



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:04 AM UTC

PDB ID : 2GOX / pdb_00002gox
Title : Crystal structure of Efb-C / C3d Complex
Authors : Hammel, M.; Geisbrecht, B.V.
Deposited on : 2006-04-14
Resolution : 2.20 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

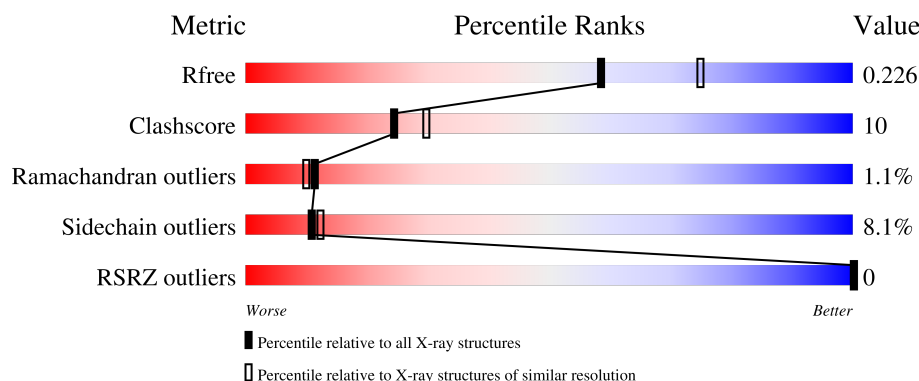
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	297	
1	C	297	
2	B	65	
2	D	65	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5991 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 Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2327	1492	393	433	9			
1	C	297	Total	C	N	O	S	0	0	0
			2327	1492	393	433	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	991	GLY	-	expression tag	UNP P01024
A	992	SER	-	expression tag	UNP P01024
A	993	ARG	-	expression tag	UNP P01024
A	994	SER	-	expression tag	UNP P01024
A	995	THR	-	expression tag	UNP P01024
A	1010	ALA	CYS	engineered mutation	UNP P01024
C	991	GLY	-	expression tag	UNP P01024
C	992	SER	-	expression tag	UNP P01024
C	993	ARG	-	expression tag	UNP P01024
C	994	SER	-	expression tag	UNP P01024
C	995	THR	-	expression tag	UNP P01024
C	1010	ALA	CYS	engineered mutation	UNP P01024

- Molecule 2 is a protein called Fibrinogen-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	65	Total	C	N	O	S	0	0	0
			513	321	95	96	1			
2	D	65	Total	C	N	O	S	0	0	0
			507	318	92	96	1			

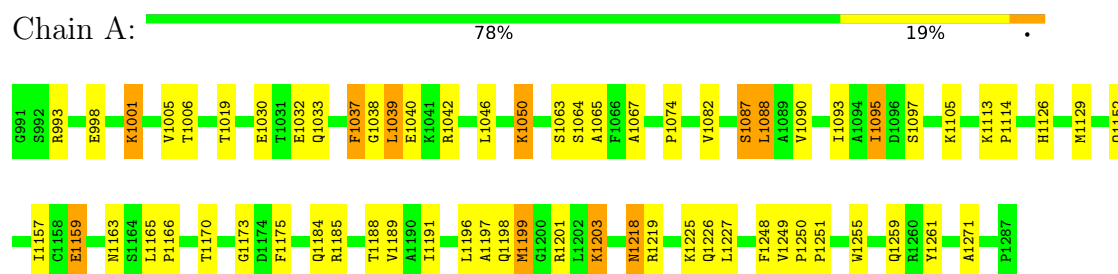
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total 145	O 145	0	0
3	B	17	Total 17	O 17	0	0
3	C	139	Total 139	O 139	0	0
3	D	16	Total 16	O 16	0	0

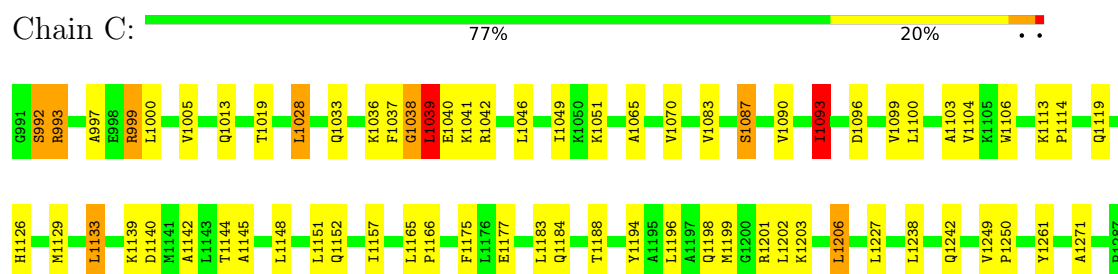
3 Residue-property plots [i](#)

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.

