



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:15 pm GMT

PDB ID : 1EER
Title : CRYSTAL STRUCTURE OF HUMAN ERYTHROPOIETIN COMPLEXED
TO ITS RECEPTOR AT 1.9 ANGSTROMS
Authors : Syed, R.S.; Li, C.
Deposited on : 1998-07-24
Resolution : 1.90 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

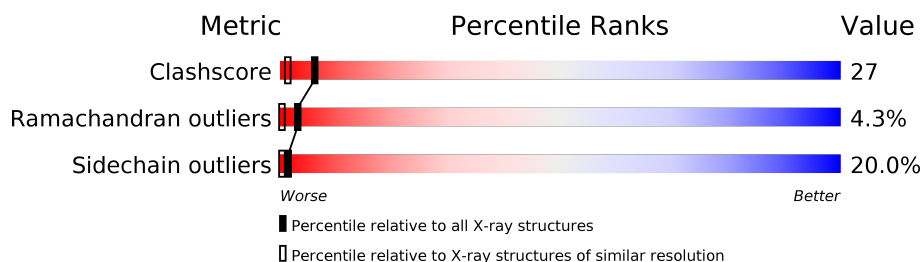
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	166	 61% 29% 8% •
2	B	227	 41% 39% 14% 6%
2	C	227	 49% 35% 9% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4917 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 ERYTHROPOIETIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1291	815	231	240	5			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	LYS	ASN	ENGINEERED	UNP P01588
A	38	LYS	ASN	ENGINEERED	UNP P01588
A	83	LYS	ASN	ENGINEERED	UNP P01588
A	121	ASN	PRO	ENGINEERED	UNP P01588
A	122	SER	PRO	ENGINEERED	UNP P01588

- Molecule 2 is a protein called ERYTHROPOIETIN RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1664	1057	293	307	7			
2	C	213	Total	C	N	O	S	0	0	0
			1664	1057	293	307	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	52	GLN	ASN	ENGINEERED	UNP P19235
B	164	GLN	ASN	ENGINEERED	UNP P19235
B	211	GLU	ALA	ENGINEERED	UNP P19235
C	52	GLN	ASN	ENGINEERED	UNP P19235
C	164	GLN	ASN	ENGINEERED	UNP P19235
C	211	GLU	ALA	ENGINEERED	UNP P19235

- Molecule 3 is water.

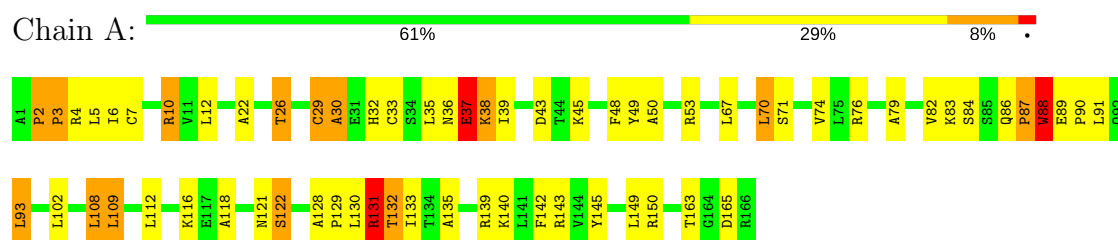
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total 118	O 118	0	0
3	B	74	Total 74	O 74	0	0
3	C	106	Total 106	O 106	0	0

