



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:08 PM UTC

PDB ID : 4IGG / pdb_00004igg
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

<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

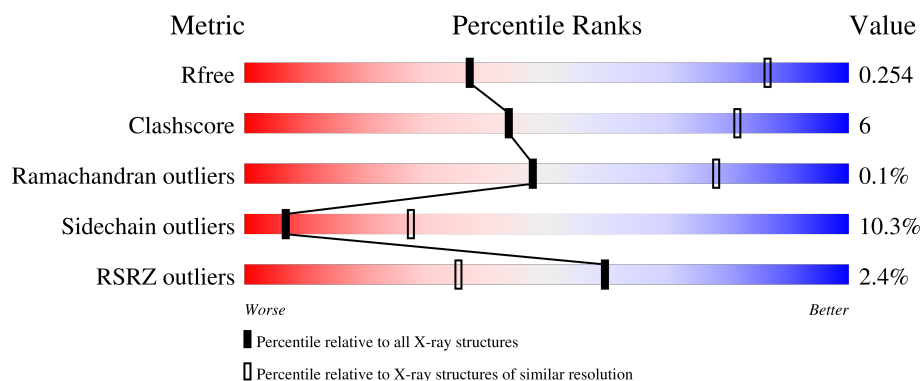
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

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	832	2% 70%18%10%
1	B	832	2% 72%18%7%

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.

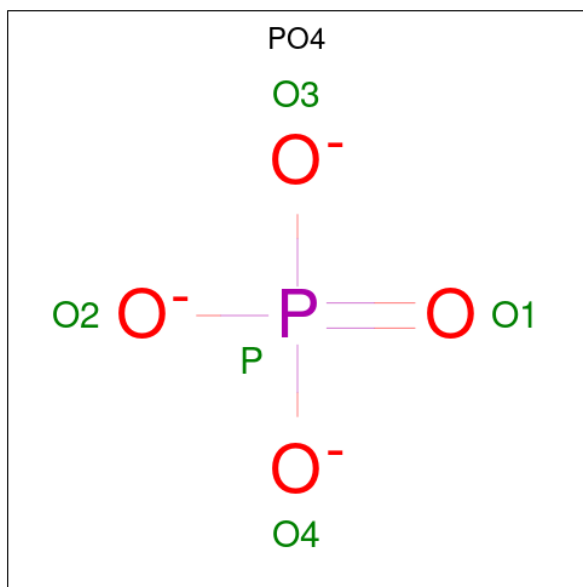
- Molecule 1 is a protein called Catenin alpha-1.

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 (CCD ID: PO4) (formula: O₄P).

