HG3	1:B:581:ASN:HD22	1.59	0.67
1:A:109:GLY:HA2	1:B:98:ARG:HH11	1.61	0.66
1:B:154:LEU:HD21	1:B:256:SER:HB2	1.77	0.66
1:A:615:SER:O	1:A:618:VAL:HG22	1.97	0.64
1:B:216:LYS:O	1:B:219:PRO:HD2	1.98	0.64
1:A:201:VAL:HA	1:A:204:ARG:HD3	1.79	0.62
1:A:389:HIS:HB3	1:A:433:VAL:HG22	1.82	0.61
1:A:577:LYS:HG3	1:A:581:ASN:HD22	1.64	0.61
1:B:237:TYR:CE1	1:B:470:ALA:HB1	2.36	0.61
1:A:151:LEU:HB3	1:B:864:PRO:HB3	1.84	0.59
1:A:249:GLN:O	1:A:252:VAL:HG22	2.03	0.59
1:B:538:LEU:HD12	1:B:591:VAL:HG13	1.83	0.58
1:A:477:SER:O	1:A:481:GLN:HG3	2.03	0.58
1:A:89:GLU:HG2	1:A:141:LEU:HD11	1.85	0.58
1:A:324:CYS:HB2	1:A:389:HIS:CD2	2.40	0.57
1:A:220:ILE:HG22	1:A:244:ILE:HD13	1.85	0.57
1:B:324:CYS:HB2	1:B:389:HIS:CD2	2.41	0.56
1:A:527:VAL:O	1:A:531:GLN:HG3	2.06	0.56
1:B:757:ASP:HA	1:B:780:LEU:HD22	1.88	0.56
1:A:757:ASP:HA	1:A:780:LEU:HD22	1.88	0.56
1:B:704:LYS:HB2	1:B:861:MET:HE3	1.88	0.56
1:B:90:LEU:O	1:B:94:VAL:HG23	2.07	0.55
1:B:673:MET:HA	1:B:676:LEU:HD13	1.87	0.55
1:A:462:PRO:HA	1:A:465:ILE:HG12	1.89	0.54
1:A:213:ILE:HG23	1:A:217:ASN:ND2	2.23	0.54
1:B:846:SER:HB3	1:B:852:LEU:H	1.72	0.54
1:B:535:VAL:HG23	1:B:598:LEU:HD12	1.89	0.54
1:B:249:GLN:O	1:B:252:VAL:HG22	2.08	0.54
1:A:568:TYR:CE1	1:A:632:ILE:HB	2.42	0.53
1:A:90:LEU:O	1:A:94:VAL:HG23	2.09	0.53
1:A:407:ALA:HB1	1:A:415:GLU:HB3	1.90	0.53
1:A:711:ASP:HA	1:A:714:VAL:HG12	1.91	0.53
1:A:124:MET:O	1:A:124:MET:HG2	2.08	0.52
1:B:430:LEU:O	1:B:433:VAL:HG22	2.10	0.51
1:B:527:VAL:O	1:B:531:GLN:HG3	2.10	0.51
1:A:402:LEU:O	1:A:405:ILE:HG13	2.10	0.51
1:B:121:ARG:O	1:B:124:MET:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:PRO:HG2	1:B:680:GLN:HB2	1.93	0.51
1:B:390:VAL:O	1:B:394:PHE:HB2	2.11	0.50
1:A:114:ASP:HB3	1:A:120:LYS:HD2	1.93	0.50
1:B:508:ILE:HD13	1:B:559:GLU:HG2	1.93	0.49
1:B:402:LEU:O	1:B:405:ILE:HG13	2.11	0.49
1:A:608:GLU:O	1:A:612:ILE:HG13	2.11	0.49
1:B:685:ALA:HA	1:B:731:ARG:HH12	1.78	0.49
1:A:161:ILE:HD13	1:A:248:LEU:HD22	1.94	0.49
1:A:508:ILE:HD13	1:A:559:GLU:HG2	1.93	0.49
1:B:553:ILE:HD13	1:B:580:SER:HB3	1.95	0.49
1:A:668:SER:H	1:A:738:ASN:HB3	1.77	0.49
1:A:271:GLN:HE22	1:A:277:GLU:HA	1.78	0.48
1:A:172:ASP:HA	1:A:175:ILE:HD12	1.95	0.48
1:A:154:LEU:CD2	1:A:256:SER:HB2	2.41	0.48
1:A:201:VAL:HA	1:A:204:ARG:CD	2.42	0.48
1:B:114:ASP:HB3	1:B:120:LYS:HD2	1.95	0.48
1:B:711:ASP:H	1:B:857:VAL:HG12	1.78	0.47
1:B:608:GLU:O	1:B:612:ILE:HG13	2.14	0.47
1:A:85:PHE:O	1:A:88:GLU:HG2	2.15	0.47
1:A:151:LEU:CB	1:B:864:PRO:HB3	2.43	0.47
1:A:246:LYS:HG3	1:A:249:GLN:HE21	1.80	0.47
1:A:415:GLU:HG2	1:A:419:TYR:CE2	2.49	0.47
1:A:230:GLN:C	1:A:232:PRO:HD3	2.35	0.47
1:B:478:LYS:H	1:B:478:LYS:HD2	1.80	0.47
1:A:357:ARG:HG3	1:A:360:ARG:HE	1.80	0.46
1:B:670:ARG:HG2	1:B:737:LYS:HA	1.97	0.46
1:A:109:GLY:HA2	1:B:98:ARG:NH1	2.29	0.46
1:B:154:LEU:CD2	1:B:256:SER:HB2	2.45	0.46
1:A:169:ASN:ND2	1:A:172:ASP:OD2	2.49	0.46