3 Residue-property plots

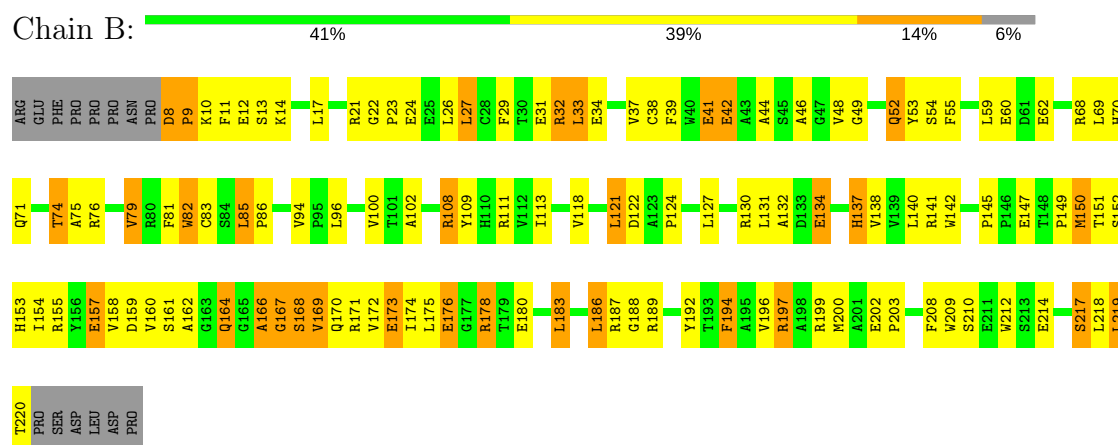
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

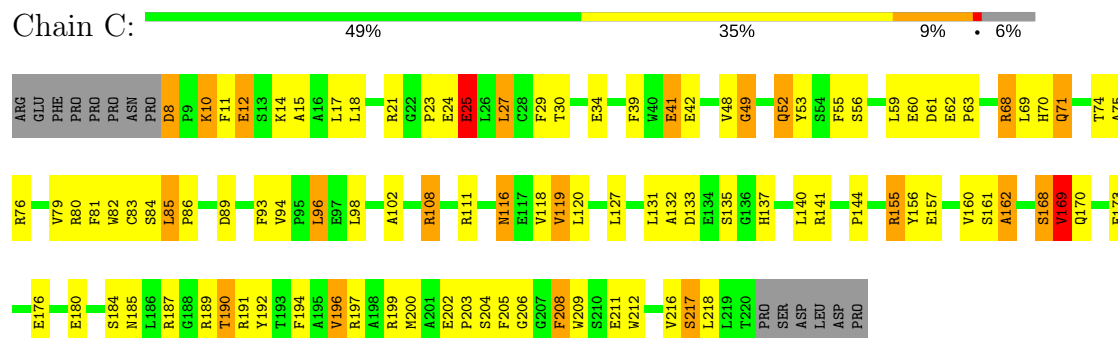
• Molecule 1: ERYTHROPOIETIN



• Molecule 2: ERYTHROPOIETIN RECEPTOR



• Molecule 2: ERYTHROPOIETIN RECEPTOR



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.40 Å 79.30 Å 136.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	93.3 (50.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.242 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4917	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

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	0.35	0/1312	0.62	0/1774
2	B	0.36	0/1709	0.61	0/2330
2	C	0.37	0/1709	0.63	0/2330
All	All	0.36	0/4730	0.62	0/6434

There are no bond length outliers.

There are no bond angle outliers.

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	1291	0	1323	58	0
2	B	1664	0	1622	104	0
2	C	1664	0	1622	90	0
3	A	118	0	0	4	0
3	B	74	0	0	3	0
3	C	106	0	0	4	0
All	All	4917	0	4567	250	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 27.