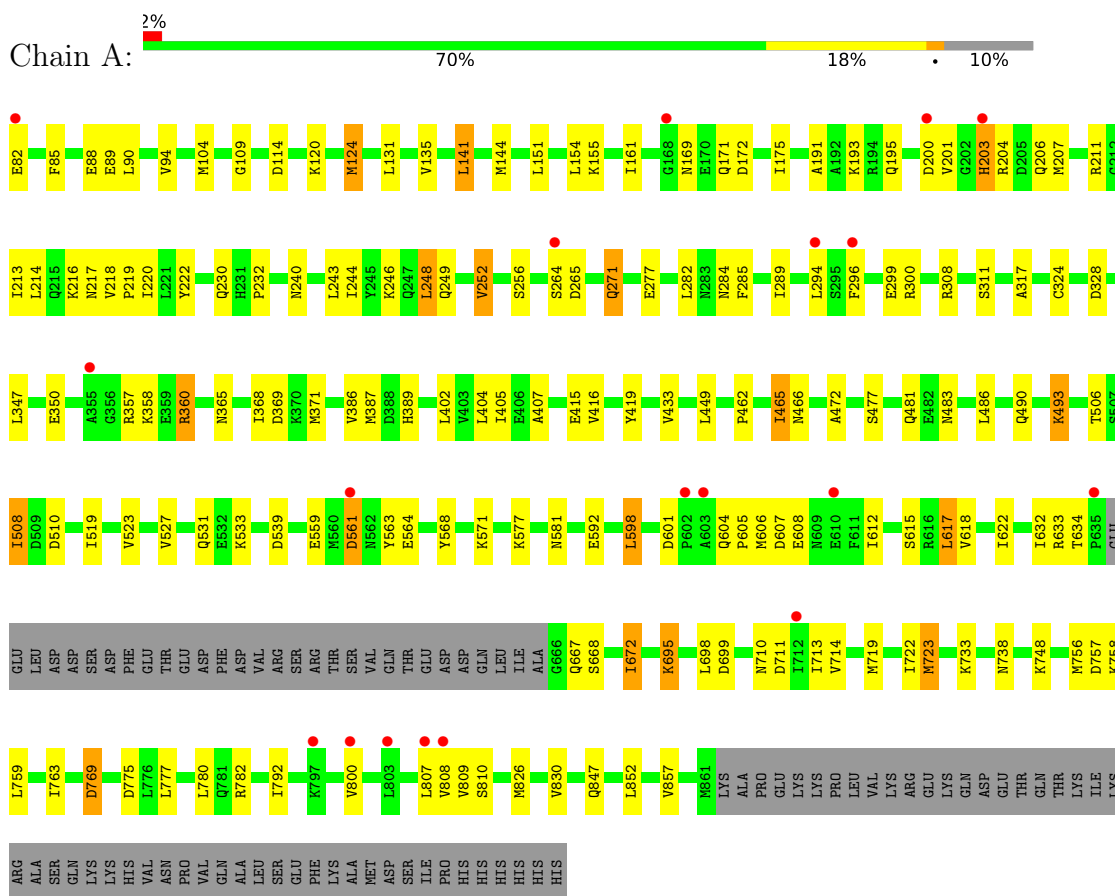


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

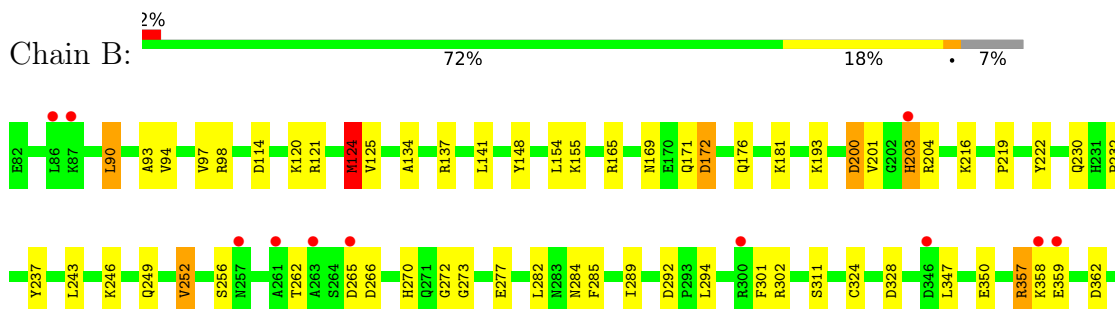
3 Residue-property plots

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: Catenin alpha-1



• Molecule 1: Catenin alpha-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 23.21 – 3.66	Depositor EDS
% Data completeness (in resolution range)	99.9 (23.21-3.66) 99.5 (23.21-3.66)	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	TNT, BUSTER 2.11.2	Depositor
R, R_{free}	0.217 , 0.241 0.229 , 0.254	Depositor DCC
R_{free} test set	1828 reflections (5.02%)	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)	0.30 , 108.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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	0.93	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.*

