



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:34 PM UTC

PDB ID : 3B71 / pdb_00003b71
Title : CD4 endocytosis motif bound to the Focal Adhesion Targeting (FAT) domain
of the Focal Adhesion Kinase
Authors : Garron, M.-L.; Arold, S.T.
Deposited on : 2007-10-30
Resolution : 2.82 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

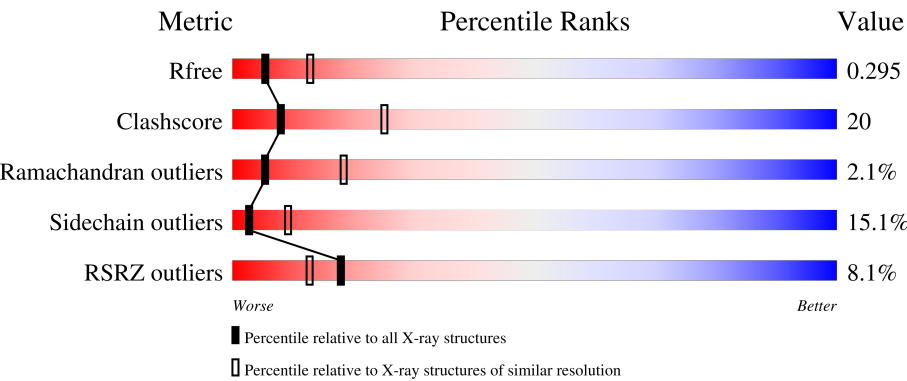
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	49%28%17%
1	B	162	46%33%7%14%
1	C	162	3%48%26%10%14%
2	D	23	48% 17%13%17%52%
2	E	23	43% 17%22%9%52%

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Mol	Chain	Length	Quality of chain
2	F	23	9%17%13%61%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3454 atoms, of which 0 are hydrogens and 0 are deuteriums.

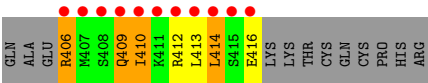
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Focal adhesion kinase 1.

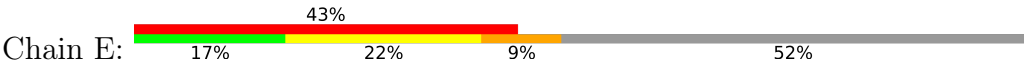
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	1	0
			1048	662	178	201	7			
1	B	139	Total	C	N	O	S	0	0	0
			1073	680	180	206	7			
1	C	139	Total	C	N	O	S	0	0	0
			1073	680	180	206	7			

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

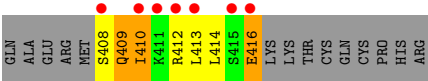
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	11	Total	C	N	O	S	0	0	0
			93	57	19	16	1			
2	E	11	Total	C	N	O	S	0	0	0
			93	57	19	16	1			
2	F	9	Total	C	N	O		0	0	0
			74	46	14	14				