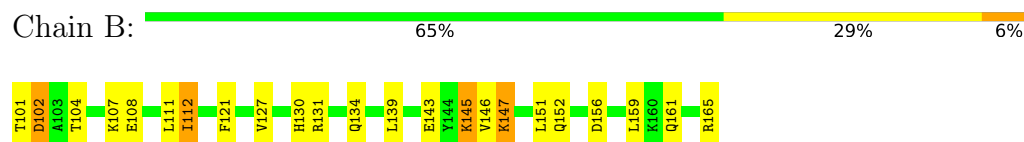
• Molecule 1: Complement C3



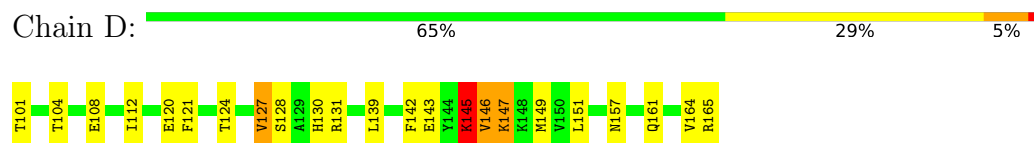
• Molecule 1: Complement C3



• Molecule 2: Fibrinogen-binding protein



• Molecule 2: Fibrinogen-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	90.94Å 90.94Å 122.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.20) 98.8 (50.00-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.181 , 0.231 (Not available) , 0.226	Depositor DCC
R_{free} test set	2519 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5991	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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 [i](#)

5.1 Standard geometry [i](#)

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	1.33	7/2376 (0.3%)	1.22	10/3219 (0.3%)
1	C	1.35	9/2376 (0.4%)	1.19	3/3219 (0.1%)
2	B	1.11	2/516 (0.4%)	1.21	2/691 (0.3%)
2	D	1.04	0/510	1.19	2/684 (0.3%)
All	All	1.30	18/5778 (0.3%)	1.20	17/7813 (0.2%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1191	ILE	CA-CB	7.10	1.62	1.54
1	C	1093	ILE	CA-CB	6.77	1.65	1.54
1	C	1103	ALA	CA-CB	6.47	1.63	1.53
1	A	1019	THR	CA-C	6.25	1.60	1.52
1	C	1249	VAL	CA-CB	6.25	1.57	1.54
1	C	1202	LEU	CA-C	6.14	1.60	1.52
1	A	1197	ALA	CA-CB	5.97	1.62	1.53
1	C	1145	ALA	CA-CB	-5.47	1.44	1.53
2	B	145	LYS	CD-CE	5.38	1.68	1.52
1	A	1087	SER	C-O	-5.33	1.18	1.24
1	C	1175	PHE	C-O	5.30	1.30	1.24
1	A	1082	VAL	CA-C	5.24	1.59	1.52
1	C	1242	GLN	N-CA	5.23	1.52	1.46
1	C	1087	SER	C-O	-5.17	1.18	1.24
2	B	145	LYS	CE-NZ	5.16	1.64	1.49
1	A	1170	THR	CA-CB	5.16	1.61	1.53
1	A	1175	PHE	C-O	5.10	1.29	1.24
1	C	1019	THR	CA-C	5.04	1.59	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1006	THR	CA-C-N	-6.59	112.87	119.99
1	A	1006	THR	C-N-CA	-6.59	112.87	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	146	VAL	N-CA-C	6.39	116.54	110.53
2	D	157	ASN	N-CA-C	6.12	117.62	111.07
1	A	1249	VAL	CA-C-N	-6.05	114.15	120.38
1	A	1249	VAL	C-N-CA	-6.05	114.15	120.38
2	D	146	VAL	N-CA-C	5.95	116.01	110.42
1	C	1250	PRO	N-CA-C	5.48	117.39	110.70
2	B	102	ASP	N-CA-C	-5.41	105.54	111.82
1	C	992	SER	N-CA-C	5.32	117.83	111.71
1	A	1097	SER	CB-CA-C	-5.12	101.97	110.68
1	C	1261	TYR	CA-CB-CG	-5.12	104.69	113.90
1	A	1065	ALA	N-CA-C	5.08	117.09	110.53
1	A	1050	LYS	CA-CB-CG	5.08	124.25	114.10
1	A	1184	GLN	N-CA-C	-5.07	107.65	113.88
1	A	1189	VAL	N-CA-C	5.01	115.62	110.36
1	A	1157	ILE	N-CA-C	-5.00	105.30	112.35

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	2327	0	2324	37	0
1	C	2327	0	2324	49	0
2	B	513	0	532	16	0
2	D	507	0	521	20	0
3	A	145	0	0	6	0
3	B	17	0	0	0	0
3	C	139	0	0	14	0
3	D	16	0	0	1	0
All	All	5991	0	5701	112	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 10.

