



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 02:47 am BST

PDB ID : 1HYN
Title : CRYSTAL STRUCTURE OF THE CYTOPLASMIC DOMAIN OF HUMAN ERYTHROCYTE BAND-3 PROTEIN
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Deposited on : 2001-01-20
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

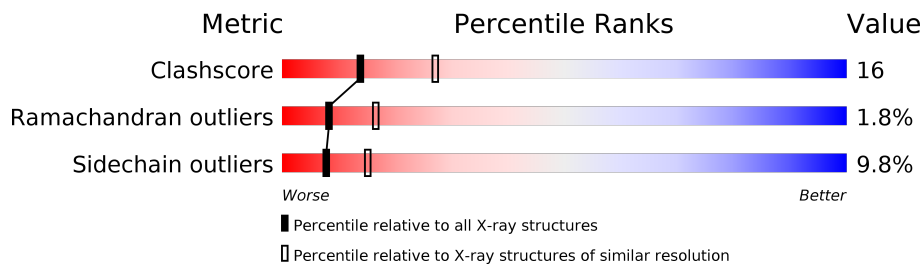
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	P	379	
1	Q	379	
1	R	379	
1	S	379	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9698 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 BAND 3 ANION TRANSPORT PROTEIN.

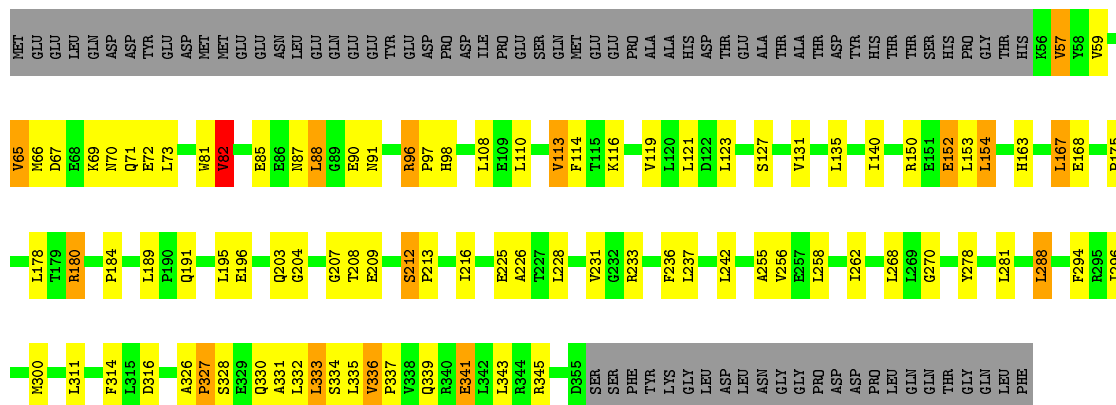
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	P	293	2318	1473	404	435	6	0	0	0
1	Q	302	2382	1511	416	449	6	0	0	0
1	R	300	2366	1502	412	446	6	0	0	0
1	S	293	2318	1473	404	435	6	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	71	Total	O	0	0
			71	71		
2	Q	87	Total	O	0	0
			87	87		
2	R	87	Total	O	0	0
			87	87		
2	S	69	Total	O	0	0
			69	69		

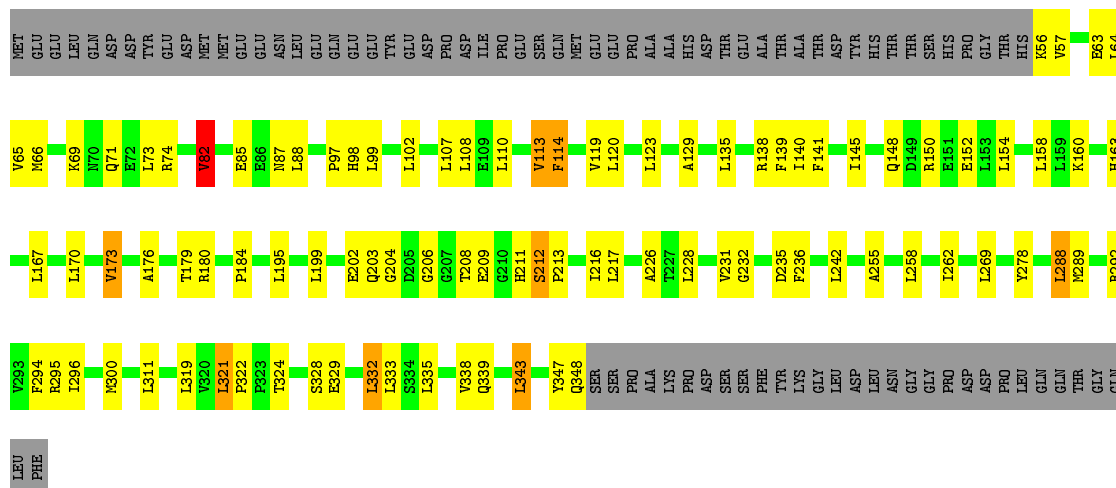
- Molecule 1: BAND 3 ANION TRANSPORT PROTEIN

