



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:03 AM UTC

PDB ID : 1K05 / pdb_00001k05
Title : Crystal structure of the Focal Adhesion Targeting Domain of Focal Adhesion Kinase
Authors : Arold, S.T.; Hoellerer, M.K.; Noble, M.E.M.
Deposited on : 2001-09-18
Resolution : 2.90 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
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

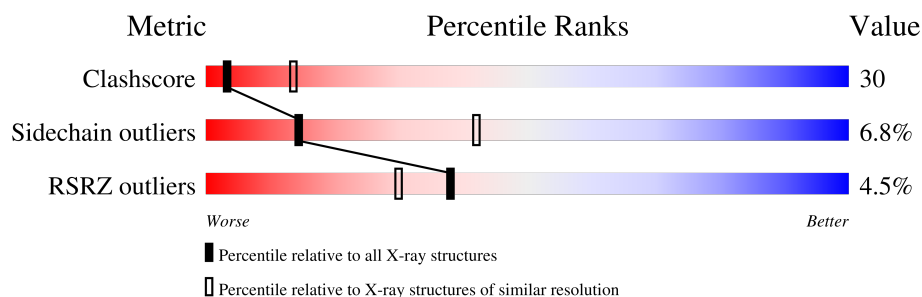
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	162	2% 42% 36% 5% • 17%
1	B	162	2% 45% 36% 6% • 12%
1	C	162	7% 41% 43% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3257 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 FOCAL ADHESION KINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			1053	664	180	202	7			
1	B	142	Total	C	N	O	S	0	0	0
			1098	695	184	212	7			
1	C	142	Total	C	N	O	S	0	0	0
			1100	695	185	213	7			

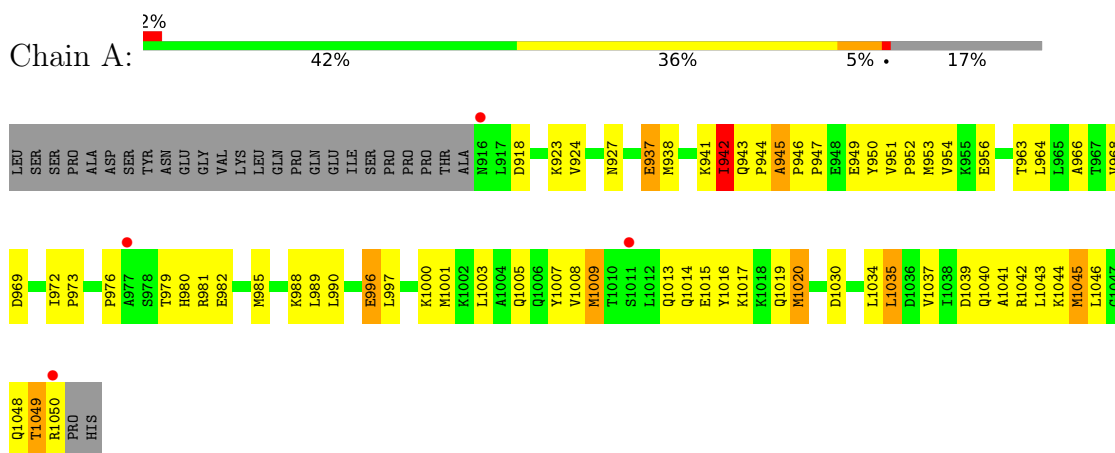
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		
2	C	5	Total	O	0	0
			5	5		