All (112) 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:1173:GLY:HA3	1:A:1199:MET:HE1	1.16	1.10
1:A:1173:GLY:CA	1:A:1199:MET:HE1	1.86	1.04
1:A:1039:LEU:HD11	2:B:165:ARG:H	1.19	1.02
2:B:134:GLN:HE22	2:B:152:GLN:HE22	1.25	0.84
2:D:101:THR:HA	2:D:104:THR:HB	1.59	0.83
1:C:1201:ARG:HD2	3:C:168:HOH:O	1.79	0.81
1:A:1037:PHE:CZ	3:A:306:HOH:O	2.34	0.81
2:D:147:LYS:HE3	2:D:151:LEU:HG	1.61	0.81
1:A:1199:MET:HE3	1:A:1201:ARG:HD3	1.63	0.80
1:A:1001:LYS:HZ2	1:A:1001:LYS:HB3	1.45	0.80
1:A:1001:LYS:HB3	1:A:1001:LYS:NZ	1.95	0.78
1:C:1152:GLN:HG2	3:C:247:HOH:O	1.82	0.78
2:B:147:LYS:HE3	2:B:151:LEU:HG	1.69	0.74
1:C:992:SER:HB3	3:C:281:HOH:O	1.89	0.72
1:A:1114:PRO:HG3	3:A:276:HOH:O	1.88	0.72
1:C:1049:ILE:HG22	1:C:1093:ILE:HD12	1.71	0.72
2:D:147:LYS:CE	2:D:151:LEU:HG	2.19	0.71
1:A:1093:ILE:HG13	1:A:1095:ILE:HD12	1.74	0.70
1:A:1030:GLU:HG3	3:A:173:HOH:O	1.91	0.69
1:A:1159:GLU:OE2	1:A:1159:GLU:HA	1.93	0.69
1:A:1042:ARG:HH22	2:B:130:HIS:HD2	1.42	0.67
1:C:1013:GLN:HG3	3:C:310:HOH:O	1.93	0.67
2:D:121:PHE:CZ	2:D:130:HIS:HB2	2.30	0.67
1:A:1039:LEU:HD11	2:B:165:ARG:N	2.02	0.66
2:D:164:VAL:HG22	2:D:165:ARG:H	1.60	0.66
1:C:993:ARG:H	1:C:993:ARG:NE	1.93	0.66
1:C:1087:SER:O	1:C:1090:VAL:HG22	1.97	0.63
1:C:1152:GLN:NE2	1:C:1198:GLN:OE1	2.31	0.63
1:C:1042:ARG:HH22	2:D:130:HIS:HD2	1.45	0.63
1:A:1218:ASN:HD21	1:A:1219:ARG:HH11	1.47	0.63
2:D:130:HIS:HE1	3:D:180:HOH:O	1.82	0.63
1:C:1148:LEU:HD21	1:C:1199:MET:CE	2.30	0.60
1:A:1001:LYS:NZ	1:A:1001:LYS:CB	2.64	0.60
1:C:997:ALA:H	1:C:1033:GLN:HE22	1.50	0.59
1:A:998:GLU:O	1:A:1001:LYS:HG2	2.03	0.58
1:A:1227:LEU:HD22	1:A:1271:ALA:CB	2.34	0.57
1:C:1148:LEU:HD21	1:C:1199:MET:HE2	1.87	0.57
1:A:1152:GLN:NE2	1:A:1198:GLN:OE1	2.37	0.57
1:A:1196:LEU:HD23	1:A:1199:MET:HE2	1.86	0.57
1:C:1070:VAL:HG22	3:C:182:HOH:O	2.05	0.56
1:C:993:ARG:H	1:C:993:ARG:CD	2.19	0.56
1:C:997:ALA:H	1:C:1033:GLN:NE2	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:LYS:CE	2:B:151:LEU:HG	2.36	0.55
1:C:999:ARG:HD2	3:C:204:HOH:O	2.06	0.55
1:A:1093:ILE:HG13	1:A:1095:ILE:CD1	2.37	0.54
1:A:1063:SER:O	1:A:1064:SER:HB2	2.08	0.53
1:C:1049:ILE:CG2	1:C:1093:ILE:HD12	2.37	0.53
2:D:146:VAL:HA	2:D:149:MET:HE2	1.89	0.53
1:A:1033:GLN:O	1:A:1037:PHE:HB3	2.08	0.53
1:C:1152:GLN:CD	3:C:247:HOH:O	2.52	0.53
1:A:1037:PHE:HZ	3:A:306:HOH:O	1.80	0.52
1:C:1196:LEU:HA	1:C:1199:MET:HE3	1.92	0.52
1:A:1042:ARG:HH22	2:B:130:HIS:CD2	2.26	0.51
1:C:1040:GLU:H	1:C:1040:GLU:CD	2.19	0.51
1:C:1039:LEU:HD21	2:D:164:VAL:HA	1.91	0.51
1:A:1185:ARG:NH1	3:A:236:HOH:O	2.41	0.51
2:B:121:PHE:CZ	2:B:130:HIS:HB2	2.46	0.51
1:C:1227:LEU:HD22	1:C:1271:ALA:CB	2.41	0.51
1:C:1152:GLN:OE1	3:C:247:HOH:O	2.19	0.51
1:C:1152:GLN:CG	3:C:247:HOH:O	2.49	0.51
2:D:104:THR:O	2:D:108:GLU:HG3	2.11	0.51