Chain R:  55% 20% 21%



- Molecule 1: BAND 3 ANION TRANSPORT PROTEIN

Chain S:  53% 22% 23%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.59Å 92.58Å 123.33Å 90.00° 131.86° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	99.0 (8.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.216 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9698	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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	P	0.41	0/2366	0.69	2/3213 (0.1%)
1	Q	0.40	0/2433	0.70	1/3305 (0.0%)
1	R	0.41	0/2416	0.70	1/3282 (0.0%)
1	S	0.42	0/2366	0.72	5/3213 (0.2%)
All	All	0.41	0/9581	0.70	9/13013 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	332	LEU	CA-CB-CG	-6.49	100.38	115.30
1	S	56	LYS	N-CA-C	-6.08	94.60	111.00
1	R	82	VAL	N-CA-C	-6.00	94.81	111.00
1	S	332	LEU	CA-CB-CG	-5.92	101.68	115.30
1	S	71	GLN	O-C-N	5.74	131.89	122.70
1	P	82	VAL	N-CA-C	-5.69	95.64	111.00
1	Q	82	VAL	N-CA-C	-5.46	96.24	111.00
1	S	82	VAL	N-CA-C	-5.25	96.81	111.00
1	S	321	LEU	CA-CB-CG	5.16	127.16	115.30

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	P	2318	0	2320	97	0
1	Q	2382	0	2378	101	0
1	R	2366	0	2366	80	0
1	S	2318	0	2320	82	0
2	P	71	0	0	3	0
2	Q	87	0	0	4	0
2	R	87	0	0	3	0
2	S	69	0	0	0	0
All	All	9698	0	9384	297	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 16.