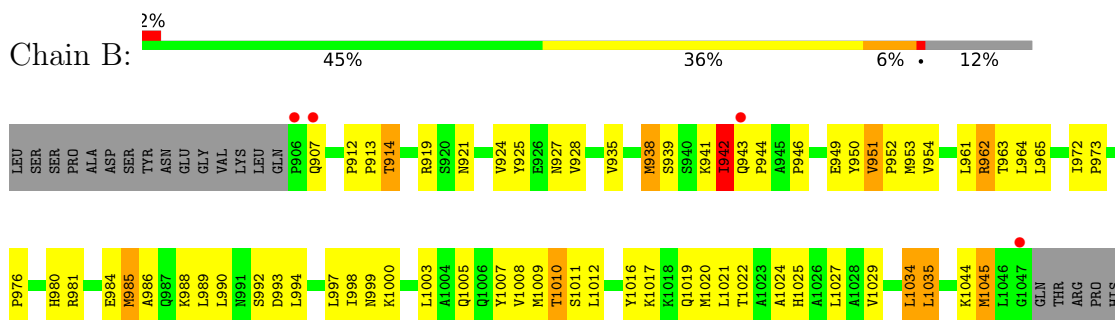
3 Residue-property plots

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.

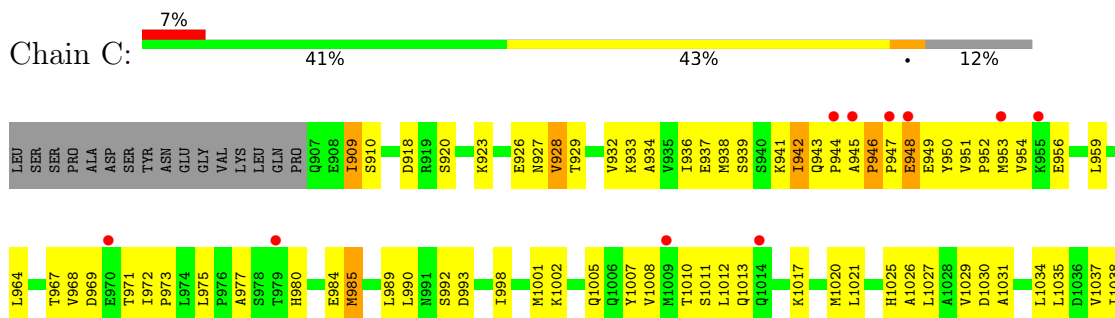
• Molecule 1: FOCAL ADHESION KINASE 1



• Molecule 1: FOCAL ADHESION KINASE 1



• Molecule 1: FOCAL ADHESION KINASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	87.48Å 222.10Å 97.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.30 – 2.90 31.30 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (31.30-2.90) 96.0 (31.30-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.245 , 0.285 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	77.8	Xtriage
Anisotropy	0.522	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3257	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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

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	0.56	0/1064	1.04	6/1438 (0.4%)
1	B	0.59	0/1113	1.05	7/1509 (0.5%)
1	C	0.53	0/1114	1.02	6/1510 (0.4%)
All	All	0.56	0/3291	1.04	19/4457 (0.4%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	942	ILE	N-CA-C	11.51	121.47	110.42
1	A	945	ALA	N-CA-C	9.20	122.35	110.39
1	A	1020	MET	N-CA-C	-7.05	103.52	111.07
1	A	945	ALA	CA-C-N	6.91	127.50	120.38
1	A	945	ALA	C-N-CA	6.91	127.50	120.38
1	B	950	TYR	CA-C-N	-6.35	116.24	120.24
1	B	950	TYR	C-N-CA	-6.35	116.24	120.24
1	C	945	ALA	CA-C-N	6.17	126.74	120.38
1	C	945	ALA	C-N-CA	6.17	126.74	120.38
1	B	951	VAL	CB-CA-C	-5.91	108.09	114.35
1	C	928	VAL	N-CA-C	-5.87	104.19	110.36
1	C	942	ILE	N-CA-C	5.78	121.36	109.34
1	B	942	ILE	N-CA-C	5.73	121.27	109.34
1	B	1034	LEU	N-CA-C	-5.53	105.15	111.07
1	B	998	ILE	N-CA-C	5.52	115.72	110.42
1	C	946	PRO	CA-C-N	5.48	126.69	119.84
1	C	946	PRO	C-N-CA	5.48	126.69	119.84
1	A	1049	THR	N-CA-C	5.09	117.38	109.60
1	B	912	PRO	N-CA-C	-5.08	105.14	110.58

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	1053	0	1106	64	0
1	B	1098	0	1149	68	0
1	C	1100	0	1149	76	0
2	A	1	0	0	0	0
2	C	5	0	0	0	0
All	All	3257	0	3404	203	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 30.