1:C:1133:LEU:HD13	1:C:1142:ALA:HB1	1.93	0.50
1:C:1042:ARG:HH22	2:D:130:HIS:CD2	2.27	0.50
2:B:108:GLU:O	2:B:112:ILE:HG12	2.11	0.50
1:C:1201:ARG:CD	3:C:168:HOH:O	2.50	0.50
1:A:1250:PRO:HD2	1:A:1251:PRO:HD3	1.94	0.49
1:C:1104:VAL:HG13	1:C:1151:LEU:HD22	1.94	0.49
1:C:1126:HIS:O	1:C:1129:MET:HG2	2.13	0.48
1:A:1199:MET:HE3	1:A:1201:ARG:CD	2.40	0.48
1:C:1038:GLY:HA3	1:C:1041:LYS:HD2	1.96	0.48
1:C:1065:ALA:HB2	1:C:1106:TRP:CD2	2.49	0.48
1:A:1126:HIS:O	1:A:1129:MET:HG2	2.14	0.47
2:D:142:PHE:O	2:D:145:LYS:HB3	2.14	0.47
2:B:156:ASP:HA	2:B:159:LEU:HD12	1.96	0.47
1:A:1227:LEU:HD21	1:A:1261:TYR:CE1	2.50	0.47
2:B:147:LYS:HD2	2:B:147:LYS:HA	1.41	0.46
1:C:1083:VAL:HA	1:C:1100:LEU:HD11	1.96	0.46
2:B:127:VAL:O	2:B:131:ARG:HG3	2.16	0.46
1:C:1140:ASP:O	1:C:1144:THR:OG1	2.28	0.45
1:C:1013:GLN:NE2	3:C:310:HOH:O	2.45	0.45
1:C:1114:PRO:HD2	3:C:61:HOH:O	2.15	0.45
1:A:1067:ALA:HB2	1:A:1074:PRO:HA	2.00	0.44
1:C:1000:LEU:HD12	1:C:1028:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1227:LEU:HD22	1:C:1271:ALA:HB2	1.99	0.44
1:C:1177:GLU:HG3	1:C:1206:LEU:HD11	1.99	0.44
2:D:121:PHE:CE1	2:D:130:HIS:HB2	2.52	0.44
2:D:161:GLN:HA	2:D:161:GLN:OE1	2.17	0.44
2:B:134:GLN:HE22	2:B:152:GLN:NE2	2.05	0.44
1:A:1173:GLY:HA2	1:A:1199:MET:HE1	1.88	0.43
1:A:1248:PHE:O	1:A:1251:PRO:HD2	2.18	0.43
1:C:1039:LEU:CD2	2:D:164:VAL:HA	2.48	0.43
1:C:1051:LYS:HE3	3:C:140:HOH:O	2.18	0.43
2:D:147:LYS:HE2	2:D:151:LEU:HG	1.99	0.43
1:A:1087:SER:O	1:A:1090:VAL:HG22	2.19	0.42
1:A:1165:LEU:HB3	1:A:1166:PRO:HD3	2.00	0.42
2:D:147:LYS:HD2	2:D:147:LYS:HA	1.44	0.42
1:A:1088:LEU:HD12	1:A:1088:LEU:HA	1.79	0.42
1:C:1096:ASP:HB3	1:C:1099:VAL:HG23	2.02	0.42
2:B:121:PHE:CE1	2:B:130:HIS:HB2	2.55	0.42
1:C:1151:LEU:HB3	1:C:1165:LEU:HD11	2.02	0.42
2:B:139:LEU:HA	2:B:139:LEU:HD23	1.70	0.41
2:D:127:VAL:O	2:D:131:ARG:HG3	2.19	0.41
2:B:107:LYS:HD3	2:B:143:GLU:OE1	2.21	0.41
1:C:1194:TYR:CE1	1:C:1238:LEU:HB3	2.55	0.41
1:C:1157:ILE:HA	2:D:139:LEU:CD2	2.50	0.41
1:C:1166:PRO:HD2	3:C:241:HOH:O	2.20	0.41
1:C:1183:LEU:HA	1:C:1183:LEU:HD23	1.88	0.41
1:A:1203:LYS:HB3	3:A:145:HOH:O	2.20	0.41
1:C:1042:ARG:HH12	2:D:130:HIS:CD2	2.39	0.40
1:A:1255:TRP:O	1:A:1259:GLN:HG2	2.21	0.40
1:C:1000:LEU:HD12	1:C:1028:LEU:CD1	2.52	0.40
1:C:1113:LYS:HD3	1:C:1119:GLN:CD	2.46	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	295/297 (99%)	287 (97%)	6 (2%)	2 (1%)	18	19
1	C	295/297 (99%)	286 (97%)	5 (2%)	4 (1%)	9	7
2	B	63/65 (97%)	60 (95%)	2 (3%)	1 (2%)	7	6
2	D	63/65 (97%)	61 (97%)	1 (2%)	1 (2%)	7	6
All	All	716/724 (99%)	694 (97%)	14 (2%)	8 (1%)	11	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1036	LYS
1	A	1037	PHE
2	B	145	LYS
1	C	1037	PHE
1	C	1039	LEU
2	D	145	LYS
1	C	1038	GLY
1	A	1038	GLY

