



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:51 PM UTC

PDB ID : 6EJM / pdb_00006ejm
Title : CRYSTAL STRUCTURE OF HUMAN CD81 LARGE EXTRACELLULAR LOOP IN COMPLEX WITH SINGLE CHAIN FV FRAGMENT 5
Authors : Kuglstatter, A.; Harris, S.F.; Villasenor, A.
Deposited on : 2017-09-22
Resolution : 2.15 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

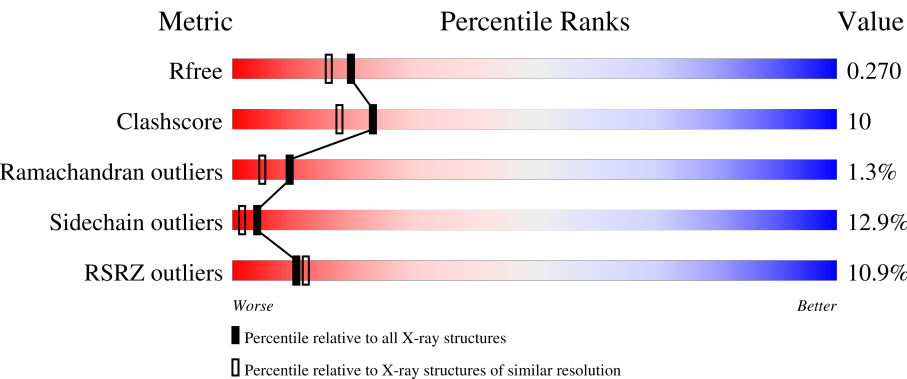
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	99	19% 66% 19% 6% • 8%
1	B	99	13% 64% 21% • • 11%
2	H	249	5% 68% 20% • 8%
2	I	249	10% 68% 19% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5072 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 CD81 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	91	Total	C	N	O	S	0	0	0
			705	440	123	138	4			
1	B	88	Total	C	N	O	S	0	0	0
			680	425	116	135	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	GLY	-	expression tag	UNP P60033
A	111	SER	-	expression tag	UNP P60033
A	203	HIS	-	expression tag	UNP P60033
A	204	HIS	-	expression tag	UNP P60033
A	205	HIS	-	expression tag	UNP P60033
A	206	HIS	-	expression tag	UNP P60033
A	207	HIS	-	expression tag	UNP P60033
A	208	HIS	-	expression tag	UNP P60033
B	110	GLY	-	expression tag	UNP P60033
B	111	SER	-	expression tag	UNP P60033
B	203	HIS	-	expression tag	UNP P60033
B	204	HIS	-	expression tag	UNP P60033
B	205	HIS	-	expression tag	UNP P60033
B	206	HIS	-	expression tag	UNP P60033
B	207	HIS	-	expression tag	UNP P60033
B	208	HIS	-	expression tag	UNP P60033