All (250) 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:B:48:VAL:HA	2:B:52:GLN:HG3	1.35	1.06
2:B:41:GLU:HG2	2:B:74:THR:HG21	1.34	1.03
2:C:162:ALA:HB2	2:C:192:TYR:HA	1.47	0.94
2:B:197:ARG:HD2	2:B:209:TRP:HB3	1.53	0.89
2:B:160:VAL:HB	2:B:170:GLN:HB3	1.57	0.87
2:B:85:LEU:HD13	2:B:86:PRO:HD2	1.59	0.84
2:C:162:ALA:CB	2:C:192:TYR:HA	2.09	0.82
2:B:127:LEU:HD12	2:B:142:TRP:HB3	1.60	0.82
2:B:48:VAL:HG22	2:B:52:GLN:HE21	1.44	0.80
1:A:87:PRO:HG3	3:A:261:HOH:O	1.81	0.79
2:C:12:GLU:HG3	3:C:246:HOH:O	1.81	0.79
1:A:32:HIS:HB3	1:A:87:PRO:HB2	1.64	0.78
2:B:197:ARG:CD	2:B:209:TRP:HB3	2.14	0.78
2:C:197:ARG:HG3	2:C:209:TRP:CE3	2.18	0.77
2:C:10:LYS:NZ	2:C:11:PHE:H	1.81	0.77
1:A:79:ALA:O	1:A:82:VAL:HG12	1.87	0.75
2:C:96:LEU:HD13	2:C:98:LEU:HD21	1.71	0.72
2:B:155:ARG:NH2	2:B:199:ARG:HD3	2.04	0.71
2:C:162:ALA:HB3	2:C:192:TYR:CD2	2.25	0.71
2:B:42:GLU:HB2	2:B:81:PHE:CE1	2.26	0.70
2:B:42:GLU:HB2	2:B:81:PHE:HE1	1.56	0.70
2:B:48:VAL:CA	2:B:52:GLN:HG3	2.20	0.69
2:B:41:GLU:CG	2:B:74:THR:HG21	2.17	0.68
2:C:93:PHE:H	2:C:116:ASN:ND2	1.92	0.67
2:B:162:ALA:HB3	2:B:167:GLY:HA3	1.76	0.67
2:C:189:ARG:HH11	2:C:189:ARG:HB3	1.58	0.67
2:C:18:LEU:HD11	2:C:120:LEU:HD12	1.77	0.66
1:A:128:ALA:O	1:A:130:LEU:HG	1.95	0.66
1:A:10:ARG:N	1:A:10:ARG:HD2	2.10	0.66
2:B:151:THR:HA	2:B:154:ILE:HD12	1.78	0.65
2:B:41:GLU:HG2	2:B:74:THR:CG2	2.19	0.65
1:A:32:HIS:HB3	1:A:87:PRO:CB	2.26	0.65
2:B:130:ARG:HG3	2:B:131:LEU:N	2.12	0.65
2:B:214:GLU:OE1	2:B:214:GLU:HA	1.95	0.65
2:C:161:SER:O	2:C:162:ALA:HB2	1.96	0.64
2:B:11:PHE:HZ	2:B:37:VAL:HG11	1.61	0.64
2:B:155:ARG:HH22	2:B:199:ARG:HD3	1.61	0.63
2:B:8:ASP:O	2:B:12:GLU:HB2	1.99	0.63
1:A:84:SER:OG	1:A:86:GLN:HG2	1.99	0.63
2:B:158:VAL:HG22	2:B:172:VAL:HB	1.79	0.63
1:A:88:TRP:HD1	1:A:91:LEU:HG	1.62	0.63
1:A:86:GLN:HB3	1:A:87:PRO:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:18:LEU:HB3	2:C:27:LEU:HD22	1.79	0.62
1:A:118:ALA:O	1:A:122:SER:HB2	1.99	0.62
2:B:188:GLY:HA2	2:B:220:THR:OG1	2.00	0.62
2:B:149:PRO:C	2:B:150:MET:HG2	2.20	0.62
2:B:142:TRP:CH2	2:B:174:ILE:HG13	2.35	0.61
2:B:27:LEU:HD12	2:B:39:PHE:CE1	2.35	0.61
1:A:32:HIS:HB3	1:A:87:PRO:CG	2.31	0.61
2:B:219:LEU:HD12	2:B:219:LEU:H	1.66	0.61
2:C:116:ASN:H	2:C:116:ASN:HD22	1.49	0.60
2:C:10:LYS:HZ1	2:C:11:PHE:H	1.47	0.60
1:A:89:GLU:N	1:A:90:PRO:CD	2.65	0.60
2:C:41:GLU:HG2	2:C:74:THR:HG21	1.84	0.60
2:B:127:LEU:CD1	2:B:142:TRP:HB3	2.31	0.60
2:B:49:GLY:O	2:B:52:GLN:HB2	2.02	0.59
1:A:49:TYR:O	1:A:53:ARG:HG3	2.02	0.59
2:C:162:ALA:HB1	2:C:191:ARG:O	2.02	0.59
1:A:6:ILE:HD12	1:A:108:LEU:HB3	1.84	0.59
2:B:48:VAL:HG13	2:B:52:GLN:NE2	2.16	0.59
2:C:14:LYS:HG2	2:C:120:LEU:HD13	1.85	0.59
2:C:71:GLN:HG2	2:C:79:VAL:CG2	2.32	0.59
2:B:85:LEU:HD13	2:B:86:PRO:CD	2.32	0.59