1:A:219:PRO:O	1:A:222:TYR:HB3	2.16	0.46
1:B:577:LYS:HG3	1:B:581:ASN:ND2	2.28	0.46
1:A:710:ASN:HB2	1:A:852:LEU:HB3	1.98	0.45
1:A:577:LYS:HG3	1:A:581:ASN:ND2	2.30	0.45
1:B:676:LEU:HD23	1:B:680:GLN:HB3	1.99	0.45
1:B:684:ILE:HD11	1:B:812:VAL:HG21	1.98	0.45
1:A:207:MET:O	1:A:211:ARG:HG3	2.17	0.45
1:A:240:ASN:HA	1:A:466:ASN:HD22	1.82	0.45
1:B:474:LYS:HB3	1:B:477:SER:HB2	1.98	0.44
1:A:777:LEU:HA	1:A:780:LEU:HD12	2.00	0.44
1:B:292:ASP:HB3	1:B:357:ARG:HH21	1.81	0.44
1:B:172:ASP:O	1:B:176:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:THR:HB	1:A:758:LYS:HE3	2.00	0.44
1:B:93:ALA:O	1:B:97:VAL:HG23	2.17	0.44
1:B:777:LEU:HA	1:B:780:LEU:HD12	2.00	0.44
1:A:563:TYR:HD2	1:A:857:VAL:HG23	1.82	0.44
1:B:550:ALA:HA	1:B:553:ILE:HD12	1.99	0.43
1:B:673:MET:HG2	1:B:730:THR:HA	2.00	0.43
1:B:750:ALA:HB2	1:B:791:ASN:HD21	1.83	0.43
1:A:711:ASP:HB2	1:A:759:LEU:HD11	2.00	0.43
1:A:200:ASP:HB3	1:A:203:HIS:HD2	1.84	0.43
1:A:465:ILE:HG13	1:A:466:ASN:N	2.33	0.43
1:B:134:ALA:HA	1:B:137:ARG:CZ	2.48	0.43
1:A:722:ILE:HD13	1:A:748:LYS:HB3	2.00	0.43
1:A:200:ASP:O	1:A:204:ARG:HG3	2.18	0.43
1:A:131:LEU:O	1:A:135:VAL:HG23	2.18	0.43
1:B:201:VAL:HA	1:B:204:ARG:HD3	2.01	0.43
1:A:191:ALA:HB1	1:A:211:ARG:HD2	2.00	0.43
1:B:410:ASN:N	1:B:410:ASN:HD22	2.17	0.42
1:B:553:ILE:HG23	1:B:576:THR:HB	2.01	0.42
1:A:195:GLN:HG3	1:A:207:MET:HB3	1.99	0.42
1:A:719:MET:O	1:A:723:MET:HB2	2.20	0.42
1:B:230:GLN:C	1:B:232:PRO:HD3	2.39	0.42
1:B:812:VAL:HG22	1:B:815:ALA:HB3	2.00	0.42
1:A:604:GLN:N	1:A:605:PRO:HD3	2.33	0.42
1:A:490:GLN:O	1:A:493:LYS:HG2	2.19	0.42
1:A:808:VAL:HG11	1:B:203:HIS:NE2	2.35	0.42
1:B:630:LEU:HD23	1:B:680:GLN:HE22	1.84	0.42
1:A:668:SER:N	1:A:738:ASN:HB3	2.33	0.42
1:B:722:ILE:HD13	1:B:748:LYS:HB3	2.01	0.42
1:A:214:LEU:O	1:A:218:VAL:HG23	2.20	0.41
1:B:634:THR:HG23	1:B:635:PRO:HD3	2.01	0.41
1:A:404:LEU:HD11	1:A:416:VAL:HG13	2.02	0.41
1:A:698:LEU:HA	1:A:830:VAL:HG23	2.03	0.41
1:B:277:GLU:CD	1:B:277:GLU:H	2.24	0.41
1:A:672:ILE:HG13	1:B:148:TYR:HD1	1.84	0.41
1:B:219:PRO:O	1:B:222:TYR:HB3	2.19	0.41
1:A:617:LEU:HD12	1:A:617:LEU:HA	1.96	0.41
1:A:523:VAL:HG11	1:A:618:VAL:CG2	2.50	0.41
1:B:272:GLY:HA2	1:B:273:GLY:HA2	1.86	0.41
1:B:412:ASN:O	1:B:416:VAL:HG22	2.21	0.41
1:B:719:MET:O	1:B:723:MET:HB2	2.20	0.41
1:A:523:VAL:HG11	1:A:618:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:SER:H	1:B:709:GLY:HA3	1.86	0.41
1:A:365:ASN:HA	1:A:368:ILE:HD12	2.03	0.40
1:A:203:HIS:HA	1:A:206:GLN:NE2	2.35	0.40
1:A:317:ALA:HA	1:B:301:PHE:CZ	2.56	0.40
1:B:493:LYS:O	1:B:497:VAL:HG23	2.21	0.40
1:A:416:VAL:HG21	1:A:472:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	746/832 (90%)	713 (96%)	33 (4%)	0	100	100
1	B	767/832 (92%)	741 (97%)	24 (3%)	2 (0%)	41	74
All	All	1513/1664 (91%)	1454 (96%)	57 (4%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	200	ASP
1	B	603	ALA