All (203) 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:976:PRO:HD3	1:A:1045:MET:HG2	1.43	1.01
1:A:1049:THR:HG22	1:A:1050:ARG:H	1.33	0.92
1:C:943:GLN:HB2	1:C:944:PRO:HD3	1.53	0.88
1:A:1013:GLN:HG3	1:A:1014:GLN:H	1.38	0.87
1:B:938:MET:HE2	1:B:954:VAL:HG22	1.57	0.85
1:B:1000:LYS:HD2	1:B:1019:GLN:HB3	1.58	0.83
1:C:942:ILE:HD13	1:C:1020:MET:HE3	1.58	0.83
1:A:1013:GLN:HG3	1:A:1014:GLN:N	1.89	0.82
1:C:972:ILE:HA	1:C:975:LEU:HD12	1.64	0.80
1:B:924:VAL:O	1:B:928:VAL:HG23	1.82	0.80
1:A:1045:MET:HA	1:A:1045:MET:HE2	1.64	0.79
1:C:964:LEU:O	1:C:968:VAL:HG23	1.84	0.77
1:B:943:GLN:HB2	1:B:944:PRO:HD3	1.66	0.75
1:B:985:MET:HE3	1:B:985:MET:HA	1.69	0.75
1:A:1008:VAL:HB	1:A:1009:MET:HE2	1.69	0.74
1:C:950:TYR:HA	1:C:953:MET:HE3	1.69	0.74
1:B:927:ASN:HD22	1:B:964:LEU:HA	1.52	0.73
1:B:985:MET:HG3	1:C:1012:LEU:HG	1.69	0.73
1:C:943:GLN:CB	1:C:944:PRO:HD3	2.19	0.72
1:B:927:ASN:ND2	1:B:963:THR:HG22	2.04	0.72
1:A:976:PRO:HD3	1:A:1045:MET:CG	2.19	0.72
1:A:942:ILE:HD11	1:A:1020:MET:HE2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:949:GLU:O	1:C:953:MET:HG3	1.91	0.71
1:A:976:PRO:CD	1:A:1045:MET:HG2	2.20	0.71
1:C:985:MET:HA	1:C:985:MET:HE3	1.73	0.70
1:C:969:ASP:O	1:C:973:PRO:HD3	1.94	0.68
1:C:1007:TYR:HB3	1:C:1010:THR:OG1	1.93	0.68
1:B:980:HIS:O	1:B:984:GLU:HG3	1.94	0.67
1:C:942:ILE:CD1	1:C:1020:MET:HE3	2.23	0.67
1:A:950:TYR:O	1:A:954:VAL:HG23	1.95	0.67
1:B:935:VAL:HG13	1:B:1024:ALA:HB1	1.78	0.66
1:B:1007:TYR:HD2	1:B:1010:THR:HG21	1.62	0.65
1:A:985:MET:HE3	1:A:985:MET:HA	1.78	0.64
1:C:923:LYS:HB3	1:C:967:THR:HG21	1.79	0.64
1:C:968:VAL:O	1:C:972:ILE:HG13	1.97	0.64
1:B:938:MET:HE1	1:B:997:LEU:HD11	1.79	0.64
1:A:972:ILE:HB	1:A:973:PRO:HD3	1.81	0.63
1:C:1025:HIS:O	1:C:1029:VAL:HG23	1.98	0.62
1:C:942:ILE:O	1:C:943:GLN:C	2.42	0.62
1:C:969:ASP:HA	1:C:972:ILE:CD1	2.30	0.62
1:A:1042:ARG:O	1:A:1046:LEU:HG	1.99	0.62
1:B:941:LYS:CB	1:B:953:MET:HE1	2.28	0.62
1:C:1017:LYS:O	1:C:1020:MET:HB3	2.00	0.61
1:B:927:ASN:HD21	1:B:963:THR:HG22	1.65	0.61
1:B:1000:LYS:HD2	1:B:1019:GLN:CB	2.31	0.61
1:B:942:ILE:HG22	1:B:943:GLN:N	2.16	0.61
1:B:941:LYS:HB2	1:B:953:MET:HE1	1.82	0.61
1:B:999:ASN:O	1:B:1003:LEU:HD12	2.01	0.61
1:C:938:MET:HE1	1:C:954:VAL:HG22	1.82	0.61
1:A:989:LEU:HD21	1:A:1030:ASP:CG	2.26	0.60
1:C:950:TYR:O	1:C:954:VAL:HG23	2.02	0.60