2:C:8:ASP:OD1	2:C:10:LYS:HE2	2.03	0.59
1:A:36:ASN:O	1:A:37:GLU:HB3	2.02	0.59
1:A:70:LEU:O	1:A:74:VAL:HG23	2.01	0.59
2:B:162:ALA:CB	2:B:167:GLY:HA3	2.31	0.59
2:C:197:ARG:HD2	2:C:212:TRP:CH2	2.38	0.58
2:B:192:TYR:O	2:B:217:SER:HA	2.03	0.58
2:C:204:SER:HB2	3:C:253:HOH:O	2.03	0.58
2:B:121:LEU:HD11	2:B:200:MET:HG2	1.84	0.58
1:A:93:LEU:HD23	1:A:93:LEU:H	1.67	0.58
1:A:29:CYS:O	1:A:30:ALA:HB3	2.03	0.58
2:C:23:PRO:O	2:C:27:LEU:HD21	2.04	0.57
2:B:189:ARG:N	2:B:220:THR:O	2.37	0.57
2:B:158:VAL:HG12	2:B:196:VAL:HG23	1.86	0.57
1:A:82:VAL:HG13	1:A:83:LYS:HD3	1.86	0.57
2:B:53:TYR:CD1	2:B:102:ALA:HA	2.39	0.57
2:B:48:VAL:HG22	2:B:52:GLN:NE2	2.15	0.57
2:C:116:ASN:ND2	2:C:116:ASN:H	2.02	0.57
2:B:122:ASP:O	2:B:145:PRO:HB3	2.04	0.56
2:B:23:PRO:O	2:B:24:GLU:HB2	2.04	0.56
2:C:190:THR:HB	2:C:192:TYR:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:PRO:HG2	2:B:196:VAL:HG13	1.86	0.56
2:B:59:LEU:HB2	2:B:62:GLU:HG3	1.88	0.56
2:C:10:LYS:HE3	2:C:10:LYS:N	2.20	0.56
1:A:88:TRP:CD1	1:A:91:LEU:HG	2.41	0.55
2:B:131:LEU:HG	2:B:218:LEU:HD21	1.88	0.55
1:A:145:TYR:CE1	1:A:149:LEU:HD11	2.42	0.55
2:B:132:ALA:C	2:B:134:GLU:H	2.08	0.55
1:A:3:PRO:HD2	1:A:7:CYS:SG	2.47	0.54
1:A:84:SER:CB	1:A:86:GLN:HG2	2.37	0.54
1:A:26:THR:HB	1:A:139:ARG:HA	1.88	0.54
2:C:42:GLU:OE1	2:C:108:ARG:NH1	2.41	0.54
2:B:32:ARG:C	2:B:34:GLU:H	2.10	0.54
2:C:53:TYR:CD1	2:C:102:ALA:HA	2.43	0.54
2:C:119:VAL:HG11	2:C:200:MET:HG3	1.91	0.53
2:B:157:GLU:HG2	2:B:197:ARG:NH1	2.23	0.53
2:C:127:LEU:O	2:C:216:VAL:HG21	2.08	0.53
2:C:21:ARG:CZ	2:C:208:PHE:HB3	2.39	0.53
2:C:48:VAL:O	2:C:52:GLN:HB2	2.09	0.53
1:A:132:THR:O	1:A:132:THR:HG22	2.07	0.53
1:A:79:ALA:O	1:A:83:LYS:HG2	2.09	0.53
2:C:119:VAL:HG13	2:C:206:GLY:O	2.09	0.53
2:C:202:GLU:HB3	2:C:203:PRO:HA	1.88	0.53
2:B:14:LYS:HD2	2:B:31:GLU:OE2	2.09	0.53
2:B:8:ASP:HB3	2:B:11:PHE:CD1	2.43	0.53
2:B:121:LEU:CD1	2:B:121:LEU:N	2.72	0.52
2:B:189:ARG:HD2	3:B:270:HOH:O	2.10	0.52
2:B:48:VAL:HG13	2:B:52:GLN:HE21	1.74	0.52
2:C:18:LEU:CD1	2:C:120:LEU:HD12	2.40	0.52
2:C:49:GLY:O	2:C:52:GLN:HB2	2.09	0.52
1:A:2:PRO:O	1:A:4:ARG:N	2.31	0.51
2:B:153:HIS:HA	2:B:176:GLU:HG3	1.92	0.51
2:C:10:LYS:NZ	2:C:11:PHE:N	2.56	0.51
2:C:17:LEU:N	2:C:17:LEU:HD23	2.25	0.51
2:B:137:HIS:CD2	2:B:137:HIS:N	2.78	0.51
2:C:137:HIS:CE1	2:C:184:SER:HB2	2.46	0.51
2:C:23:PRO:HB2	2:C:25:GLU:HB2	1.93	0.51
2:C:161:SER:O	2:C:162:ALA:CB	2.60	0.50
2:C:197:ARG:HD2	2:C:212:TRP:CZ2	2.47	0.50
2:B:118:VAL:O	2:B:118:VAL:HG23	2.10	0.50
2:B:159:ASP:O	2:B:194:PHE:HA	2.12	0.50
2:C:10:LYS:HE3	2:C:10:LYS:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PHE:CD2	2:B:33:LEU:HB3	2.47	0.49
2:C:41:GLU:CG	2:C:74:THR:HG21	2.41	0.49
2:B:60:GLU:HG3	3:B:253:HOH:O	2.12	0.49