● Molecule 2: T-cell surface glycoprotein CD4



● Molecule 2: T-cell surface glycoprotein CD4



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.07Å 220.47Å 97.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 2.82 29.00 – 2.82	Depositor EDS
% Data completeness (in resolution range)	93.8 (29.00-2.82) 93.8 (29.00-2.82)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.241 , 0.307 0.233 , 0.295	Depositor DCC
R_{free} test set	459 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3454	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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	1.06	3/1064 (0.3%)	1.21	8/1439 (0.6%)
1	B	1.13	4/1087 (0.4%)	1.28	6/1474 (0.4%)
1	C	0.96	1/1087 (0.1%)	1.23	5/1474 (0.3%)
2	D	0.69	0/92	1.14	0/119
2	E	0.87	0/92	0.93	0/119
2	F	1.13	0/73	1.11	1/95 (1.1%)
All	All	1.04	8/3495 (0.2%)	1.23	20/4720 (0.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	951	VAL	CA-CB	-7.39	1.50	1.54
1	C	979	THR	CA-CB	5.98	1.57	1.53
1	A	954	VAL	CA-CB	-5.73	1.47	1.54
1	B	911	PRO	CA-C	5.62	1.54	1.51
1	B	1024	ALA	CA-CB	-5.48	1.44	1.53
1	B	928	VAL	CA-C	5.39	1.59	1.52
1	A	968	VAL	CA-CB	-5.19	1.48	1.54
1	A	1026	ALA	CA-CB	-5.06	1.45	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	911	PRO	CA-C-N	-8.27	111.86	120.38
1	B	911	PRO	C-N-CA	-8.27	111.86	120.38
1	C	980	HIS	N-CA-C	-7.36	104.28	113.55
1	B	910	SER	N-CA-C	6.71	119.03	108.55
1	A	946	PRO	CA-C-N	6.46	126.39	119.28
1	A	946	PRO	C-N-CA	6.46	126.39	119.28
1	C	1032	LYS	N-CA-C	-6.40	104.73	112.54
1	C	972	ILE	CB-CA-C	-6.17	107.81	114.35
1	B	942	ILE	N-CA-C	6.10	116.88	110.72
1	A	950	TYR	N-CA-C	6.08	120.54	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	924	VAL	N-CA-C	-5.76	104.89	110.42
1	B	911	PRO	N-CA-C	5.73	115.97	110.47
1	A	957	VAL	CB-CA-C	-5.58	104.71	112.02
1	A	983	ILE	CB-CA-C	-5.39	105.08	111.81
2	F	409	GLN	N-CA-C	-5.33	105.92	112.90
1	C	983	ILE	CB-CA-C	-5.29	105.15	112.24
1	B	963	THR	N-CA-C	-5.09	105.73	111.28
1	A	945	ALA	CA-C-N	5.06	125.59	120.38
1	A	945	ALA	C-N-CA	5.06	125.59	120.38
1	C	910	SER	N-CA-C	5.05	120.96	109.81

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	1048	0	1096	26	0
1	B	1073	0	1127	47	0
1	C	1073	0	1127	47	0
2	D	93	0	104	10	0
2	E	93	0	104	10	0
2	F	74	0	82	4	0
All	All	3454	0	3640	139	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 20.