All (297) 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:S:73:LEU:HD13	1:S:184:PRO:HB3	1.29	1.11
1:R:73:LEU:HD13	1:R:184:PRO:HB3	1.30	1.08
1:Q:73:LEU:HD13	1:Q:184:PRO:HB3	1.36	1.07
1:S:87:ASN:HD21	1:S:98:HIS:HE1	1.12	0.98
1:P:73:LEU:O	1:P:159:LEU:HD13	1.66	0.95
1:P:332:LEU:HD22	1:Q:335:LEU:HD22	1.52	0.90
1:P:332:LEU:HB3	1:Q:335:LEU:HB3	1.55	0.88
1:Q:256:VAL:HG21	1:Q:262:ILE:HD11	1.57	0.84
1:R:333:LEU:HD21	1:S:99:LEU:H	1.42	0.84
1:R:330:GLN:O	1:R:333:LEU:HD22	1.77	0.84
1:P:73:LEU:HD13	1:P:184:PRO:HB3	1.58	0.84
1:P:341:GLU:HG2	1:Q:195:LEU:HD13	1.59	0.84
1:R:73:LEU:HD13	1:R:184:PRO:CB	2.10	0.80
1:Q:331:ALA:HB1	1:Q:335:LEU:HD12	1.63	0.80
1:Q:325:ASP:O	1:Q:327:PRO:HD3	1.81	0.79
1:R:335:LEU:HB3	1:S:332:LEU:HB3	1.65	0.79
1:P:333:LEU:HD13	1:Q:332:LEU:HD21	1.69	0.75
1:R:335:LEU:HB3	1:S:332:LEU:HD22	1.67	0.74
1:Q:87:ASN:HD21	1:Q:98:HIS:HE1	1.36	0.74
1:S:208:THR:HB	1:S:212:SER:HB3	1.69	0.73
1:R:335:LEU:O	1:S:332:LEU:HD13	1.89	0.73
1:Q:180:ARG:HG3	1:Q:236:PHE:HB3	1.71	0.72
1:S:87:ASN:ND2	1:S:98:HIS:HE1	1.88	0.72
1:Q:333:LEU:HD23	1:Q:334:SER:N	2.04	0.72
1:Q:333:LEU:HD23	1:Q:334:SER:H	1.55	0.71
1:S:343:LEU:HD22	1:S:347:TYR:HE1	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:332:LEU:CB	1:Q:335:LEU:HB3	2.20	0.69
1:R:195:LEU:HD21	1:S:338:VAL:HG13	1.75	0.68
1:R:333:LEU:HD21	1:S:99:LEU:N	2.07	0.68
1:Q:226:ALA:HB3	1:Q:262:ILE:HD13	1.75	0.67
1:R:327:PRO:HB2	1:R:330:GLN:HB2	1.77	0.67
1:S:289:MET:CE	1:S:295:ARG:HG3	2.24	0.67
1:P:209:GLU:HB2	1:P:212:SER:OG	1.95	0.67
1:P:199:LEU:HD12	1:Q:337:PRO:HB2	1.75	0.67
1:R:339:GLN:HG3	1:S:332:LEU:HD11	1.77	0.66
1:P:256:VAL:HG21	1:P:262:ILE:HD11	1.77	0.66
1:S:226:ALA:HB3	1:S:262:ILE:HD13	1.77	0.66
1:R:87:ASN:HD21	1:R:98:HIS:HE1	1.42	0.66
1:S:87:ASN:HD21	1:S:98:HIS:CE1	2.04	0.66
1:S:163:HIS:HE1	1:S:255:ALA:O	1.78	0.65
1:R:127:SER:O	1:R:131:VAL:HG23	1.96	0.65
1:R:333:LEU:HD23	1:R:334:SER:N	2.11	0.65
1:R:191:GLN:OE1	1:R:191:GLN:HA	1.97	0.65
1:P:98:HIS:HA	1:Q:333:LEU:HG	1.77	0.65
1:P:195:LEU:HG	1:Q:345:ARG:HH21	1.62	0.65
1:R:88:LEU:HD13	1:R:167:LEU:HD12	1.79	0.65
1:R:335:LEU:HB3	1:S:332:LEU:CB	2.27	0.65
1:S:296:ILE:HG22	1:S:300:MET:CE	2.27	0.65
1:S:180:ARG:HG2	1:S:236:PHE:HB3	1.79	0.64
1:S:329:GLU:O	1:S:333:LEU:HB2	1.97	0.64
1:R:333:LEU:HD11	1:S:98:HIS:HA	1.79	0.64
1:Q:70:ASN:ND2	1:Q:72:GLU:HG3	2.12	0.63
1:R:335:LEU:C	1:S:332:LEU:HD13	2.20	0.62
1:P:123:LEU:HD22	1:P:125:GLU:HG2	1.80	0.62
1:Q:252:GLU:HB3	2:Q:5859:HOH:O	1.98	0.62
1:R:332:LEU:HD21	1:S:333:LEU:HD13	1.80	0.62
1:S:66:MET:HB2	1:S:176:ALA:HB2	1.81	0.62
1:Q:189:LEU:HD11	1:S:141:PHE:CZ	2.35	0.62
1:R:296:ILE:O	1:R:300:MET:HG3	1.99	0.62
1:P:341:GLU:HG2	1:Q:195:LEU:CD1	2.30	0.61
1:S:343:LEU:HD22	1:S:347:TYR:CE1	2.35	0.61
1:Q:84:LEU:HB2	1:Q:216:ILE:HD11	1.82	0.61
1:Q:231:VAL:CG1	1:Q:278:TYR:HB3	2.30	0.61
1:S:85:GLU:O	1:S:97:PRO:HA	2.00	0.61
1:P:233:ARG:NH1	1:P:278:TYR:HB2	2.15	0.60
1:P:99:LEU:HB2	1:Q:333:LEU:HD21	1.83	0.60
1:Q:345:ARG:HG2	1:Q:345:ARG:HH11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:87:ASN:OD1	1:P:98:HIS:HE1	1.85	0.60
1:R:59:VAL:HB	1:R:81:TRP:HB2	1.84	0.59
1:P:73:LEU:O	1:P:159:LEU:CD1	2.47	0.59
1:Q:296:ILE:O	1:Q:300:MET:HG3	2.03	0.59
1:P:141:PHE:CE1	1:R:189:LEU:HD11	2.39	0.58
1:P:141:PHE:CE2	1:R:189:LEU:HD21	2.39	0.58
1:R:140:ILE:HD11	1:R:150:ARG:HB2	1.86	0.58