2:B:55:PHE:CD2	2:B:100:VAL:HG22	2.48	0.49
2:B:121:LEU:N	2:B:121:LEU:HD12	2.27	0.49
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.47	0.49
2:B:166:ALA:O	2:B:167:GLY:C	2.51	0.49
2:B:48:VAL:CG2	2:B:52:GLN:HE21	2.19	0.49
2:C:199:ARG:HB3	2:C:209:TRP:CE3	2.47	0.49
1:A:89:GLU:N	1:A:90:PRO:HD3	2.26	0.49
2:B:59:LEU:O	2:B:62:GLU:HB2	2.12	0.48
2:B:187:ARG:O	2:B:220:THR:OG1	2.20	0.48
2:B:155:ARG:HG2	2:B:173:GLU:OE2	2.13	0.48
2:B:197:ARG:HD3	2:B:210:SER:O	2.13	0.48
2:C:155:ARG:HA	2:C:176:GLU:HA	1.95	0.48
2:C:155:ARG:NH2	2:C:199:ARG:HD3	2.29	0.48
2:B:23:PRO:O	2:B:24:GLU:CB	2.61	0.48
2:B:42:GLU:C	2:B:44:ALA:H	2.15	0.48
2:B:71:GLN:OE1	2:B:79:VAL:HG11	2.13	0.48
2:B:142:TRP:HH2	2:B:174:ILE:HG13	1.77	0.48
2:C:34:GLU:O	2:C:34:GLU:HG3	2.14	0.48
2:B:137:HIS:CE1	2:B:186:LEU:H	2.32	0.47
1:A:38:LYS:HB2	1:A:38:LYS:HE2	1.63	0.47
2:C:27:LEU:HD13	2:C:39:PHE:CE2	2.48	0.47
2:C:62:GLU:HB3	2:C:63:PRO:HD2	1.96	0.47
1:A:84:SER:HB3	1:A:86:GLN:HG2	1.96	0.47
2:B:26:LEU:HB2	2:B:109:TYR:CD2	2.49	0.47
2:B:178:ARG:HG3	2:B:178:ARG:HH11	1.80	0.47
2:C:144:PRO:HB3	2:C:156:TYR:OH	2.14	0.47
1:A:150:ARG:HD2	2:B:203:PRO:O	2.15	0.47
2:B:141:ARG:HD2	2:B:180:GLU:OE1	2.15	0.47
1:A:145:TYR:O	1:A:149:LEU:HG	2.14	0.47
1:A:128:ALA:O	1:A:129:PRO:C	2.53	0.47
1:A:140:LYS:HG3	1:A:143:ARG:NH2	2.30	0.47
1:A:32:HIS:HD2	3:A:240:HOH:O	1.97	0.47
2:C:23:PRO:C	2:C:25:GLU:H	2.17	0.47
2:C:52:GLN:HB3	2:C:53:TYR:CE2	2.49	0.47
2:C:48:VAL:CG1	2:C:52:GLN:HG3	2.44	0.47
2:C:21:ARG:NE	2:C:208:PHE:HB3	2.31	0.46
2:C:85:LEU:HD22	2:C:86:PRO:HD2	1.97	0.46
2:B:197:ARG:HD3	3:B:286:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:VAL:HG21	2:B:183:LEU:CD2	2.45	0.46
2:B:197:ARG:HH11	2:B:197:ARG:CG	2.28	0.46
2:B:153:HIS:HD2	2:B:176:GLU:OE2	1.99	0.46
2:C:189:ARG:NH1	2:C:189:ARG:HB3	2.30	0.45
2:C:52:GLN:HB3	2:C:53:TYR:CD2	2.51	0.45
2:C:157:GLU:HG3	2:C:173:GLU:OE2	2.16	0.45
1:A:163:THR:O	1:A:163:THR:HG22	2.16	0.45
2:B:9:PRO:C	2:B:11:PHE:N	2.70	0.45
2:C:10:LYS:HZ2	2:C:11:PHE:N	2.15	0.45
2:C:48:VAL:HG12	2:C:52:GLN:HG3	1.97	0.45
2:C:10:LYS:HZ1	2:C:11:PHE:HB3	1.82	0.45
1:A:43:ASP:OD2	1:A:45:LYS:HE2	2.17	0.44
1:A:71:SER:HA	1:A:102:LEU:HD13	1.99	0.44
2:C:157:GLU:OE1	2:C:197:ARG:HD3	2.17	0.44
1:A:35:LEU:HD13	1:A:39:ILE:HD12	1.99	0.44
2:B:132:ALA:C	2:B:134:GLU:N	2.71	0.44
2:B:70:HIS:HB2	2:B:82:TRP:CD2	2.52	0.44
2:B:111:ARG:NH2	2:B:113:ILE:HG21	2.33	0.44
2:B:214:GLU:OE1	2:B:214:GLU:CA	2.65	0.44
2:B:197:ARG:HG3	2:B:197:ARG:NH1	2.33	0.44
2:C:8:ASP:CG	2:C:10:LYS:NZ	2.71	0.44
2:C:141:ARG:HH11	2:C:180:GLU:HB2	1.83	0.43
1:A:26:THR:HG21	1:A:142:PHE:HD2	1.83	0.43
2:B:219:LEU:H	2:B:219:LEU:CD1	2.27	0.43
2:C:10:LYS:HZ2	2:C:11:PHE:H	1.62	0.43
2:C:140:LEU:O	2:C:180:GLU:HA	2.18	0.43
