



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:28 PM GMT

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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

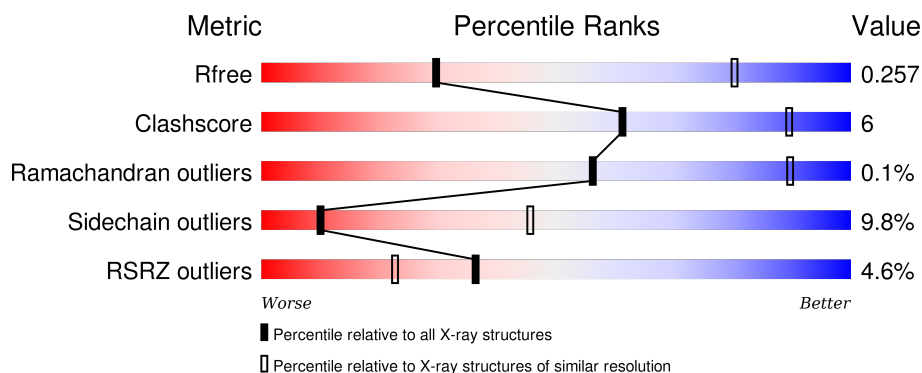
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1010 (3.82-3.50)
Clashscore	102246	1125 (3.82-3.50)
Ramachandran outliers	100387	1079 (3.82-3.50)
Sidechain outliers	100360	1078 (3.82-3.50)
RSRZ outliers	91569	1017 (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 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 $\leq 5\%$. 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	832	
1	B	832	

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			

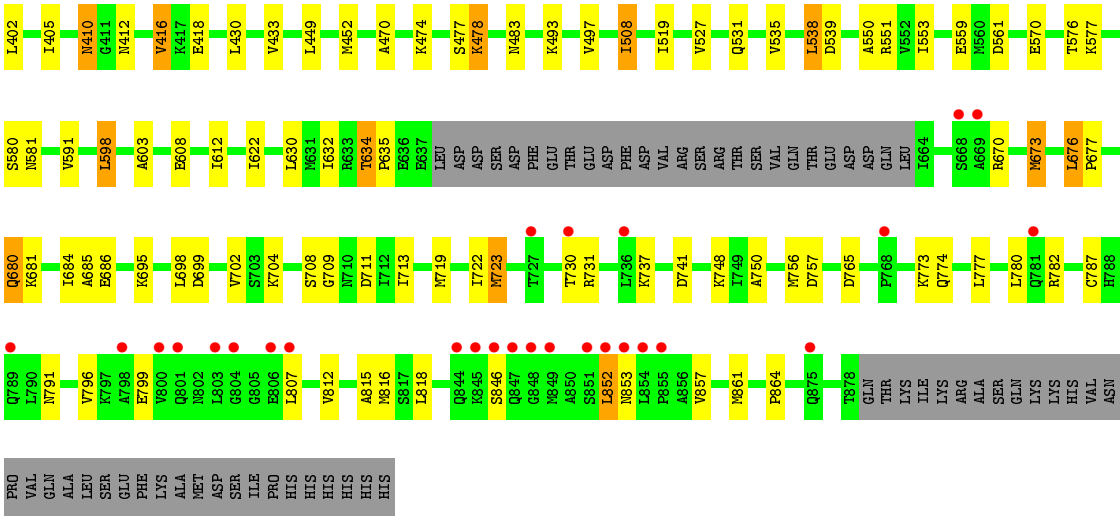
There are 14 discrepancies between the modelled and reference sequences:

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: O₄P).



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		



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
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.67Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.217 , 0.241 0.232 , 0.257	Depositor DCC
R_{free} test set	1822 reflections (5.30%)	DCC
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
Estimated twinning fraction	0.015 for -h,-k,l 0.039 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 36368 reflections	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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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