1:P:345:ARG:O	1:P:348:GLN:HG2	2.03	0.58
1:Q:69:LYS:HG3	1:Q:70:ASN:H	1.69	0.58
1:Q:87:ASN:HD21	1:Q:98:HIS:CE1	2.20	0.57
1:P:296:ILE:O	1:P:300:MET:HG3	2.04	0.57
1:R:231:VAL:CG1	1:R:278:TYR:HB3	2.35	0.57
1:R:339:GLN:CG	1:S:332:LEU:HD11	2.35	0.57
1:P:141:PHE:CZ	1:R:189:LEU:HD11	2.40	0.57
1:Q:139:PHE:HB3	1:Q:145:ILE:HG12	1.87	0.57
1:P:127:SER:O	1:P:131:VAL:HG23	2.05	0.57
1:P:332:LEU:HD13	1:Q:335:LEU:CA	2.35	0.56
1:R:73:LEU:CD1	1:R:184:PRO:HB3	2.20	0.56
1:P:99:LEU:HD13	1:Q:321:LEU:HD21	1.88	0.56
1:Q:209:GLU:HB3	1:Q:212:SER:HB2	1.87	0.56
1:P:148:GLN:HG3	2:P:5942:HOH:O	2.06	0.55
1:R:335:LEU:HB3	1:S:332:LEU:CD2	2.36	0.55
1:R:335:LEU:CB	1:S:332:LEU:HD22	2.36	0.55
1:S:179:THR:HA	1:S:235:ASP:OD2	2.07	0.55
1:S:57:VAL:HG21	1:S:295:ARG:HD3	1.88	0.55
1:R:242:LEU:HD12	1:R:268:LEU:HD21	1.88	0.55
1:S:163:HIS:CE1	1:S:255:ALA:O	2.60	0.55
1:P:332:LEU:HD13	1:Q:335:LEU:C	2.27	0.55
1:Q:90:GLU:O	1:Q:167:LEU:HD21	2.06	0.55
1:P:65:VAL:CG2	1:P:173:VAL:HG21	2.37	0.55
1:Q:73:LEU:HD13	1:Q:184:PRO:CB	2.24	0.54
1:Q:212:SER:N	1:Q:213:PRO:HD2	2.23	0.54
1:R:233:ARG:HA	1:R:270:GLY:O	2.08	0.54
1:P:66:MET:HA	1:P:72:GLU:O	2.07	0.54
1:R:152:GLU:HB2	2:R:5950:HOH:O	2.07	0.54
1:P:234:ALA:HB3	1:P:237:LEU:HD12	1.89	0.54
1:P:292:ARG:HG3	1:P:292:ARG:HH11	1.72	0.54
1:Q:261:PRO:HG3	2:Q:5859:HOH:O	2.07	0.54
1:S:82:VAL:HB	1:S:216:ILE:HG12	1.90	0.54
1:Q:70:ASN:HD22	1:Q:72:GLU:HG3	1.73	0.53
1:R:119:VAL:HG12	1:R:121:LEU:HG	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:57:VAL:HA	1:R:225:GLU:O	2.08	0.53
1:S:288:LEU:HD22	1:S:294:PHE:CG	2.43	0.53
1:S:195:LEU:HD22	1:S:199:LEU:CD2	2.37	0.53
1:S:57:VAL:CG2	1:S:295:ARG:HD3	2.39	0.53
1:P:116:LYS:NZ	1:P:239:GLN:HE22	2.05	0.53
1:S:179:THR:HG22	1:S:180:ARG:N	2.24	0.53
1:Q:87:ASN:ND2	1:Q:98:HIS:HE1	2.04	0.53
1:P:139:PHE:HB3	1:P:145:ILE:HG12	1.89	0.52
1:P:199:LEU:HD21	1:Q:341:GLU:HG3	1.91	0.52
1:S:209:GLU:HB2	1:S:212:SER:HB2	1.91	0.52
1:R:226:ALA:HB3	1:R:262:ILE:HD13	1.90	0.52
1:R:345:ARG:HH11	1:R:345:ARG:HG2	1.75	0.52
1:R:341:GLU:HG3	1:S:199:LEU:HD21	1.92	0.52
1:S:73:LEU:HD13	1:S:184:PRO:CB	2.20	0.52
1:P:90:GLU:O	1:P:167:LEU:HD11	2.10	0.52
1:P:226:ALA:HB3	1:P:262:ILE:HD13	1.92	0.52
1:P:99:LEU:H	1:Q:333:LEU:HD21	1.74	0.52
1:Q:109:GLU:O	1:Q:113:VAL:HG22	2.09	0.52
1:R:180:ARG:HG3	1:R:236:PHE:HB3	1.92	0.52
1:R:331:ALA:HB1	1:R:335:LEU:HD12	1.91	0.52
1:S:98:HIS:HD2	1:S:99:LEU:O	1.92	0.52
1:R:212:SER:N	1:R:213:PRO:HD2	2.25	0.52
1:Q:97:PRO:HB3	1:Q:216:ILE:HD12	1.92	0.51
1:Q:93:ALA:CB	1:Q:204:GLY:HA3	2.41	0.51
1:R:256:VAL:HG21	1:R:262:ILE:HD11	1.92	0.51
1:R:85:GLU:O	1:R:97:PRO:HA	2.10	0.51
1:P:65:VAL:HG21	1:P:173:VAL:HG21	1.93	0.51
1:P:129:ALA:HA	1:P:158:LEU:HD21	1.93	0.51
1:P:68:GLU:HG2	1:P:174:LYS:HG3	1.93	0.51
1:R:163:HIS:HE1	1:R:255:ALA:O	1.93	0.50
1:P:233:ARG:HH11	1:P:278:TYR:HB2	1.75	0.50
1:Q:105:TRP:CE3	1:Q:275:HIS:HB3	2.46	0.50
1:S:139:PHE:HB3	1:S:145:ILE:HG12	1.93	0.50
1:P:332:LEU:HD11	1:Q:339:GLN:HB2	1.92	0.50
1:R:314:PHE:CZ	1:S:322:PRO:HB3	2.46	0.50
1:P:69:LYS:HB2	1:P:170:LEU:O	2.12	0.50
1:P:98:HIS:CA	1:Q:333:LEU:HG	2.40	0.50
1:Q:82:VAL:O	1:Q:83:GLN:HB2	2.12	0.50
1:R:175:PRO:HB3	1:R:191:GLN:HE21	1.76	0.49
1:P:108:LEU:O	1:P:112:ARG:HG3	2.13	0.49
1:P:273:ALA:HB3	1:P:276:ILE:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:332:LEU:HD13	1:Q:335:LEU:HA	1.95	0.49
1:P:323:PRO:HG3	1:Q:317:CYS:HB2	1.95	0.49