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	621/698 (89%)	568 (92%)	53 (8%)	10	40
1	B	640/698 (92%)	570 (89%)	70 (11%)	6	29
All	All	1261/1396 (90%)	1138 (90%)	123 (10%)	8	33

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	MET
1	A	141	LEU
1	A	171	GLN
1	A	193	LYS
1	A	207	MET
1	A	243	LEU
1	A	264	SER
1	A	265	ASP
1	A	271	GLN
1	A	286	ASP
1	A	289	ILE
1	A	294	LEU
1	A	299	GLU
1	A	300	ARG
1	A	308	ARG
1	A	311	SER
1	A	328	ASP
1	A	347	LEU
1	A	350	GLU
1	A	358	LYS
1	A	365	ASN
1	A	369	ASP
1	A	386	VAL
1	A	449	LEU
1	A	465	ILE
1	A	486	LEU
1	A	508	ILE
1	A	539	ASP
1	A	551	ARG
1	A	561	ASP
1	A	564	GLU
1	A	571	LYS
1	A	598	LEU
1	A	601	ASP
1	A	605	PRO

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Mol	Chain	Res	Type
1	A	606	MET
1	A	617	LEU
1	A	633	ARG
1	A	667	GLN
1	A	695	LYS
1	A	698	LEU
1	A	699	ASP
1	A	723	MET
1	A	741	ASP
1	A	756	MET
1	A	763	ILE
1	A	769	ASP
1	A	775	ASP
1	A	782	ARG
1	A	800	VAL
1	A	807	LEU
1	A	818	LEU
1	A	847	GLN
1	B	90	LEU
1	B	124	MET
1	B	141	LEU
1	B	165	ARG
1	B	172	ASP
1	B	181	LYS
1	B	186	LYS
1	B	193	LYS
1	B	200	ASP
1	B	243	LEU
1	B	246	LYS
1	B	262	THR
1	B	265	ASP
1	B	266	ASP
1	B	270	HIS
1	B	284	ASN
1	B	286	ASP
1	B	294	LEU
1	B	311	SER
1	B	328	ASP
1	B	347	LEU
1	B	350	GLU
1	B	357	ARG
1	B	358	LYS

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Mol	Chain	Res	Type
1	B	359	GLU
1	B	362	ASP
1	B	369	ASP
1	B	379	ARG
1	B	387	MET
1	B	410	ASN
1	B	416	VAL
1	B	418	GLU
1	B	449	LEU
1	B	452	MET
1	B	478	LYS
1	B	483	ASN
1	B	508	ILE
1	B	538	LEU
1	B	539	ASP
1	B	551	ARG
1	B	561	ASP
1	B	570	GLU
1	B	598	LEU
1	B	632	ILE
1	B	634	THR
1	B	673	MET
1	B	676	LEU
1	B	680	GLN
1	B	681	LYS
1	B	686	GLU
1	B	695	LYS
1	B	698	LEU
1	B	699	ASP
1	B	702	VAL
1	B	713	ILE
1	B	723	MET
1	B	741	ASP
1	B	756	MET
1	B	765	ASP
1	B	773	LYS
1	B	774	GLN
1	B	782	ARG
1	B	787	CYS
1	B	796	VAL
1	B	799	GLU
1	B	807	LEU