1:B:919:ARG:HD2	1:B:925:TYR:CD2	2.36	0.59
1:A:1049:THR:HG22	1:A:1050:ARG:N	2.12	0.59
1:A:1005:GLN:O	1:A:1008:VAL:HG22	2.02	0.59
1:C:928:VAL:HG21	1:C:1035:LEU:HB2	1.84	0.59
1:B:949:GLU:O	1:B:952:PRO:HG2	2.02	0.58
1:C:1035:LEU:HD23	1:C:1035:LEU:O	2.03	0.58
1:A:927:ASN:ND2	1:A:963:THR:HG22	2.18	0.58
1:A:923:LYS:O	1:A:924:VAL:C	2.44	0.58
1:A:1003:LEU:HD13	1:A:1016:TYR:CE1	2.38	0.58
1:C:971:THR:HG22	1:C:975:LEU:HD11	1.86	0.57
1:C:943:GLN:HB2	1:C:944:PRO:CD	2.31	0.57
1:A:943:GLN:HB2	1:A:944:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:PRO:HG3	1:A:950:TYR:OH	2.05	0.56
1:B:976:PRO:HG3	1:B:1045:MET:HG2	1.86	0.56
1:B:1000:LYS:HE3	1:B:1019:GLN:OE1	2.05	0.56
1:C:950:TYR:CA	1:C:953:MET:HE3	2.35	0.56
1:A:1040:GLN:O	1:A:1041:ALA:C	2.48	0.56
1:A:1005:GLN:O	1:A:1008:VAL:CG2	2.54	0.56
1:B:942:ILE:HG23	1:B:1017:LYS:HD3	1.89	0.55
1:B:1012:LEU:HG	1:C:985:MET:HG3	1.89	0.55
1:A:1008:VAL:O	1:A:1013:GLN:HB3	2.07	0.55
1:B:972:ILE:HB	1:B:973:PRO:HD3	1.88	0.54
1:C:1002:LYS:O	1:C:1005:GLN:HB2	2.07	0.54
1:C:1007:TYR:CE2	1:C:1012:LEU:HD12	2.42	0.54
1:A:953:MET:O	1:A:956:GLU:HB2	2.06	0.54
1:B:1003:LEU:HD22	1:B:1016:TYR:CZ	2.42	0.54
1:C:942:ILE:HD13	1:C:1020:MET:CE	2.36	0.54
1:C:968:VAL:HG13	1:C:1038:ILE:HD11	1.90	0.53
1:A:982:GLU:HG2	1:A:1037:VAL:HG11	1.90	0.53
1:C:909:ILE:C	1:C:909:ILE:HD13	2.33	0.53
1:C:1007:TYR:O	1:C:1013:GLN:HB2	2.08	0.53
1:B:946:PRO:HD2	1:B:949:GLU:HG3	1.90	0.53
1:C:932:VAL:O	1:C:936:ILE:HG13	2.10	0.52
1:B:942:ILE:CG2	1:B:943:GLN:N	2.72	0.52
1:B:951:VAL:N	1:B:952:PRO:HD2	2.25	0.52
1:B:994:LEU:O	1:B:997:LEU:HB3	2.10	0.52
1:C:948:GLU:HA	1:C:948:GLU:OE1	2.09	0.52
1:A:985:MET:CE	1:A:988:LYS:HD2	2.40	0.51
1:C:1005:GLN:O	1:C:1008:VAL:HG23	2.11	0.51
1:A:1045:MET:HA	1:A:1045:MET:CE	2.38	0.51
1:A:938:MET:HE2	1:A:954:VAL:HG22	1.93	0.51
1:C:941:LYS:O	1:C:944:PRO:HD2	2.10	0.51
1:C:947:PRO:HG2	1:C:1008:VAL:HG13	1.92	0.51
1:A:1007:TYR:O	1:A:1008:VAL:O	2.30	0.50
1:B:989:LEU:HD12	1:B:989:LEU:O	2.12	0.50
1:A:1044:LYS:HE3	1:B:921:ASN:HD21	1.77	0.50
1:A:976:PRO:HG3	1:A:1045:MET:HE3	1.93	0.50
1:C:973:PRO:C	1:C:975:LEU:H	2.20	0.50
1:A:951:VAL:HG22	1:A:1001:MET:SD	2.52	0.50
1:C:1035:LEU:HD23	1:C:1035:LEU:C	2.36	0.49
1:A:1043:LEU:HD13	1:A:1048:GLN:OE1	2.12	0.48
1:B:976:PRO:O	1:B:980:HIS:HD2	1.95	0.48