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	243/245 (99%)	223 (92%)	20 (8%)	10	12
1	C	243/245 (99%)	230 (95%)	13 (5%)	20	26
2	B	55/59 (93%)	48 (87%)	7 (13%)	4	4
2	D	54/59 (92%)	46 (85%)	8 (15%)	3	2
All	All	595/608 (98%)	547 (92%)	48 (8%)	11	12

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	993	ARG
1	A	1001	LYS
1	A	1005	VAL

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Mol	Chain	Res	Type
1	A	1032	GLU
1	A	1039	LEU
1	A	1040	GLU
1	A	1046	LEU
1	A	1050	LYS
1	A	1088	LEU
1	A	1095	ILE
1	A	1105	LYS
1	A	1113	LYS
1	A	1159	GLU
1	A	1163	ASN
1	A	1188	THR
1	A	1199	MET
1	A	1203	LYS
1	A	1218	ASN
1	A	1225	LYS
1	A	1226	GLN
2	B	101	THR
2	B	102	ASP
2	B	104	THR
2	B	111	LEU
2	B	112	ILE
2	B	147	LYS
2	B	161	GLN
1	C	993	ARG
1	C	999	ARG
1	C	1005	VAL
1	C	1028	LEU
1	C	1039	LEU
1	C	1046	LEU
1	C	1093	ILE
1	C	1133	LEU
1	C	1139	LYS
1	C	1184	GLN
1	C	1188	THR
1	C	1203	LYS
1	C	1206	LEU
2	D	112	ILE
2	D	120	GLU
2	D	124	THR
2	D	127	VAL
2	D	128	SER

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Mol	Chain	Res	Type
2	D	143	GLU
2	D	145	LYS
2	D	147	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1033	GLN
1	A	1152	GLN
1	A	1161	GLN
1	A	1182	ASN
1	A	1198	GLN
1	A	1218	ASN
1	A	1277	GLN
2	B	130	HIS
2	B	152	GLN
2	B	161	GLN
1	C	1013	GLN
1	C	1033	GLN
1	C	1152	GLN
1	C	1163	ASN
1	C	1182	ASN
1	C	1198	GLN
1	C	1226	GLN
1	C	1242	GLN
1	C	1257	ASN
2	D	115	GLN
2	D	116	ASN
2	D	130	HIS
2	D	134	GLN
2	D	152	GLN

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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	297/297 (100%)	-1.34	0 100 100	27, 36, 59, 72	0
1	C	297/297 (100%)	-1.32	0 100 100	27, 36, 60, 68	0
2	B	65/65 (100%)	-0.97	0 100 100	44, 59, 76, 87	0
2	D	65/65 (100%)	-0.95	0 100 100	44, 58, 81, 88	0
All	All	724/724 (100%)	-1.27	0 100 100	27, 39, 66, 88	0

There are no RSRZ outliers to report.

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.