2:C:211:GLU:HG2	3:C:310:HOH:O	2.17	0.43
2:B:132:ALA:N	2:B:137:HIS:O	2.49	0.43
1:A:4:ARG:O	1:A:6:ILE:N	2.52	0.43
2:C:48:VAL:HG12	2:C:52:GLN:HA	2.01	0.43
1:A:38:LYS:H	1:A:38:LYS:NZ	2.16	0.42
2:B:189:ARG:H	2:B:220:THR:C	2.22	0.42
1:A:86:GLN:OE1	1:A:86:GLN:HA	2.20	0.42
2:C:200:MET:HB3	2:C:205:PHE:CB	2.49	0.42
2:C:41:GLU:HG3	2:C:80:ARG:HB2	2.01	0.42
1:A:83:LYS:O	1:A:84:SER:CB	2.67	0.42
2:C:60:GLU:O	2:C:61:ASP:HB2	2.20	0.42
2:B:111:ARG:NH2	2:B:113:ILE:CG2	2.83	0.42
1:A:33:CYS:SG	1:A:88:TRP:CD1	3.13	0.42
2:B:160:VAL:HG21	2:B:183:LEU:HD22	2.02	0.42
1:A:12:LEU:O	1:A:12:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:GLN:C	2:B:166:ALA:H	2.24	0.41
2:C:15:ALA:HB1	2:C:39:PHE:CE2	2.55	0.41
2:C:184:SER:HA	3:C:319:HOH:O	2.19	0.41
1:A:50:ALA:HB2	3:A:262:HOH:O	2.20	0.41
2:C:29:PHE:HA	2:C:118:VAL:O	2.20	0.41
2:C:30:THR:HG23	2:C:119:VAL:HB	2.02	0.41
2:C:70:HIS:HB2	2:C:82:TRP:CE2	2.55	0.41
1:A:22:ALA:HB1	1:A:142:PHE:CD1	2.55	0.41
2:C:127:LEU:HD13	2:C:196:VAL:HG22	2.03	0.41
2:C:192:TYR:O	2:C:217:SER:HA	2.21	0.41
1:A:43:ASP:HA	1:A:133:ILE:HD12	2.03	0.41
2:B:130:ARG:O	2:B:138:VAL:HG13	2.21	0.41
2:B:197:ARG:HG3	2:B:197:ARG:HH11	1.85	0.41
2:B:197:ARG:HG3	2:B:212:TRP:CH2	2.56	0.41
2:B:131:LEU:HG	2:B:218:LEU:CD2	2.48	0.41
2:C:21:ARG:NH1	2:C:21:ARG:HB3	2.35	0.41
2:C:68:ARG:H	2:C:68:ARG:HG2	1.47	0.41
1:A:29:CYS:O	1:A:30:ALA:CB	2.66	0.41
1:A:131:ARG:HB3	1:A:132:THR:H	1.72	0.41
2:B:131:LEU:H	2:B:131:LEU:HD12	1.86	0.41
2:B:159:ASP:OD1	2:B:169:VAL:HG12	2.21	0.41
2:B:32:ARG:C	2:B:34:GLU:N	2.74	0.41
2:B:41:GLU:HA	2:B:79:VAL:O	2.21	0.41
2:C:48:VAL:O	2:C:49:GLY:O	2.39	0.41
2:C:70:HIS:O	2:C:81:PHE:HA	2.20	0.41
1:A:129:PRO:HD3	3:A:243:HOH:O	2.20	0.41
2:B:29:PHE:HE2	2:B:31:GLU:HG3	1.86	0.41
2:B:26:LEU:HD11	2:B:38:CYS:HB3	2.03	0.41
1:A:74:VAL:HG21	1:A:102:LEU:CD1	2.51	0.40
1:A:32:HIS:HB3	1:A:87:PRO:HG2	2.01	0.40
2:B:22:GLY:O	2:B:27:LEU:HD21	2.21	0.40
2:C:59:LEU:HD22	2:C:94:VAL:CG1	2.51	0.40
2:B:111:ARG:HH21	2:B:113:ILE:HG22	1.86	0.40
2:C:12:GLU:HG2	2:C:80:ARG:HH12	1.86	0.40
2:B:178:ARG:NH1	2:B:178:ARG:HG3	2.36	0.40
2:C:168:SER:O	2:C:169:VAL:HG22	2.22	0.40
2:C:79:VAL:O	2:C:79:VAL:HG13	2.21	0.40
1:A:135:ALA:HB1	1:A:140:LYS:HB3	2.03	0.40
1:A:67:LEU:HD22	1:A:109:LEU:HD22	2.03	0.40
2:C:74:THR:C	2:C:76:ARG:H	2.22	0.40
2:B:108:ARG:HG2	2:B:109:TYR:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:23:PRO:C	2:C:25:GLU:N	2.74	0.40
2:C:48:VAL:HG12	2:C:52:GLN:CA	2.52	0.40
2:C:85:LEU:HD13	2:C:89:ASP:HB2	2.02	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	164/166 (99%)	150 (92%)	5 (3%)	9 (6%)	2	0
2	B	211/227 (93%)	181 (86%)	21 (10%)	9 (4%)	3	0
2	C	211/227 (93%)	186 (88%)	18 (8%)	7 (3%)	4	0
All	All	586/620 (94%)	517 (88%)	44 (8%)	25 (4%)	3	0