1:R:65:VAL:O	1:R:73:LEU:HD12	2.13	0.49
1:S:119:VAL:O	1:S:120:LEU:HD23	2.12	0.49
1:Q:178:LEU:HD11	1:Q:182:GLY:HA2	1.94	0.49
1:P:148:GLN:NE2	1:P:148:GLN:H	2.10	0.49
1:S:292:ARG:HD2	1:S:347:TYR:HE2	1.77	0.48
1:Q:189:LEU:HD11	1:S:141:PHE:CE1	2.47	0.48
1:Q:93:ALA:HB1	1:Q:204:GLY:HA3	1.96	0.48
1:Q:92:GLY:HA2	1:Q:167:LEU:HD13	1.94	0.48
1:S:212:SER:N	1:S:213:PRO:CD	2.77	0.48
1:Q:67:ASP:HA	1:Q:173:VAL:HA	1.94	0.48
1:P:73:LEU:C	1:P:159:LEU:HD13	2.33	0.48
1:Q:174:LYS:HD2	1:Q:175:PRO:HD2	1.96	0.48
1:S:292:ARG:HH11	1:S:292:ARG:HG3	1.79	0.48
1:S:65:VAL:O	1:S:73:LEU:HD12	2.13	0.48
1:P:73:LEU:O	1:P:159:LEU:HD22	2.14	0.48
1:P:91:ASN:HD21	1:P:204:GLY:HA2	1.78	0.48
1:R:335:LEU:O	1:R:336:VAL:HG23	2.13	0.48
1:Q:180:ARG:H	1:Q:180:ARG:HD2	1.77	0.48
1:R:180:ARG:HG2	1:R:180:ARG:HH11	1.78	0.48
1:R:96:ARG:HG2	1:R:203:GLN:HE22	1.79	0.48
1:P:206:GLY:N	1:P:210:GLY:HA2	2.29	0.47
1:P:333:LEU:CD1	1:Q:332:LEU:HD21	2.43	0.47
1:Q:334:SER:O	1:Q:338:VAL:HB	2.14	0.47
1:R:82:VAL:HB	1:R:216:ILE:HG12	1.97	0.47
1:R:91:ASN:O	1:R:168:GLU:HG2	2.14	0.47
1:R:108:LEU:HD13	1:S:108:LEU:HD13	1.96	0.47
1:S:319:LEU:HD21	1:S:335:LEU:HD22	1.95	0.47
1:P:288:LEU:HD22	1:P:294:PHE:CG	2.49	0.47
1:S:208:THR:HB	1:S:212:SER:CB	2.42	0.47
1:S:74:ARG:HH11	1:S:74:ARG:HG2	1.78	0.47
1:Q:69:LYS:HG2	1:Q:170:LEU:O	2.15	0.47
1:Q:341:GLU:O	1:Q:345:ARG:HG3	2.15	0.47
1:S:231:VAL:HG13	1:S:278:TYR:HB3	1.95	0.47
1:R:70:ASN:HB3	1:R:72:GLU:HG3	1.96	0.47
1:P:338:VAL:HA	1:Q:199:LEU:HD21	1.97	0.47
1:P:119:VAL:HG12	1:P:121:LEU:HG	1.96	0.47
1:P:231:VAL:HG13	1:P:278:TYR:HB3	1.96	0.47
1:Q:163:HIS:HE1	1:Q:255:ALA:O	1.98	0.47
1:S:296:ILE:HG22	1:S:300:MET:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:87:ASN:ND2	1:R:98:HIS:HE1	2.10	0.46
1:Q:199:LEU:HD13	1:Q:200:PHE:CE1	2.51	0.46
1:P:67:ASP:OD1	1:P:72:GLU:HG3	2.16	0.46
1:R:333:LEU:C	1:R:333:LEU:HD23	2.35	0.46
1:R:258:LEU:HB3	2:R:6068:HOH:O	2.14	0.46
1:S:232:GLY:O	1:S:269:LEU:HA	2.15	0.46
1:P:73:LEU:CD1	1:P:184:PRO:HB3	2.39	0.46
1:P:338:VAL:HG21	1:Q:101:HIS:ND1	2.31	0.46
1:Q:55:HIS:HD2	1:Q:223:ASP:O	1.98	0.46
1:P:289:MET:CE	1:P:295:ARG:HG3	2.45	0.46
1:Q:180:ARG:HH11	1:Q:180:ARG:HG2	1.81	0.46
1:P:141:PHE:CD2	1:R:189:LEU:HD21	2.50	0.46
1:S:203:GLN:HB2	1:S:206:GLY:O	2.15	0.46
1:S:113:VAL:HG13	1:S:242:LEU:HB2	1.97	0.45
1:Q:231:VAL:HG11	1:Q:278:TYR:HB3	1.97	0.45
1:S:99:LEU:HA	1:S:99:LEU:HD23	1.78	0.45
1:S:328:SER:O	1:S:332:LEU:HD12	2.17	0.45
1:P:139:PHE:O	1:P:144:GLN:HB2	2.16	0.45
1:P:332:LEU:HD11	1:Q:339:GLN:HG3	1.97	0.45
1:S:120:LEU:HD21	1:S:138:ARG:HG2	1.99	0.45
1:P:237:LEU:O	1:P:271:PRO:HB3	2.17	0.45
1:S:343:LEU:CD2	1:S:347:TYR:HE1	2.25	0.45
1:R:333:LEU:CD1	1:S:98:HIS:HA	2.46	0.45
1:R:116:LYS:HE3	2:R:5834:HOH:O	2.17	0.44
1:P:329:GLU:O	1:P:333:LEU:HB2	2.17	0.44
1:Q:156:ALA:HA	1:Q:159:LEU:HG	1.98	0.44
1:S:63:GLU:HG2	1:S:231:VAL:HB	1.98	0.44
1:P:96:ARG:HD2	1:P:200:PHE:HD2	1.81	0.44
1:P:99:LEU:HD12	1:Q:331:ALA:HA	1.98	0.44
1:R:96:ARG:HE	1:R:203:GLN:HE22	1.66	0.44
1:S:226:ALA:HB3	1:S:262:ILE:CD1	2.44	0.44
1:P:123:LEU:HD12	1:P:245:VAL:HG11	2.00	0.44
1:P:319:LEU:HD22	1:P:335:LEU:HD13	1.99	0.44
1:P:68:GLU:O	1:P:71:GLN:NE2	2.50	0.44
1:P:98:HIS:HA	1:Q:333:LEU:CG	2.45	0.44
1:Q:336:VAL:HB	1:Q:337:PRO:CD	2.48	0.44
1:R:336:VAL:HB	1:R:337:PRO:CD	2.47	0.44
1:P:99:LEU:HG	1:Q:330:GLN:O	2.18	0.43
1:Q:122:ASP:N	1:Q:246:ARG:O	2.51	0.43