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

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	0.71	2/5825 (0.0%)	1.30	14/7848 (0.2%)
1	B	0.75	4/5999 (0.1%)	1.37	9/8080 (0.1%)
All	All	0.73	6/11824 (0.1%)	1.33	23/15928 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	HIS	CG-ND1	7.60	1.46	1.38
1	B	203	HIS	CE1-NE2	6.29	1.38	1.32
1	B	203	HIS	CD2-NE2	6.01	1.44	1.37
1	A	203	HIS	CE1-NE2	5.12	1.37	1.32
1	B	124	MET	SD-CE	-5.03	1.67	1.79
1	A	203	HIS	CG-ND1	5.01	1.43	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	561	ASP	CA-CB-CG	9.30	121.90	112.60
1	A	296	PHE	CA-CB-CG	6.40	120.20	113.80
1	A	360	ARG	CA-C-N	5.74	128.24	120.38
1	A	360	ARG	C-N-CA	5.74	128.24	120.38
1	A	769	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	265	ASP	CA-CB-CG	5.60	118.20	112.60
1	B	416	VAL	N-CA-CB	5.55	116.67	110.62
1	B	252	VAL	N-CA-CB	5.37	116.83	110.55
1	A	252	VAL	N-CA-CB	5.29	116.75	110.55
1	A	82	GLU	CA-C-N	5.22	128.51	121.05
1	A	82	GLU	C-N-CA	5.22	128.51	121.05
1	B	523	VAL	N-CA-CB	5.21	118.40	110.58
1	A	792	ILE	CA-C-N	5.19	127.49	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	792	ILE	C-N-CA	5.19	127.49	120.38
1	A	607	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	810	SER	CA-C-N	5.11	125.61	119.94
1	A	810	SER	C-N-CA	5.11	125.61	119.94
1	B	706	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	412	ASN	CA-C-N	5.07	128.79	120.63
1	B	412	ASN	C-N-CA	5.07	128.79	120.63
1	B	125	VAL	CA-C-N	5.03	127.27	120.38
1	B	125	VAL	C-N-CA	5.03	127.27	120.38
1	B	169	ASN	CA-CB-CG	5.03	117.63	112.60

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	83	0
1	B	5938	0	6038	69	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
All	All	11714	0	11894	143	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 (143) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:MET:HE1	1:A:506:THR:HB	1.77	0.66
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: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:B:704:LYS:HB2	1:B:861:MET:HE3	1.89	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:230:GLN:C	1:A:232:PRO:HD3	2.35	0.51
1:A:387:MET:HE3	1:A:510:ASP:HB2	1.91	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:MET:HE1	1:B:870:VAL:HA	1.94	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:B:285:PHE:HE1	1:B:371:MET:HE2	1.79	0.48
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:104:MET:HE2	1:B:97:VAL:HG11	1.96	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:B:230:GLN:C	1:B:232:PRO:HD3	2.39	0.47
1:A:415:GLU:HG2	1:A:419:TYR:CE2	2.49	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:A:723:MET:HE3	1:A:826:MET:SD	2.55	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:A:695:LYS:HA	1:A:826:MET:HE2	1.96	0.46
1:B:277:GLU:CD	1:B:277:GLU:H	2.24	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:A:285:PHE:HE1	1:A:371:MET:HE2	1.81	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASN:HA	1:A:466:ASN:HD22	1.82	0.45
1:B:387:MET:HE3	1:B:390:VAL:HB	1.99	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
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:A:277:GLU:H	1:A:277:GLU:CD	2.26	0.43
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:VAL:HG11	1:A:618:VAL:CG2	2.50	0.41
1:B:726:MET:HE2	1:B:818:LEU:HD11	2.02	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
1:B:285:PHE:CE1	1:B:371:MET:HE2	2.56	0.41
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
1:A:285:PHE:CE1	1:A:371:MET:HE2	2.57	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%)	36	64
All	All	1513/1664 (91%)	1454 (96%)	57 (4%)	2 (0%)	48	78

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%)	566 (91%)	55 (9%)	9	31
1	B	640/698 (92%)	565 (88%)	75 (12%)	5	23
All	All	1261/1396 (90%)	1131 (90%)	130 (10%)	7	27