1:B:1007:TYR:CD2	1:B:1010:THR:HG21	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:949:GLU:C	1:C:952:PRO:HD2	2.38	0.48
1:A:1044:LYS:HE3	1:B:921:ASN:ND2	2.27	0.48
1:B:1007:TYR:HB3	1:B:1010:THR:CG2	2.43	0.48
1:A:947:PRO:C	1:A:949:GLU:H	2.19	0.48
1:A:1007:TYR:CD1	1:A:1016:TYR:CE2	3.02	0.48
1:B:961:LEU:HG	1:B:965:LEU:CD1	2.43	0.48
1:C:956:GLU:O	1:C:959:LEU:HB3	2.14	0.48
1:B:1003:LEU:HD22	1:B:1016:TYR:CE1	2.49	0.48
1:A:945:ALA:HA	1:A:946:PRO:HD3	1.63	0.47
1:B:981:ARG:HA	1:B:984:GLU:OE1	2.14	0.47
1:A:979:THR:O	1:A:980:HIS:C	2.56	0.47
1:C:933:LYS:O	1:C:934:ALA:C	2.57	0.47
1:C:951:VAL:N	1:C:952:PRO:HD2	2.28	0.47
1:C:969:ASP:HA	1:C:972:ILE:HD11	1.96	0.47
1:B:986:ALA:CB	1:B:1034:LEU:HD13	2.45	0.47
1:B:990:LEU:O	1:B:993:ASP:HB2	2.15	0.47
1:A:1009:MET:HE2	1:A:1009:MET:H	1.80	0.47
1:C:947:PRO:HG3	1:C:950:TYR:OH	2.15	0.47
1:B:939:SER:HB2	1:B:1021:LEU:HD22	1.97	0.47
1:B:985:MET:HA	1:B:985:MET:CE	2.42	0.47
1:C:918:ASP:C	1:C:920:SER:H	2.23	0.47
1:B:961:LEU:HD13	1:B:1027:LEU:HD11	1.97	0.46
1:C:927:ASN:O	1:C:928:VAL:C	2.58	0.46
1:A:945:ALA:O	1:A:1017:LYS:NZ	2.48	0.46
1:B:1005:GLN:O	1:B:1008:VAL:HG23	2.15	0.46
1:C:990:LEU:HD21	1:C:1031:ALA:CA	2.46	0.46
1:C:985:MET:HA	1:C:985:MET:CE	2.44	0.46
1:A:947:PRO:HA	1:A:950:TYR:CZ	2.52	0.45
1:B:1017:LYS:O	1:B:1020:MET:HB2	2.15	0.45
1:C:977:ALA:HA	1:C:980:HIS:CD2	2.51	0.45
1:C:938:MET:CE	1:C:954:VAL:HG22	2.44	0.45
1:C:939:SER:HA	1:C:1021:LEU:HD21	1.99	0.45
1:B:980:HIS:O	1:B:981:ARG:C	2.60	0.45
1:C:989:LEU:O	1:C:992:SER:HB3	2.17	0.45
1:A:990:LEU:CD1	1:A:1034:LEU:HD22	2.47	0.45
1:B:941:LYS:HB2	1:B:953:MET:CE	2.46	0.45
1:C:943:GLN:CB	1:C:944:PRO:CD	2.90	0.45
1:A:969:ASP:O	1:A:973:PRO:HD3	2.17	0.44
1:A:1035:LEU:HD22	1:A:1039:ASP:OD2	2.17	0.44
1:A:1013:GLN:HG3	1:A:1014:GLN:HG2	1.99	0.44
1:B:928:VAL:HG21	1:B:1035:LEU:HG	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1025:HIS:O	1:B:1029:VAL:HG23	2.17	0.44
1:C:942:ILE:HG22	1:C:943:GLN:N	2.33	0.44
1:A:964:LEU:HD21	1:A:1034:LEU:HD23	1.99	0.44
1:B:993:ASP:O	1:B:994:LEU:C	2.60	0.44
1:A:1016:TYR:HA	1:A:1019:GLN:NE2	2.33	0.44
1:C:926:GLU:O	1:C:929:THR:HB	2.18	0.44
1:B:976:PRO:O	1:B:980:HIS:CD2	2.70	0.44
1:B:985:MET:HG2	1:C:1011:SER:OG	2.17	0.44
1:C:946:PRO:HA	1:C:947:PRO:HD3	1.83	0.44
1:C:972:ILE:O	1:C:975:LEU:HB2	2.18	0.43