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Mol	Chain	Res	Type
1	B	816	MET
1	B	818	LEU
1	B	852	LEU
1	B	853	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	203	HIS
1	A	206	GLN
1	A	217	ASN
1	A	226	GLN
1	A	240	ASN
1	A	249	GLN
1	A	271	GLN
1	A	288	GLN
1	A	428	ASN
1	A	466	ASN
1	A	494	GLN
1	A	581	ASN
1	A	604	GLN
1	A	827	ASN
1	A	847	GLN
1	B	123	ASN
1	B	226	GLN
1	B	284	ASN
1	B	410	ASN
1	B	581	ASN
1	B	675	GLN
1	B	680	GLN
1	B	788	HIS
1	B	824	ASN
1	B	827	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	#$|Z| > 2$
2	PO4	B	1001	-	4,4,4	1.20	1 (25%)	6,6,6	0.41	0
2	PO4	A	1001	-	4,4,4	1.21	1 (25%)	6,6,6	0.52	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	PO4	P-O1	2.29	1.56	1.50
2	A	1001	PO4	P-O1	2.24	1.56	1.50

There are no bond angle outliers.

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	750/832 (90%)	0.53	30 (4%)	38	27	49, 117, 184, 241	8 (1%)
1	B	771/832 (92%)	0.58	40 (5%)	27	19	72, 122, 195, 262	8 (1%)
All	All	1521/1664 (91%)	0.55	70 (4%)	32	22	49, 120, 192, 262	16 (1%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	270	HIS	10.9
1	B	848	GLY	6.6
1	B	853	ASN	6.5
1	B	265	ASP	6.1
1	B	264	SER	5.4
1	B	271	GLN	5.3
1	B	272	GLY	5.1
1	B	269	GLN	4.9
1	A	355	ALA	4.8
1	B	669	ALA	4.8
1	A	296	PHE	4.4
1	B	847	GLN	4.0
1	A	707	ASP	3.9
1	B	852	LEU	3.7
1	B	845	LYS	3.7
1	B	803	LEU	3.6
1	A	731	ARG	3.6
1	B	263	ALA	3.5
1	A	809	VAL	3.4
1	B	668	SER	3.3
1	B	736	LEU	3.1
1	B	854	LEU	3.1
1	B	730	THR	3.1
1	A	267	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	849	MET	3.0
1	A	603	ALA	2.8
1	B	849	MET	2.8
1	A	733	LYS	2.7
1	B	262	THR	2.7
1	A	297	SER	2.6
1	A	299	GLU	2.6
1	B	800	VAL	2.6
1	A	706	ASP	2.6
1	B	846	SER	2.5
1	A	806	GLU	2.5
1	B	789	GLN	2.5
1	A	850	ALA	2.5
1	A	803	LEU	2.5
1	B	273	GLY	2.5
1	B	261	ALA	2.4
1	B	798	ALA	2.4
1	B	804	GLY	2.4
1	B	257	ASN	2.4
1	A	698	LEU	2.4
1	B	362	ASP	2.3
1	A	275	GLY	2.3
1	B	781	GLN	2.3
1	A	303	PRO	2.3
1	A	819	ILE	2.3
1	B	359	GLU	2.3
1	B	807	LEU	2.3
1	A	726	MET	2.2
1	B	82	GLU	2.2
1	A	737	LYS	2.2
1	B	855	PRO	2.2
1	A	87	LYS	2.2
1	A	702	VAL	2.2
1	A	356	GLY	2.2
1	A	808	VAL	2.2
1	B	875	GLN	2.1
1	B	851	SER	2.1
1	A	832	THR	2.1
1	A	633	ARG	2.1
1	B	768	PRO	2.1
1	A	708	SER	2.1
1	A	796	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	872	ARG	2.0
1	B	727	THR	2.0
1	B	806	GLU	2.0
1	A	845	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
2	PO4	B	1001	5/5	0.79	0.42	190,196,200,202	0
2	PO4	A	1001	5/5	0.92	0.21	141,143,149,150	0

6.5 Other polymers ⓘ

There are no such residues in this entry.