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

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:B:757:ASP:HA	1:B:780:LEU:HD22	1.88	0.56
1:A:527:VAL:O	1:A:531:GLN:HG3	2.06	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:673:MET:HA	1:B:676:LEU:HD13	1.87	0.55
1:B:90:LEU:O	1:B:94:VAL:HG23	2.07	0.55
1:A:462:PRO:HA	1:A:465:ILE:HG12	1.89	0.54
1:B:846:SER:HB3	1:B:852:LEU:H	1.72	0.54
1:A:213:ILE:HG23	1:A:217:ASN:ND2	2.23	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:508:ILE:HD13	1:A:559:GLU:HG2	1.93	0.49
1:A:161:ILE:HD13	1:A:248:LEU:HD22	1.94	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: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:169:ASN:ND2	1:A:172:ASP:OD2	2.49	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:B:777:LEU:HA	1:B:780:LEU:HD12	2.00	0.44
1:B:93:ALA:O	1:B:97:VAL:HG23	2.17	0.44
1:A:634:THR:HB	1:A:758:LYS:HE3	2.00	0.44
1:A:563:TYR:HD2	1:A:857:VAL:HG23	1.82	0.44
1:B:673:MET:HG2	1:B:730:THR:HA	2.00	0.43
1:B:550:ALA:HA	1:B:553:ILE:HD12	1.99	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:553:ILE:HG23	1:B:576:THR:HB	2.01	0.42
1:B:410:ASN:HD22	1:B:410:ASN:N	2.17	0.42
1:A:195:GLN:HG3	1:A:207:MET:HB3	1.99	0.42
1:B:812:VAL:HG22	1:B:815:ALA:HB3	2.00	0.42
1:B:230:GLN:C	1:B:232:PRO:HD3	2.39	0.42
1:A:719:MET:O	1:A:723:MET:HB2	2.20	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:B:630:LEU:HD23	1:B:680:GLN:HE22	1.84	0.42
1:A:808:VAL:HG11	1:B:203:HIS:NE2	2.35	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:H	1:B:277:GLU:CD	2.24	0.41
1:B:219:PRO:O	1:B:222:TYR:HB3	2.19	0.41
1:A:672:ILE:HG13	1:B:148:TYR:HD1	1.84	0.41
1:A:617:LEU:HA	1:A:617:LEU:HD12	1.96	0.41
1:A:523:VAL:HG11	1:A:618:VAL:CG2	2.50	0.41
1:B:412:ASN:O	1:B:416:VAL:HG22	2.21	0.41
1:B:272:GLY:HA2	1:B:273:GLY:HA2	1.86	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 [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	746/832 (90%)	713 (96%)	33 (4%)	0	100	100
1	B	767/832 (92%)	741 (97%)	24 (3%)	2 (0%)	46	83
All	All	1513/1664 (91%)	1454 (96%)	57 (4%)	2 (0%)	56	90

All (2) Ramachandran outliers are listed below:

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

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	621/698 (89%)	568 (92%)	53 (8%)	13	53
1	B	640/698 (92%)	570 (89%)	70 (11%)	8	41
All	All	1261/1396 (90%)	1138 (90%)	123 (10%)	10	45

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

Some 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 ⓘ

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](#)

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	A	1001	-	4,4,4	0.80	0	6,6,6	0.28	0
2	PO4	B	1001	-	4,4,4	0.73	0	6,6,6	0.27	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
2	PO4	A	1001	-	-	0/0/0/0	0/0/0/0
2	PO4	B	1001	-	-	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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.55	29 (3%)	43 28	49, 117, 184, 241	8 (1%)
1	B	771/832 (92%)	0.60	41 (5%)	30 18	72, 122, 195, 262	8 (1%)
All	All	1521/1664 (91%)	0.58	70 (4%)	36 23	49, 120, 192, 262	16 (1%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	270	HIS	10.5
1	B	853	ASN	6.6
1	B	848	GLY	6.5
1	B	265	ASP	6.2
1	B	264	SER	5.6
1	B	271	GLN	5.3
1	B	272	GLY	5.0
1	B	269	GLN	4.9
1	A	355	ALA	4.9
1	B	669	ALA	4.8
1	A	296	PHE	4.4
1	B	847	GLN	4.1
1	A	707	ASP	4.0
1	B	852	LEU	3.7
1	B	803	LEU	3.6
1	B	845	LYS	3.6
1	A	731	ARG	3.5
1	B	263	ALA	3.5
1	B	668	SER	3.4
1	A	809	VAL	3.4
1	B	736	LEU	3.1
1	B	730	THR	3.1
1	B	854	LEU	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	B	262	THR	2.7
1	A	297	SER	2.7
1	A	733	LYS	2.7
1	A	299	GLU	2.7
1	A	706	ASP	2.6
1	A	806	GLU	2.6
1	B	846	SER	2.6
1	B	800	VAL	2.6
1	B	789	GLN	2.6
1	A	850	ALA	2.6
1	A	803	LEU	2.5
1	B	273	GLY	2.5
1	B	798	ALA	2.4
1	B	257	ASN	2.4
1	B	261	ALA	2.4
1	B	362	ASP	2.4
1	B	804	GLY	2.4
1	A	698	LEU	2.4
1	B	781	GLN	2.3
1	B	359	GLU	2.3
1	A	303	PRO	2.3
1	A	275	GLY	2.3
1	A	819	ILE	2.3
1	B	82	GLU	2.3
1	B	807	LEU	2.2
1	A	726	MET	2.2
1	B	851	SER	2.2
1	A	702	VAL	2.2
1	B	855	PRO	2.2
1	A	356	GLY	2.2
1	B	875	GLN	2.2
1	A	808	VAL	2.2
1	A	737	LYS	2.2
1	A	87	LYS	2.1
1	A	832	THR	2.1
1	A	708	SER	2.1
1	B	806	GLU	2.1
1	B	768	PRO	2.1
1	B	727	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	796	VAL	2.0
1	A	633	ARG	2.0
1	B	801	GLN	2.0
1	B	844	GLN	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
2	PO4	B	1001	5/5	0.79	0.42	2.38	190,196,200,202	0
2	PO4	A	1001	5/5	0.92	0.21	-3.53	141,143,149,150	0

6.5 Other polymers [i](#)

There are no such residues in this entry.