1:R:66:MET:HA	1:R:72:GLU:O	2.18	0.43
1:Q:98:HIS:HD2	1:Q:99:LEU:O	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:113:VAL:HG13	1:R:242:LEU:HB2	2.00	0.43
1:R:153:LEU:HD11	1:R:237:LEU:HD21	1.99	0.43
1:P:194:SER:O	1:P:198:GLN:HG3	2.18	0.43
1:P:219:LYS:O	1:P:221:PRO:HD3	2.19	0.43
1:P:57:VAL:HG21	1:P:295:ARG:HD3	2.00	0.43
1:P:85:GLU:O	1:P:97:PRO:HA	2.18	0.43
1:R:330:GLN:HA	1:R:333:LEU:HD13	2.01	0.43
1:S:129:ALA:HA	1:S:158:LEU:HD21	2.00	0.43
1:Q:119:VAL:HG12	1:Q:121:LEU:HG	2.01	0.43
1:Q:123:LEU:HG	1:Q:125:GLU:HG2	2.00	0.43
1:Q:300:MET:HG2	2:Q:5897:HOH:O	2.19	0.43
1:S:195:LEU:HD22	1:S:199:LEU:HD21	2.00	0.43
1:Q:74:ARG:HH11	1:Q:74:ARG:HG2	1.83	0.43
1:Q:189:LEU:HD21	1:S:141:PHE:CD2	2.54	0.42
1:S:102:LEU:CD1	1:S:107:LEU:HD21	2.49	0.42
1:Q:330:GLN:O	1:Q:333:LEU:HD22	2.19	0.42
1:P:332:LEU:CD1	1:Q:339:GLN:HB2	2.49	0.42
1:P:335:LEU:HD23	1:Q:101:HIS:NE2	2.34	0.42
1:R:196:GLU:H	1:R:196:GLU:CD	2.23	0.42
1:P:290:SER:O	1:P:295:ARG:NH2	2.53	0.42
1:P:321:LEU:HD23	1:Q:101:HIS:HD2	1.84	0.42
1:Q:128:LEU:HD21	2:Q:6082:HOH:O	2.19	0.42
1:R:339:GLN:CB	1:S:332:LEU:HD11	2.50	0.42
1:P:98:HIS:HA	1:Q:333:LEU:CD1	2.50	0.42
1:S:209:GLU:CB	1:S:212:SER:HB2	2.49	0.42
1:Q:330:GLN:O	1:Q:333:LEU:CD2	2.68	0.42
1:P:99:LEU:H	1:Q:333:LEU:CD2	2.32	0.42
1:P:331:ALA:HA	1:Q:99:LEU:HD22	2.02	0.42
1:S:319:LEU:CD2	1:S:335:LEU:HD22	2.50	0.42
1:R:150:ARG:HH12	1:R:154:LEU:HD12	1.85	0.42
1:R:288:LEU:HD22	1:R:294:PHE:CG	2.54	0.42
1:P:257:GLU:HG3	2:P:6024:HOH:O	2.19	0.41
1:S:140:ILE:HD11	1:S:150:ARG:HB2	2.02	0.41
1:P:273:ALA:HB3	1:P:276:ILE:HG22	2.01	0.41
1:P:56:LYS:O	1:P:57:VAL:HG23	2.20	0.41
1:Q:335:LEU:O	1:Q:336:VAL:HG23	2.20	0.41
1:R:231:VAL:HG11	1:R:278:TYR:HB3	2.02	0.41
1:S:296:ILE:HG22	1:S:300:MET:HE1	2.00	0.41
1:S:69:LYS:HB2	1:S:170:LEU:O	2.19	0.41
1:P:212:SER:N	1:P:213:PRO:CD	2.83	0.41
1:R:326:ALA:HA	1:R:327:PRO:HD3	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:231:VAL:CG1	1:P:278:TYR:HB3	2.51	0.41
1:Q:234:ALA:HB3	1:Q:237:LEU:HG	2.01	0.41
1:S:217:LEU:HD22	1:S:258:LEU:HD11	2.03	0.41
1:Q:233:ARG:HA	1:Q:270:GLY:O	2.20	0.41
1:P:67:ASP:HA	1:P:173:VAL:HG23	2.03	0.41
1:Q:153:LEU:HD11	1:Q:237:LEU:HD21	2.02	0.41
1:P:332:LEU:HD22	1:Q:335:LEU:CD2	2.38	0.41
1:Q:73:LEU:HD12	1:Q:73:LEU:HA	1.93	0.41
1:Q:237:LEU:HD12	1:Q:270:GLY:HA2	2.03	0.41
1:R:207:GLY:C	1:R:209:GLU:H	2.23	0.41
1:R:343:LEU:HD13	1:S:324:THR:O	2.20	0.41
1:R:67:ASP:OD1	1:R:72:GLU:HB2	2.21	0.41
1:Q:167:LEU:HD23	1:Q:167:LEU:C	2.41	0.41
1:Q:207:GLY:C	1:Q:209:GLU:H	2.25	0.41
1:S:110:LEU:O	1:S:114:PHE:HB2	2.20	0.41
1:P:116:LYS:HE3	2:P:5933:HOH:O	2.20	0.41
1:R:345:ARG:NH1	1:R:345:ARG:HG2	2.36	0.41
1:R:337:PRO:HB2	1:S:199:LEU:HD12	2.03	0.41
1:R:333:LEU:CG	1:S:98:HIS:HA	2.51	0.41
1:S:65:VAL:HG21	1:S:173:VAL:HG21	2.03	0.40
1:P:108:LEU:HD13	1:Q:108:LEU:HD13	2.04	0.40
1:Q:180:ARG:NH1	1:Q:180:ARG:HG2	2.37	0.40
1:P:189:LEU:HA	1:P:190:PRO:HD3	1.93	0.40
1:P:116:LYS:HZ2	1:P:239:GLN:HE22	1.70	0.40
1:R:67:ASP:OD2	1:R:70:ASN:HB2	2.21	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	P	291/379 (77%)	275 (94%)	14 (5%)	2 (1%)	22 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	300/379 (79%)	279 (93%)	11 (4%)	10 (3%)	4	6
1	R	298/379 (79%)	280 (94%)	12 (4%)	6 (2%)	7	14
1	S	291/379 (77%)	275 (94%)	13 (4%)	3 (1%)	15	32
All	All	1180/1516 (78%)	1109 (94%)	50 (4%)	21 (2%)	8	16