- Molecule 2 is a protein called SINGLE CHAIN FV FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	229	Total	C	N	O	S	0	0	0
			1733	1100	289	337	7			
2	I	227	Total	C	N	O	S	0	0	0
			1725	1096	287	335	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total 16	O 16	0	0
3	B	17	Total 17	O 17	0	0
3	H	100	Total 100	O 100	0	0
3	I	96	Total 96	O 96	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.35Å 100.50Å 116.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.57 – 2.15 41.57 – 2.15	Depositor EDS
% Data completeness (in resolution range)	85.1 (41.57-2.15) 85.1 (41.57-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.215 , 0.278 0.209 , 0.270	Depositor DCC
R_{free} test set	2064 reflections (4.33%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5072	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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	1.17	0/715	1.19	5/964 (0.5%)
1	B	1.20	0/688	1.15	1/927 (0.1%)
2	H	1.15	0/1769	1.18	7/2397 (0.3%)
2	I	1.14	1/1761 (0.1%)	1.20	3/2387 (0.1%)
All	All	1.16	1/4933 (0.0%)	1.18	16/6675 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	237	VAL	CA-CB	7.31	1.59	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	VAL	N-CA-C	7.05	118.01	111.45
2	H	278	GLY	N-CA-C	-6.99	103.59	112.54
2	I	278	GLY	N-CA-C	-6.65	103.64	112.82
2	I	222	SER	N-CA-C	-6.54	100.78	110.20
2	I	86	VAL	CB-CA-C	-6.00	105.74	111.44
1	A	119	ILE	N-CA-CB	5.83	120.30	110.56
1	B	117	ASP	N-CA-C	5.76	117.55	111.28
1	A	198	PHE	CA-C-N	-5.39	114.03	122.65
1	A	198	PHE	C-N-CA	-5.39	114.03	122.65
2	H	207	ASP	N-CA-C	5.35	122.19	110.80
2	H	86	VAL	CB-CA-C	-5.34	106.17	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	178	MET	CG-SD-CE	-5.25	89.35	100.90
2	H	136	SER	N-CA-C	-5.18	103.47	110.68
2	H	133	TYR	CA-C-N	5.16	128.18	120.95
2	H	133	TYR	C-N-CA	5.16	128.18	120.95
1	A	180	ASN	N-CA-C	5.03	117.84	110.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	206	THR	Peptide