1:C:1047:GLY:C	1:C:1048:GLN:HG3	2.43	0.43
1:C:939:SER:HA	1:C:1021:LEU:CD2	2.48	0.43
1:A:942:ILE:CG2	1:A:943:GLN:N	2.81	0.43
1:A:938:MET:HG3	1:A:953:MET:HB3	2.01	0.43
1:B:986:ALA:HB3	1:B:1034:LEU:HD13	2.01	0.43
1:C:969:ASP:O	1:C:973:PRO:CD	2.66	0.43
1:A:937:GLU:OE2	1:A:941:LYS:HD2	2.19	0.43
1:A:964:LEU:O	1:A:968:VAL:HG23	2.19	0.43
1:B:962:ARG:O	1:B:963:THR:C	2.60	0.43
1:B:913:PRO:O	1:B:914:THR:C	2.62	0.43
1:C:947:PRO:O	1:C:951:VAL:HG23	2.19	0.43
1:C:972:ILE:N	1:C:973:PRO:CD	2.82	0.42
1:C:1026:ALA:O	1:C:1027:LEU:C	2.62	0.42
1:C:946:PRO:HD2	1:C:949:GLU:OE1	2.19	0.42
1:B:976:PRO:HG2	1:B:1044:LYS:HD3	2.01	0.42
1:B:976:PRO:HD3	1:B:1045:MET:CG	2.49	0.42
1:B:1010:THR:HG23	1:B:1011:SER:N	2.33	0.42
1:B:942:ILE:O	1:B:943:GLN:C	2.61	0.42
1:B:980:HIS:CD2	1:B:980:HIS:H	2.36	0.42
1:A:1013:GLN:C	1:A:1015:GLU:N	2.77	0.42
1:A:918:ASP:OD2	1:A:918:ASP:C	2.62	0.42
1:C:998:ILE:O	1:C:1001:MET:HB3	2.19	0.42
1:C:1012:LEU:HD23	1:C:1012:LEU:HA	1.86	0.42
1:C:937:GLU:OE2	1:C:941:LYS:HE3	2.20	0.42
1:C:972:ILE:HG13	1:C:972:ILE:H	1.54	0.41
1:A:989:LEU:CD2	1:A:1030:ASP:CG	2.92	0.41
1:A:1008:VAL:HG12	1:A:1009:MET:N	2.35	0.41
1:A:942:ILE:HD11	1:A:1020:MET:CE	2.47	0.41
1:A:1013:GLN:C	1:A:1015:GLU:H	2.29	0.41
1:A:951:VAL:N	1:A:952:PRO:HD2	2.34	0.41
1:A:1049:THR:CG2	1:A:1050:ARG:H	2.15	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1045:MET:C	1:C:1047:GLY:H	2.28	0.41
1:B:949:GLU:C	1:B:952:PRO:HD2	2.46	0.41
1:C:1037:VAL:O	1:C:1040:GLN:N	2.53	0.41
1:A:966:ALA:O	1:A:969:ASP:HB2	2.20	0.41
1:B:942:ILE:HD11	1:B:1020:MET:CE	2.50	0.41
1:A:938:MET:HE1	1:A:997:LEU:HD21	2.03	0.41
1:A:947:PRO:C	1:A:949:GLU:N	2.79	0.41
1:A:996:GLU:O	1:A:1000:LYS:HG2	2.21	0.41
1:B:951:VAL:N	1:B:952:PRO:CD	2.83	0.41
1:C:923:LYS:HB3	1:C:967:THR:CG2	2.49	0.41
1:C:972:ILE:CA	1:C:975:LEU:HD12	2.43	0.41
1:B:976:PRO:CD	1:B:1045:MET:HG2	2.51	0.41
1:C:990:LEU:CD1	1:C:1034:LEU:HD22	2.51	0.41
1:B:961:LEU:HG	1:B:965:LEU:HD12	2.03	0.40
1:B:999:ASN:OD1	1:B:999:ASN:N	2.53	0.40
1:B:976:PRO:CG	1:B:1045:MET:HG2	2.50	0.40
1:C:993:ASP:OD2	1:C:1030:ASP:OD2	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	118/142 (83%)	111 (94%)	7 (6%)	18	48
1	B	124/142 (87%)	111 (90%)	13 (10%)	6	22
1	C	124/142 (87%)	119 (96%)	5 (4%)	28	62
All	All	366/426 (86%)	341 (93%)	25 (7%)	14	42