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	327	PRO
1	Q	204	GLY
1	R	57	VAL
1	R	336	VAL
1	Q	56	LYS
1	Q	202	GLU
1	Q	336	VAL
1	S	202	GLU
1	P	69	LYS
1	P	82	VAL
1	Q	205	ASP
1	Q	327	PRO
1	R	204	GLY
1	Q	69	LYS
1	Q	328	SER
1	S	82	VAL
1	Q	82	VAL
1	R	208	THR
1	S	204	GLY
1	R	82	VAL
1	Q	259	PRO

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	P	251/327 (77%)	221 (88%)	30 (12%)	5	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	259/327 (79%)	235 (91%)	24 (9%)	9	17
1	R	257/327 (79%)	232 (90%)	25 (10%)	8	15
1	S	251/327 (77%)	230 (92%)	21 (8%)	11	21
All	All	1018/1308 (78%)	918 (90%)	100 (10%)	8	15

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	64	LEU
1	P	69	LYS
1	P	70	ASN
1	P	88	LEU
1	P	96	ARG
1	P	114	PHE
1	P	123	LEU
1	P	135	LEU
1	P	139	PHE
1	P	148	GLN
1	P	154	LEU
1	P	160	LYS
1	P	168	GLU
1	P	173	VAL
1	P	183	ASP
1	P	190	PRO
1	P	192	HIS
1	P	195	LEU
1	P	203	GLN
1	P	205	ASP
1	P	211	HIS
1	P	223	ASP
1	P	228	LEU
1	P	281	LEU
1	P	288	LEU
1	P	311	LEU
1	P	321	LEU
1	P	333	LEU
1	P	339	GLN
1	P	346	ARG
1	Q	64	LEU
1	Q	65	VAL
1	Q	68	GLU