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	MET
1	A	141	LEU
1	A	155	LYS
1	A	171	GLN
1	A	193	LYS
1	A	243	LEU
1	A	248	LEU
1	A	264	SER
1	A	271	GLN
1	A	282	LEU
1	A	284	ASN
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	369	ASP
1	A	386	VAL
1	A	449	LEU
1	A	465	ILE
1	A	483	ASN
1	A	486	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	493	LYS
1	A	508	ILE
1	A	539	ASP
1	A	561	ASP
1	A	564	GLU
1	A	571	LYS
1	A	592	GLU
1	A	598	LEU
1	A	601	ASP
1	A	606	MET
1	A	617	LEU
1	A	633	ARG
1	A	667	GLN
1	A	672	ILE
1	A	695	LYS
1	A	699	ASP
1	A	713	ILE
1	A	723	MET
1	A	733	LYS
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	809	VAL
1	A	847	GLN
1	B	90	LEU
1	B	124	MET
1	B	141	LEU
1	B	155	LYS
1	B	165	ARG
1	B	171	GLN
1	B	172	ASP
1	B	181	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	266	ASP
1	B	270	HIS
1	B	282	LEU
1	B	284	ASN
1	B	289	ILE
1	B	294	LEU
1	B	302	ARG
1	B	311	SER
1	B	328	ASP
1	B	347	LEU
1	B	350	GLU
1	B	357	ARG
1	B	358	LYS
1	B	359	GLU
1	B	362	ASP
1	B	369	ASP
1	B	386	VAL
1	B	387	MET
1	B	410	ASN
1	B	416	VAL
1	B	418	GLU
1	B	449	LEU
1	B	465	ILE
1	B	478	LYS
1	B	483	ASN
1	B	508	ILE
1	B	538	LEU
1	B	539	ASP
1	B	567	VAL
1	B	570	GLU
1	B	592	GLU
1	B	598	LEU
1	B	604	GLN
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	699	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	702	VAL
1	B	713	ILE
1	B	723	MET
1	B	747	LYS
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	801	GLN
1	B	807	LEU
1	B	808	VAL
1	B	816	MET
1	B	818	LEU
1	B	838	VAL
1	B	852	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	123	ASN
1	A	169	ASN
1	A	176	GLN
1	A	203	HIS
1	A	215	GLN
1	A	217	ASN
1	A	226	GLN
1	A	240	ASN
1	A	249	GLN
1	A	260	GLN
1	A	271	GLN
1	A	288	GLN
1	A	398	ASN
1	A	412	ASN
1	A	428	ASN
1	A	466	ASN
1	A	581	ASN
1	A	604	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	687	GLN
1	A	692	GLN
1	A	738	ASN
1	A	774	GLN
1	A	820	GLN
1	A	824	ASN
1	A	831	GLN
1	A	844	GLN
1	A	853	ASN
1	B	100	GLN
1	B	123	ASN
1	B	176	GLN
1	B	215	GLN
1	B	226	GLN
1	B	257	ASN
1	B	398	ASN
1	B	410	ASN
1	B	463	GLN
1	B	581	ASN
1	B	590	GLN
1	B	675	GLN
1	B	680	GLN
1	B	692	GLN
1	B	781	GLN
1	B	791	ASN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	1.25	1 (25%)	6,6,6	0.44	0
2	PO4	A	1001	-	4,4,4	1.27	1 (25%)	6,6,6	0.56	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	2.40	1.56	1.50
2	A	1001	PO4	P-O1	2.36	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%)	0.15	19 (2%) 58 35	49, 117, 184, 241	8 (1%)
1	B	771/832 (92%)	0.12	17 (2%) 62 37	72, 121, 195, 262	8 (1%)
All	All	1521/1664 (91%)	0.14	36 (2%) 59 35	49, 120, 192, 262	16 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	798	ALA	4.3
1	B	359	GLU	3.9
1	B	203	HIS	3.6
1	B	300	ARG	3.5
1	B	803	LEU	3.5
1	A	800	VAL	3.4
1	A	602	PRO	3.4
1	A	294	LEU	3.3
1	B	86	LEU	3.3
1	B	87	LYS	3.3
1	A	355	ALA	3.1
1	B	483	ASN	3.0
1	B	261	ALA	2.8
1	A	264	SER	2.7
1	A	712	ILE	2.5
1	A	603	ALA	2.4
1	A	635	PRO	2.4
1	B	358	LYS	2.4
1	B	257	ASN	2.4
1	A	82	GLU	2.4
1	B	263	ALA	2.4
1	A	200	ASP	2.3
1	B	854	LEU	2.3
1	A	296	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	803	LEU	2.3
1	B	346	ASP	2.3
1	B	710	ASN	2.2
1	A	808	VAL	2.2
1	A	561	ASP	2.1
1	A	203	HIS	2.1
1	B	763	ILE	2.1
1	A	807	LEU	2.1
1	A	797	LYS	2.1
1	A	610	GLU	2.0
1	A	168	GLY	2.0
1	B	265	ASP	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($\text{\AA}^2$)	Q<0.9
2	PO4	B	1001	5/5	0.84	0.15	190,196,200,202	0
2	PO4	A	1001	5/5	0.88	0.09	141,143,149,150	0

6.5 Other polymers [i](#)

There are no such residues in this entry.