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	705	0	688	19	0
1	B	680	0	669	22	0
2	H	1733	0	1720	28	0
2	I	1725	0	1714	40	0
3	A	16	0	0	1	0
3	B	17	0	0	0	0
3	H	100	0	0	1	0
3	I	96	0	0	3	0
All	All	5072	0	4791	99	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 (99) 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)
2:I:178:MET:HE3	2:I:269:GLN:HG2	1.28	1.09
2:H:178:MET:HE3	2:H:269:GLN:HG2	1.33	1.07
1:A:123:VAL:HG22	1:B:119:ILE:HD11	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:176:VAL:HG12	2:I:178:MET:HE2	1.49	0.94
2:H:227:ILE:HD11	2:H:230:VAL:O	1.74	0.86
1:A:132:GLN:HG3	1:A:165:LEU:HD11	1.55	0.85
2:H:178:MET:CE	2:H:269:GLN:HG2	2.09	0.83
1:A:162:LEU:HD12	1:A:165:LEU:HD12	1.63	0.81
2:H:151:THR:HG23	3:H:337:HOH:O	1.79	0.81
1:A:123:VAL:CG2	1:B:119:ILE:HD11	2.11	0.81
2:I:178:MET:HE3	2:I:269:GLN:CG	2.10	0.80
2:H:205:ASP:HB3	2:H:207:ASP:HB2	1.64	0.78
2:I:176:VAL:CG1	2:I:178:MET:HE2	2.14	0.76
2:H:176:VAL:HG12	2:H:178:MET:HE2	1.68	0.76
2:I:218:ARG:NH2	2:I:260:GLU:HA	2.01	0.75
2:H:178:MET:HE3	2:H:269:GLN:CG	2.16	0.74
1:A:177:SER:HB2	1:A:180:ASN:HB2	1.69	0.73
2:I:205:ASP:HB3	2:I:207:ASP:HB2	1.71	0.73
2:I:201:GLN:HG3	3:I:314:HOH:O	1.89	0.72
1:A:162:LEU:CD1	1:A:165:LEU:HD12	2.21	0.71
2:I:40:VAL:HG22	2:I:64:GLY:HA3	1.72	0.71
1:A:202:LEU:HB2	1:B:149:THR:HG23	1.73	0.70
2:I:256:ARG:HH11	2:I:256:ARG:HG2	1.57	0.69
1:B:141:ASN:HB2	1:B:144:LYS:HG3	1.75	0.68
1:B:166:THR:O	1:B:169:VAL:HG22	1.92	0.68
2:I:178:MET:CE	2:I:269:GLN:HG2	2.18	0.68
2:H:40:VAL:HG22	2:H:64:GLY:HA3	1.75	0.68
2:I:207:ASP:OD1	2:I:211:TYR:OH	2.07	0.64
1:A:123:VAL:HG22	1:B:119:ILE:CD1	2.24	0.63
2:H:176:VAL:HG12	2:H:178:MET:CE	2.30	0.62
2:H:207:ASP:OD2	2:H:211:TYR:OH	2.13	0.60
2:H:198:LYS:HE3	2:H:249:ASP:OD2	2.01	0.60
2:I:50:VAL:HG11	2:I:124:LEU:HD23	1.85	0.59
2:I:176:VAL:CG1	2:I:178:MET:CE	2.81	0.58
2:H:188:THR:O	2:H:191:GLN:HB3	2.05	0.56
1:A:114:VAL:H	1:B:129:GLN:HE22	1.53	0.56
1:B:169:VAL:HG23	1:B:170:LEU:N	2.20	0.55
2:H:76:ARG:HD3	2:H:84:GLU:OE1	2.05	0.55
2:I:207:ASP:HB3	2:I:209:LYS:H	1.72	0.55
1:B:168:SER:HA	1:B:171:LYS:HD3	1.89	0.54
2:I:179:THR:HG22	3:I:356:HOH:O	2.07	0.54
2:H:106:PHE:CZ	2:H:121:LEU:HD22	2.42	0.54
2:I:218:ARG:HH21	2:I:260:GLU:HA	1.71	0.54
1:B:177:SER:HB3	1:B:180:ASN:OD1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLN:O	1:A:129:GLN:HG3	2.09	0.52
1:A:173:ASN:HA	3:A:301:HOH:O	2.09	0.52
1:A:161:THR:HG22	1:A:162:LEU:HD23	1.93	0.51
1:B:168:SER:HA	1:B:171:LYS:CD	2.41	0.50