All (139) 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:950:TYR:HA	1:B:953:MET:HE2	1.37	1.03
1:C:942:ILE:HG23	1:C:943:GLN:N	1.82	0.94
1:C:977:ALA:HA	1:C:980:HIS:NE2	1.84	0.91
1:C:1003:LEU:O	1:C:1006:GLN:HB2	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:950:TYR:HA	1:B:953:MET:CE	2.00	0.90
1:B:1008:VAL:HA	1:B:1013:GLN:OE1	1.74	0.85
1:C:942:ILE:CG2	1:C:943:GLN:H	1.90	0.83
1:C:942:ILE:HG23	1:C:943:GLN:H	1.37	0.83
2:D:413:LEU:HA	2:D:416:GLU:CD	2.06	0.80
2:F:412:ARG:O	2:F:416:GLU:HB3	1.82	0.79
1:C:942:ILE:CG2	1:C:943:GLN:N	2.47	0.78
1:B:943:GLN:HB3	1:B:944:PRO:HD3	1.66	0.78
1:B:956:GLU:OE2	1:B:956:GLU:HA	1.82	0.77
1:C:977:ALA:HA	1:C:980:HIS:CD2	2.19	0.77
1:C:968:VAL:O	1:C:972:ILE:HG13	1.86	0.76
2:E:406:ARG:O	2:E:410:ILE:HG22	1.86	0.76
2:D:406:ARG:HH11	2:D:406:ARG:HB3	1.49	0.76
1:B:950:TYR:CA	1:B:953:MET:HE2	2.18	0.71
1:C:980:HIS:O	1:C:984:GLU:HG2	1.92	0.70
2:E:408:SER:OG	2:E:412:ARG:NH1	2.24	0.69
1:B:1001:MET:HB2	1:B:1020:MET:HE3	1.75	0.69
1:B:995:GLY:HA3	2:E:406:ARG:HH21	1.58	0.69
1:A:1043:LEU:HD13	1:A:1048:GLN:HG2	1.76	0.68
1:A:998:ILE:CG2	1:A:1002:LYS:HE3	2.25	0.67
1:A:998:ILE:HG22	1:A:1002:LYS:HE3	1.78	0.66
1:C:985:MET:HA	1:C:985:MET:HE2	1.78	0.65
1:A:942:ILE:HG21	1:A:1021:LEU:HD11	1.80	0.64
1:C:977:ALA:HA	1:C:980:HIS:HE2	1.62	0.63
1:B:979:THR:O	1:B:983:ILE:HD12	1.99	0.63
1:C:1007:TYR:O	1:C:1013:GLN:HB3	1.98	0.63
1:B:937:GLU:HA	1:B:937:GLU:OE1	1.99	0.62
1:C:962:ARG:HG3	1:C:962:ARG:HH11	1.63	0.62
1:A:1012:LEU:O	1:A:1013:GLN:C	2.42	0.62
1:B:976:PRO:HB2	1:B:979:THR:HG23	1.83	0.60
1:C:938:MET:O	1:C:942:ILE:HB	2.01	0.60
2:D:414:LEU:HD22	2:D:414:LEU:O	2.01	0.60
2:D:412:ARG:HB2	2:D:412:ARG:NH1	2.17	0.60
1:C:951:VAL:HB	1:C:952:PRO:HD3	1.84	0.59
1:B:949:GLU:C	1:B:952:PRO:HD2	2.27	0.59
1:B:998:ILE:HD13	2:E:409:GLN:HB3	1.84	0.59
1:B:950:TYR:HE2	1:B:1013:GLN:NE2	1.99	0.59
1:C:969:ASP:O	1:C:973:PRO:HD3	2.04	0.58
2:D:409:GLN:HA	2:D:412:ARG:NH2	2.19	0.58
1:B:949:GLU:O	1:B:952:PRO:HD2	2.05	0.57
1:C:979:THR:O	1:C:979:THR:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:910:SER:HB2	1:C:911:PRO:HD2	1.88	0.55
1:B:980:HIS:O	1:B:984:GLU:HG3	2.06	0.55
2:F:408:SER:N	2:F:410:ILE:HG23	2.22	0.55