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	937	GLU
1	A	942	ILE
1	A	981	ARG
1	A	996	GLU
1	A	1009	MET
1	A	1035	LEU
1	A	1045	MET
1	B	907	GLN
1	B	914	THR
1	B	938	MET
1	B	942	ILE
1	B	962	ARG
1	B	985	MET
1	B	988	LYS
1	B	992	SER
1	B	1009	MET
1	B	1010	THR
1	B	1022	THR
1	B	1035	LEU
1	B	1045	MET
1	C	909	ILE
1	C	910	SER
1	C	948	GLU
1	C	984	GLU
1	C	985	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1005	GLN
1	A	1006	GLN
1	A	1013	GLN
1	B	921	ASN
1	B	927	ASN
1	B	980	HIS
1	C	927	ASN
1	C	991	ASN
1	C	999	ASN
1	C	1033	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	135/162 (83%)	0.28	4 (2%)	52	43	47, 72, 95, 113	0
1	B	142/162 (87%)	0.06	4 (2%)	55	46	45, 69, 87, 123	0
1	C	142/162 (87%)	0.48	11 (7%)	19	16	62, 82, 115, 128	0
All	All	419/486 (86%)	0.27	19 (4%)	38	30	45, 74, 108, 128	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	906	PRO	7.4
1	B	907	GLN	3.4
1	C	1047	GLY	2.7
1	A	977	ALA	2.6
1	B	943	GLN	2.6
1	C	947	PRO	2.6
1	C	945	ALA	2.5
1	C	1009	MET	2.4
1	C	944	PRO	2.4
1	B	1047	GLY	2.3
1	C	953	MET	2.3
1	A	1011	SER	2.3
1	C	1014	GLN	2.2
1	C	970	GLU	2.2
1	A	916	ASN	2.1
1	A	1050	ARG	2.1
1	C	948	GLU	2.1
1	C	979	THR	2.0
1	C	955	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.