2:I:76:ARG:HD3	2:I:84:GLU:OE1	2.12	0.50
1:B:154:LEU:O	1:B:155:ASP:HB3	2.12	0.48
1:A:131:LEU:HD11	1:A:169:VAL:HG21	1.94	0.48
2:I:218:ARG:CZ	2:I:260:GLU:HA	2.43	0.48
1:A:177:SER:O	1:A:179:SER:N	2.43	0.48
2:I:179:THR:HB	2:I:198:LYS:HB3	1.95	0.48
1:A:114:VAL:HG13	1:B:129:GLN:NE2	2.29	0.47
2:H:205:ASP:HB3	2:H:207:ASP:CB	2.38	0.47
2:H:106:PHE:CE2	2:H:121:LEU:HD22	2.49	0.47
1:B:148:LYS:O	1:B:152:GLU:HB2	2.14	0.47
2:I:176:VAL:HG11	2:I:178:MET:CE	2.43	0.47
2:I:185:LEU:HB3	2:I:283:LEU:HD23	1.97	0.47
2:I:60:CYS:HB3	2:I:117:LEU:HB3	1.97	0.46
1:B:177:SER:HB2	1:B:180:ASN:HB2	1.98	0.46
2:I:218:ARG:HH11	2:I:218:ARG:HB3	1.81	0.46
2:I:178:MET:HE1	2:I:203:LEU:HD21	1.98	0.46
2:I:256:ARG:HH11	2:I:256:ARG:CG	2.24	0.45
2:I:207:ASP:HB3	2:I:209:LYS:HG3	1.98	0.45
2:I:218:ARG:HB3	2:I:218:ARG:NH1	2.32	0.45
2:H:176:VAL:CG1	2:H:178:MET:CE	2.96	0.44
2:H:207:ASP:HB3	2:H:209:LYS:H	1.82	0.44
2:I:44:GLU:OE1	2:I:145:GLY:HA3	2.18	0.44
2:H:212:LEU:HG	2:H:213:THR:N	2.27	0.44
2:I:233:LEU:HD23	2:I:237:VAL:O	2.18	0.44
2:H:79:PRO:HD3	2:H:129:THR:O	2.17	0.44
2:H:146:GLN:H	2:H:146:GLN:CD	2.25	0.44
2:I:146:GLN:H	2:I:146:GLN:CD	2.25	0.44
2:I:206:THR:C	2:I:208:GLY:H	2.26	0.43
2:I:186:SER:HA	2:I:284:ASP:O	2.19	0.42
2:H:268:LEU:HG	2:H:277:PHE:CE2	2.54	0.42
2:H:106:PHE:N	2:H:106:PHE:CD1	2.87	0.42
2:I:216:LEU:HD11	2:I:218:ARG:HG2	2.01	0.42
1:B:174:LEU:C	1:B:176:PRO:HD3	2.44	0.42
2:H:191:GLN:HG3	2:H:192:PRO:HD2	2.02	0.42
2:H:214:TRP:HB2	2:H:227:ILE:HG23	2.01	0.42
1:B:119:ILE:O	1:B:123:VAL:HG23	2.20	0.42
2:I:189:ILE:H	2:I:189:ILE:HG13	1.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:50:VAL:HG22	3:I:360:HOH:O	2.20	0.42
2:H:215:LEU:HD13	2:H:225:ARG:HA	2.02	0.41
2:I:206:THR:C	2:I:208:GLY:N	2.78	0.41
2:I:228:TYR:O	2:I:229:LEU:C	2.61	0.41
1:A:123:VAL:HA	1:B:119:ILE:HD11	2.03	0.41
2:I:256:ARG:CG	2:I:256:ARG:NH1	2.82	0.41
1:A:149:THR:HG22	1:B:197:LEU:HD12	2.02	0.41
1:A:184:ASN:HD21	2:I:205:ASP:CG	2.29	0.41
2:H:240:ARG:NH2	2:H:261:ASP:OD1	2.54	0.41
2:I:212:LEU:HG	2:I:213:THR:N	2.35	0.41
1:A:197:LEU:HD12	1:B:149:THR:HG22	2.04	0.40
2:H:270:GLY:HA2	2:H:275:LEU:HD12	2.02	0.40
1:B:169:VAL:CG2	1:B:170:LEU:N	2.84	0.40
1:B:154:LEU:O	1:B:155:ASP:CB	2.69	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	87/99 (88%)	82 (94%)	4 (5%)	1 (1%)	11	7
1	B	84/99 (85%)	77 (92%)	5 (6%)	2 (2%)	4	1
2	H	225/249 (90%)	214 (95%)	8 (4%)	3 (1%)	9	5
2	I	223/249 (90%)	218 (98%)	3 (1%)	2 (1%)	14	9
All	All	619/696 (89%)	591 (96%)	20 (3%)	8 (1%)	9	5