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	131	ARG
2	B	46	ALA
2	B	137	HIS
2	B	164	GLN
2	B	166	ALA
2	B	168	SER
2	C	132	ALA
2	C	169	VAL
1	A	3	PRO
1	A	30	ALA
2	B	9	PRO
2	B	167	GLY
2	C	25	GLU

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Mol	Chain	Res	Type
2	C	49	GLY
2	C	162	ALA
1	A	2	PRO
1	A	37	GLU
1	A	87	PRO
1	A	88	TRP
1	A	132	THR
2	B	75	ALA
2	C	75	ALA
2	C	170	GLN
2	B	33	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	137/138 (99%)	120 (88%)	17 (12%)	5	2
2	B	176/190 (93%)	131 (74%)	45 (26%)	0	0
2	C	176/190 (93%)	140 (80%)	36 (20%)	1	0
All	All	489/518 (94%)	391 (80%)	98 (20%)	1	0

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	26	THR
1	A	29	CYS
1	A	37	GLU
1	A	38	LYS
1	A	70	LEU
1	A	76	ARG
1	A	88	TRP
1	A	93	LEU
1	A	108	LEU
1	A	109	LEU

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Mol	Chain	Res	Type
1	A	112	LEU
1	A	116	LYS
1	A	121	ASN
1	A	122	SER
1	A	131	ARG
1	A	165	ASP
2	B	8	ASP
2	B	10	LYS
2	B	13	SER
2	B	17	LEU
2	B	21	ARG
2	B	27	LEU
2	B	32	ARG
2	B	41	GLU
2	B	42	GLU
2	B	52	GLN
2	B	54	SER
2	B	68	ARG
2	B	69	LEU
2	B	74	THR
2	B	76	ARG
2	B	79	VAL
2	B	82	TRP
2	B	83	CYS
2	B	85	LEU
2	B	94	VAL
2	B	96	LEU
2	B	108	ARG
2	B	121	LEU
2	B	134	GLU
2	B	140	LEU
2	B	147	GLU
2	B	150	MET
2	B	152	SER
2	B	157	GLU
2	B	161	SER
2	B	168	SER
2	B	169	VAL
2	B	171	ARG
2	B	173	GLU
2	B	175	LEU
2	B	176	GLU