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Mol	Chain	Res	Type
1	Q	88	LEU
1	Q	110	LEU
1	Q	114	PHE
1	Q	135	LEU
1	Q	152	GLU
1	Q	155	ARG
1	Q	180	ARG
1	Q	199	LEU
1	Q	211	HIS
1	Q	214	SER
1	Q	216	ILE
1	Q	223	ASP
1	Q	228	LEU
1	Q	252	GLU
1	Q	253	LEU
1	Q	281	LEU
1	Q	288	LEU
1	Q	311	LEU
1	Q	321	LEU
1	Q	333	LEU
1	Q	356	SER
1	R	65	VAL
1	R	69	LYS
1	R	71	GLN
1	R	88	LEU
1	R	90	GLU
1	R	96	ARG
1	R	110	LEU
1	R	113	VAL
1	R	114	PHE
1	R	123	LEU
1	R	135	LEU
1	R	152	GLU
1	R	154	LEU
1	R	167	LEU
1	R	178	LEU
1	R	180	ARG
1	R	212	SER
1	R	228	LEU
1	R	281	LEU
1	R	288	LEU
1	R	311	LEU

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Mol	Chain	Res	Type
1	R	316	ASP
1	R	328	SER
1	R	333	LEU
1	R	341	GLU
1	S	64	LEU
1	S	88	LEU
1	S	113	VAL
1	S	114	PHE
1	S	123	LEU
1	S	135	LEU
1	S	148	GLN
1	S	152	GLU
1	S	154	LEU
1	S	160	LYS
1	S	167	LEU
1	S	173	VAL
1	S	211	HIS
1	S	212	SER
1	S	228	LEU
1	S	288	LEU
1	S	311	LEU
1	S	321	LEU
1	S	339	GLN
1	S	343	LEU
1	S	348	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	71	GLN
1	P	98	HIS
1	P	144	GLN
1	P	148	GLN
1	P	163	HIS
1	P	239	GLN
1	Q	55	HIS
1	Q	70	ASN
1	Q	87	ASN
1	Q	98	HIS
1	Q	134	GLN
1	Q	163	HIS
1	Q	186	GLN

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Mol	Chain	Res	Type
1	Q	203	GLN
1	R	87	ASN
1	R	98	HIS
1	R	134	GLN
1	R	144	GLN
1	R	163	HIS
1	S	87	ASN
1	S	98	HIS
1	S	101	HIS
1	S	144	GLN
1	S	163	HIS
1	S	239	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 carbohydrates 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

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.