1:C:950:TYR:O	1:C:954:VAL:HG23	2.07	0.55
1:B:931:LEU:O	1:B:931:LEU:HD12	2.07	0.54
1:C:950:TYR:HA	1:C:953:MET:HB2	1.89	0.54
2:D:412:ARG:HB2	2:D:412:ARG:HH11	1.71	0.54
1:C:977:ALA:C	1:C:979:THR:H	2.16	0.53
2:E:406:ARG:C	2:E:410:ILE:HG22	2.33	0.53
1:A:943:GLN:OE1	1:A:1014:GLN:HG3	2.08	0.53
1:B:943:GLN:HB3	1:B:944:PRO:CD	2.37	0.53
1:C:982:GLU:HG2	1:C:1037:VAL:HG11	1.91	0.52
1:B:942:ILE:O	1:B:943:GLN:C	2.52	0.52
1:A:1033:ASN:O	1:A:1037:VAL:HG23	2.10	0.51
2:E:407:MET:HA	2:E:410:ILE:CG2	2.41	0.51
1:B:1008:VAL:HG22	1:B:1008:VAL:O	2.10	0.51
1:A:971:THR:O	1:A:972:ILE:C	2.54	0.50
2:F:409:GLN:HA	2:F:412:ARG:HB2	1.94	0.50
1:C:983:ILE:O	1:C:984:GLU:C	2.55	0.50
1:B:1034:LEU:O	1:B:1035:LEU:C	2.54	0.49
1:B:1018:LYS:HA	1:B:1021:LEU:HD12	1.94	0.49
1:A:972:ILE:HB	1:A:973:PRO:HD3	1.95	0.49
1:B:919:ARG:HD2	1:B:925:TYR:CD2	2.48	0.49
1:A:961:LEU:HD23	1:A:994:LEU:HD22	1.95	0.48
1:C:977:ALA:O	1:C:979:THR:N	2.46	0.48
1:B:950:TYR:CA	1:B:953:MET:CE	2.85	0.48
2:E:406:ARG:N	2:E:406:ARG:HE	2.12	0.48
1:C:938:MET:HE1	1:C:954:VAL:HG22	1.95	0.48
1:A:937:GLU:OE2	1:A:941:LYS:HE3	2.13	0.48
1:A:971:THR:HG22	1:A:975:LEU:HD11	1.96	0.48
2:F:410:ILE:HG13	2:F:414:LEU:HD12	1.96	0.47
1:C:971:THR:C	1:C:973:PRO:HD2	2.40	0.47
1:A:993:ASP:CB	1:A:1027:LEU:HD13	2.45	0.47
1:B:1003:LEU:O	1:B:1007:TYR:HD1	1.97	0.47
1:C:931:LEU:HD23	1:C:1031:ALA:HB2	1.96	0.47
1:A:986:ALA:HB3	1:A:1034:LEU:HD13	1.96	0.47
1:C:1037:VAL:O	1:C:1038:ILE:C	2.57	0.46
1:B:909:ILE:O	1:B:909:ILE:HG23	2.15	0.46
1:B:990:LEU:HD22	1:B:1027:LEU:HD12	1.98	0.45
1:B:950:TYR:CE2	1:B:1013:GLN:NE2	2.81	0.45
1:B:994:LEU:HD23	2:E:410:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:990:LEU:HD12	1:C:990:LEU:N	2.32	0.45
1:A:993:ASP:HB2	1:A:1027:LEU:CD1	2.47	0.45
1:A:965:LEU:HD22	1:A:987:GLN:HG2	1.99	0.45
1:A:976:PRO:HD3	1:A:1045:MET:SD	2.57	0.45
1:C:942:ILE:HG21	1:C:1021:LEU:HD21	1.99	0.45
1:C:964:LEU:O	1:C:968:VAL:HG23	2.17	0.45
1:C:932:VAL:O	1:C:933:LYS:C	2.61	0.44
1:C:972:ILE:HG22	1:C:980:HIS:ND1	2.33	0.44
1:C:977:ALA:C	1:C:979:THR:N	2.75	0.44
2:E:407:MET:CA	2:E:410:ILE:HG22	2.47	0.44
1:A:918:ASP:HB3	1:B:1045:MET:SD	2.58	0.44
1:A:1042:ARG:O	1:A:1046:LEU:N	2.46	0.44