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	177	SER

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Mol	Chain	Res	Type
2	H	207	ASP
2	I	207	ASP
1	B	114	VAL
2	H	247	GLY
2	I	256	ARG
1	A	178	GLY
2	H	189	ILE

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	81/87 (93%)	70 (86%)	11 (14%)	3	1
1	B	79/87 (91%)	72 (91%)	7 (9%)	9	5
2	H	191/196 (97%)	164 (86%)	27 (14%)	3	1
2	I	191/196 (97%)	166 (87%)	25 (13%)	4	1
All	All	542/566 (96%)	472 (87%)	70 (13%)	4	1

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	VAL
1	A	116	LYS
1	A	119	ILE
1	A	125	GLN
1	A	136	VAL
1	A	159	SER
1	A	161	THR
1	A	162	LEU
1	A	167	THR
1	A	169	VAL
1	A	176	PRO
1	B	115	ASN
1	B	119	ILE
1	B	152	GLU

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Mol	Chain	Res	Type
1	B	163	THR
1	B	168	SER
1	B	177	SER
1	B	179	SER
2	H	41	MET
2	H	51	LYS
2	H	52	PRO
2	H	55	SER
2	H	58	LEU
2	H	76	ARG
2	H	124	LEU
2	H	126	SER
2	H	127	GLU
2	H	146	GLN
2	H	151	THR
2	H	184	THR
2	H	189	ILE
2	H	207	ASP
2	H	215	LEU
2	H	216	LEU
2	H	221	GLN
2	H	224	LYS
2	H	226	LEU
2	H	227	ILE
2	H	235	SER
2	H	239	ASP
2	H	246	SER
2	H	256	ARG
2	H	268	LEU
2	H	275	LEU
2	H	283	LEU
2	I	42	LEU
2	I	44	GLU
2	I	50	VAL
2	I	51	LYS
2	I	76	ARG
2	I	124	LEU
2	I	126	SER
2	I	127	GLU
2	I	146	GLN
2	I	149	SER
2	I	153	SER

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Mol	Chain	Res	Type
2	I	187	VAL
2	I	188	THR
2	I	206	THR
2	I	212	LEU
2	I	215	LEU
2	I	216	LEU
2	I	227	ILE
2	I	231	SER
2	I	239	ASP
2	I	242	THR
2	I	256	ARG
2	I	268	LEU
2	I	275	LEU
2	I	285	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	A	173	ASN
1	B	129	GLN
1	B	173	ASN
2	H	115	ASN
2	H	221	GLN
2	I	120	GLN
2	I	201	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	91/99 (91%)	0.86	19 (20%) 2 3	24, 39, 79, 84	0
1	B	88/99 (88%)	0.67	13 (14%) 5 6	21, 37, 70, 74	0
2	H	229/249 (91%)	0.18	13 (5%) 29 33	18, 33, 56, 60	0
2	I	227/249 (91%)	0.43	24 (10%) 11 12	20, 36, 60, 69	0
All	All	635/696 (91%)	0.43	69 (10%) 10 12	18, 35, 64, 84	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	40	VAL	4.9
1	A	170	LEU	4.6
1	B	113	PHE	4.6
2	I	40	VAL	4.5
1	A	169	VAL	4.4
1	A	136	VAL	4.2
1	B	170	LEU	3.9
1	A	165	LEU	3.9
1	B	169	VAL	3.8
1	A	140	ALA	3.6
1	B	114	VAL	3.5
2	H	154	SER	3.5
2	H	255	SER	3.4
1	B	136	VAL	3.4
2	I	254	ILE	3.3
2	I	285	LEU	3.3
1	A	167	THR	3.2
2	I	206	THR	3.2
2	H	156	GLY	3.1
1	A	205	HIS	3.1
2	H	235	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	I	283	LEU	3.0
1	B	164	ALA	2.9
1	A	173	ASN	2.8
2	H	189	ILE	2.8
2	I	207	ASP	2.8
2	I	189	ILE	2.7
1	A	113	PHE	2.7
2	I	286	LYS	2.7
2	H	188	THR	2.6
2	I	257	VAL	2.6
1	A	161	THR	2.6
1	A	134	ALA	2.5
1	A	135	VAL	2.5
2	I	208	GLY	2.5
2	H	187	VAL	2.4
2	H	184	THR	2.4
1	A	174	LEU	2.4
2	I	183	LEU	2.4
1	A	162	LEU	2.4
1	A	160	SER	2.4
1	B	168	SER	2.4
1	B	167	THR	2.4
2	I	256	ARG	2.4
1	A	178	GLY	2.4
1	A	163	THR	2.4
2	I	193	ALA	2.3
2	I	255	SER	2.3
1	A	114	VAL	2.3
2	I	260	GLU	2.2
1	B	177	SER	2.2
1	B	135	VAL	2.2
1	B	173	ASN	2.2
2	I	237	VAL	2.2
2	I	232	LYS	2.2
2	H	285	LEU	2.2
2	I	258	GLU	2.1
2	I	236	GLY	2.1
2	H	192	PRO	2.1
2	H	239	ASP	2.1
2	I	284	ASP	2.1
2	I	195	ILE	2.1
2	I	234	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	I	259	ALA	2.1
1	A	172	ASN	2.0
1	B	163	THR	2.0
1	B	160	SER	2.0
2	H	283	LEU	2.0
2	I	190	GLY	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.