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Mol	Chain	Res	Type
2	B	178	ARG
2	B	183	LEU
2	B	186	LEU
2	B	194	PHE
2	B	197	ARG
2	B	202	GLU
2	B	208	PHE
2	B	217	SER
2	B	219	LEU
2	C	8	ASP
2	C	10	LYS
2	C	12	GLU
2	C	24	GLU
2	C	25	GLU
2	C	27	LEU
2	C	41	GLU
2	C	52	GLN
2	C	55	PHE
2	C	56	SER
2	C	68	ARG
2	C	69	LEU
2	C	71	GLN
2	C	83	CYS
2	C	84	SER
2	C	85	LEU
2	C	96	LEU
2	C	108	ARG
2	C	111	ARG
2	C	116	ASN
2	C	119	VAL
2	C	131	LEU
2	C	133	ASP
2	C	135	SER
2	C	155	ARG
2	C	160	VAL
2	C	168	SER
2	C	169	VAL
2	C	185	ASN
2	C	187	ARG
2	C	190	THR
2	C	194	PHE
2	C	196	VAL

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Mol	Chain	Res	Type
2	C	208	PHE
2	C	217	SER
2	C	218	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	121	ASN
2	B	52	GLN
2	B	153	HIS
2	B	170	GLN
2	C	116	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 carbohydrates 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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.