1:A:976:PRO:HD3	1:A:1045:MET:HB2	2.00	0.44
1:C:1034:LEU:O	1:C:1037:VAL:HG23	2.18	0.44
1:B:961:LEU:HD12	1:B:961:LEU:O	2.18	0.43
1:C:938:MET:HE3	1:C:938:MET:HB2	1.76	0.43
1:C:937:GLU:O	1:C:938:MET:C	2.61	0.43
1:A:983:ILE:O	1:A:984:GLU:C	2.62	0.43
1:B:911:PRO:O	1:B:912:PRO:C	2.59	0.43
1:A:950:TYR:HA	1:A:953:MET:HE2	2.00	0.43
1:B:1001:MET:O	1:B:1005:GLN:HG3	2.19	0.42
1:C:972:ILE:N	1:C:973:PRO:HD2	2.33	0.42
1:C:980:HIS:C	1:C:984:GLU:HG2	2.44	0.42
1:A:1038:ILE:O	1:A:1041:ALA:HB3	2.19	0.42
1:B:910:SER:HB2	1:B:911:PRO:HD2	2.00	0.42
1:A:950:TYR:CB	1:A:953:MET:HE2	2.49	0.42
1:B:959:LEU:HD23	1:B:959:LEU:HA	1.92	0.42
1:C:969:ASP:O	1:C:973:PRO:CD	2.67	0.42
1:B:913:PRO:O	1:B:914:THR:C	2.63	0.42
1:B:994:LEU:O	1:B:995:GLY:C	2.62	0.42
1:B:929:THR:O	1:B:933:LYS:HG2	2.19	0.42
1:C:1045:MET:O	1:C:1045:MET:HG2	2.20	0.42
2:D:410:ILE:H	2:D:410:ILE:HG13	1.74	0.41
1:C:981:ARG:HE	1:C:981:ARG:HB3	1.61	0.41
1:C:1025:HIS:O	1:C:1026:ALA:C	2.62	0.41
2:D:412:ARG:HH11	2:D:412:ARG:CB	2.32	0.41
1:B:1010:THR:HB	1:C:981:ARG:HH22	1.85	0.41
1:C:1034:LEU:O	1:C:1035:LEU:C	2.62	0.41
1:B:945:ALA:HA	1:B:946:PRO:HD3	1.89	0.41
1:B:1028:ALA:O	1:B:1029:VAL:C	2.62	0.41
1:C:939:SER:O	1:C:940:SER:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:987:GLN:O	1:A:988:LYS:C	2.63	0.41
1:B:937:GLU:O	1:B:938:MET:C	2.64	0.41
2:D:409:GLN:HE21	2:D:409:GLN:C	2.29	0.41
1:B:950:TYR:HA	1:B:953:MET:HE3	1.94	0.41
2:E:409:GLN:O	2:E:413:LEU:N	2.32	0.40
1:A:916:ASN:HB3	1:A:917:LEU:H	1.63	0.40
1:B:1044:LYS:HB3	1:B:1044:LYS:HE2	1.81	0.40
1:C:1013:GLN:HG3	1:C:1014:GLN:N	2.35	0.40
1:B:942:ILE:HG21	1:B:1021:LEU:HD21	2.03	0.40
1:B:948:GLU:H	1:B:948:GLU:HG3	1.41	0.40
1:B:950:TYR:O	1:B:951:VAL:C	2.64	0.40
2:D:406:ARG:HH11	2:D:406:ARG:CB	2.27	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	133/162 (82%)	123 (92%)	8 (6%)	2 (2%)	8	26
1	B	137/162 (85%)	125 (91%)	11 (8%)	1 (1%)	18	45
1	C	137/162 (85%)	115 (84%)	16 (12%)	6 (4%)	2	6
2	D	9/23 (39%)	9 (100%)	0	0	100	100
2	E	9/23 (39%)	3 (33%)	6 (67%)	0	100	100
2	F	7/23 (30%)	4 (57%)	3 (43%)	0	100	100
All	All	432/555 (78%)	379 (88%)	44 (10%)	9 (2%)	5	18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	942	ILE

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Mol	Chain	Res	Type
1	C	978	SER
1	A	1013	GLN
1	C	970	GLU
1	C	923	LYS
1	C	941	LYS
1	C	1035	LEU
1	A	1011	SER
1	B	1034	LEU

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	118/142 (83%)	106 (90%)	12 (10%)	7	22
1	B	121/142 (85%)	107 (88%)	14 (12%)	5	17
1	C	121/142 (85%)	97 (80%)	24 (20%)	1	4
2	D	11/22 (50%)	7 (64%)	4 (36%)	0	0
2	E	11/22 (50%)	9 (82%)	2 (18%)	2	5
2	F	9/22 (41%)	6 (67%)	3 (33%)	0	0
All	All	391/492 (80%)	332 (85%)	59 (15%)	3	9

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	940	SER
1	A	942	ILE
1	A	951	VAL
1	A	978	SER
1	A	988	LYS
1	A	1011	SER
1	A	1013	GLN
1	A	1021	LEU
1	A	1032	LYS
1	A	1043	LEU

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Mol	Chain	Res	Type
1	A	1044	LYS
1	A	1049	THR
1	B	909	ILE
1	B	921	ASN
1	B	923	LYS
1	B	939	SER
1	B	940	SER
1	B	941	LYS
1	B	948	GLU
1	B	963	THR
1	B	978	SER
1	B	979	THR
1	B	988	LYS
1	B	992	SER
1	B	1021	LEU
1	B	1044	LYS
1	C	909	ILE
1	C	923	LYS
1	C	933	LYS
1	C	936	ILE
1	C	938	MET
1	C	939	SER
1	C	940	SER
1	C	941	LYS
1	C	942	ILE
1	C	955	LYS
1	C	959	LEU
1	C	962	ARG
1	C	970	GLU
1	C	974	LEU
1	C	979	THR
1	C	985	MET
1	C	988	LYS
1	C	991	ASN
1	C	992	SER
1	C	1009	MET
1	C	1032	LYS
1	C	1037	VAL
1	C	1038	ILE
1	C	1046	LEU
2	D	406	ARG
2	D	409	GLN

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Mol	Chain	Res	Type
2	D	410	ILE
2	D	414	LEU
2	E	406	ARG
2	E	407	MET
2	F	410	ILE
2	F	413	LEU
2	F	416	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	927	ASN
1	B	1006	GLN
1	C	991	ASN
1	C	1005	GLN
2	D	409	GLN

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 ⓘ

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	134/162 (82%)	0.03	1 (0%) 84 78	20, 36, 48, 53	1 (0%)
1	B	139/162 (85%)	-0.15	2 (1%) 73 64	26, 35, 43, 49	0
1	C	139/162 (85%)	0.33	5 (3%) 46 37	26, 37, 48, 56	0
2	D	11/23 (47%)	4.75	11 (100%) 0 0	53, 54, 58, 58	11 (100%)
2	E	11/23 (47%)	3.26	10 (90%) 0 0	40, 44, 48, 48	11 (100%)
2	F	9/23 (39%)	3.25	7 (77%) 0 0	34, 36, 38, 40	9 (100%)
All	All	443/555 (79%)	0.33	36 (8%) 18 13	20, 36, 50, 58	32 (7%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	407	MET	6.7
2	D	411	LYS	6.0
2	E	407	MET	5.9
2	D	415	SER	5.8
2	D	414	LEU	5.5
1	C	909	ILE	5.1
2	D	408	SER	5.1
2	F	412	ARG	4.7
2	F	416	GLU	4.7
2	D	410	ILE	4.7
2	E	406	ARG	4.6
2	D	413	LEU	4.4
2	D	406	ARG	4.3
2	F	415	SER	4.1
2	F	411	LYS	3.8
2	F	408	SER	3.6
2	D	409	GLN	3.5
2	E	409	GLN	3.4
2	F	410	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	416	GLU	3.3
2	E	408	SER	3.3
2	E	416	GLU	3.1
2	E	411	LYS	3.1
2	D	412	ARG	3.0
2	E	412	ARG	2.9
2	E	413	LEU	2.8
2	E	410	ILE	2.8
1	C	1008	VAL	2.7
1	C	1047	GLY	2.4
1	B	1014	GLN	2.4
1	C	1013	GLN	2.4
1	C	981	ARG	2.3
1	B	1047	GLY	2.2
2	E	414	LEU	2.2
2	F	413	LEU	2.1
1	A	943	GLN	2.1

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.