Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 09:30 PM EDT

PDB ID	:	2VSG
Title	:	A Structural Motif in the Variant Surface Glycoproteins of Trypanosoma Brucei
Authors	:	Blum, M.L.; Down, J.A.; Metcalf, P.; Freymann, D.M.; Wiley, D.C.
Deposited on	:	1998-11-19
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

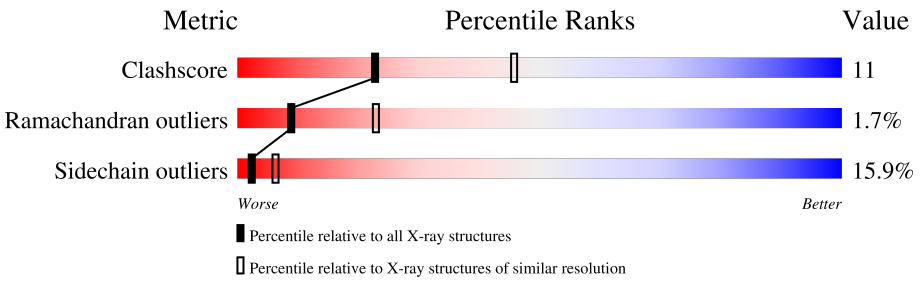
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	358	63% 31% 6% •
1	B	358	65% 26% 8% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5455 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 VARIANT SURFACE GLYCOPROTEIN ILTAT 1.24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	358	2686	1669	460	549	8	0	0	0
1	B	358	2686	1669	460	549	8	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	43	43	43	0	0
2	B	40	40	40	0	0

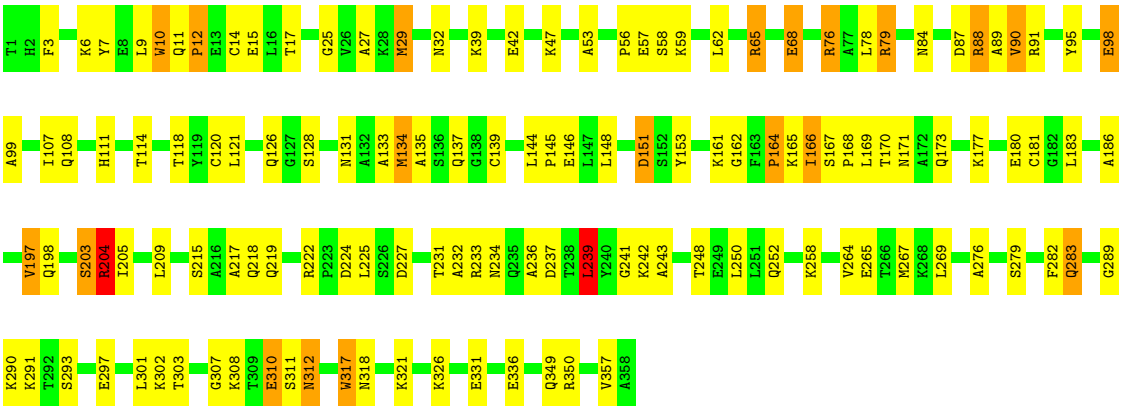
3 Residue-property plots (i)

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. 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. 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.

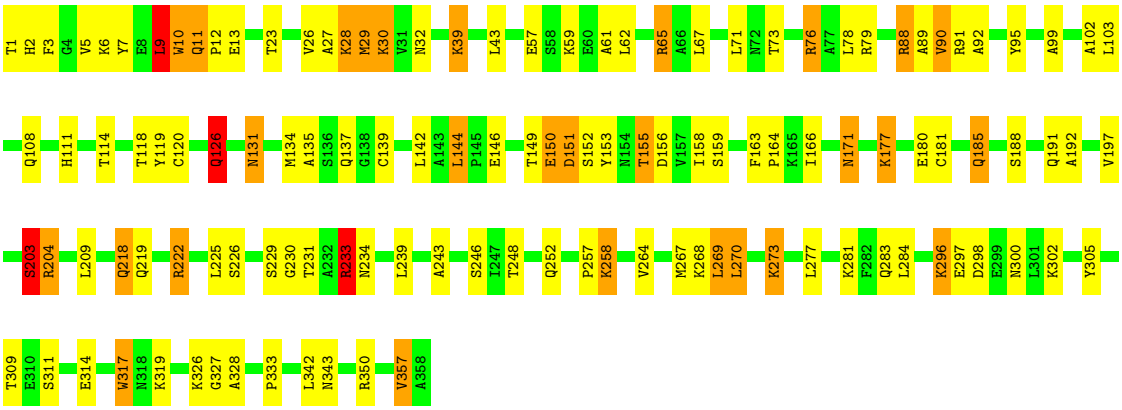
• Molecule 1: VARIANT SURFACE GLYCOPROTEIN ILTAT 1.24

Chain A: 63% 31% 6% •



• Molecule 1: VARIANT SURFACE GLYCOPROTEIN ILTAT 1.24

Chain B: 65% 26% 8% •



4 Data and refinement statistics (i)

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	55.10Å 98.80Å 172.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	81.0 (6.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5455	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	0.75	0/2724	1.47	36/3681 (1.0%)
1	B	0.77	0/2724	1.46	32/3681 (0.9%)
All	All	0.76	0/5448	1.47	68/7362 (0.9%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	204	ARG	NE-CZ-NH1	14.29	127.45	120.30
1	B	79	ARG	NE-CZ-NH2	-13.54	113.53	120.30
1	A	79	ARG	NE-CZ-NH2	-13.49	113.55	120.30
1	A	79	ARG	NE-CZ-NH1	12.91	126.76	120.30
1	B	79	ARG	NE-CZ-NH1	11.36	125.98	120.30
1	A	204	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	B	88	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	B	317	TRP	CD1-CG-CD2	9.20	113.66	106.30
1	B	65	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	B	9	LEU	CA-CB-CG	8.62	135.13	115.30
1	A	317	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	B	10	TRP	CD1-CG-CD2	8.13	112.80	106.30
1	A	65	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	A	134	MET	CG-SD-CE	-8.03	87.35	100.20
1	A	88	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	B	317	TRP	CE2-CD2-CG	-7.74	101.11	107.30
1	B	76	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	A	10	TRP	CD1-CG-CD2	7.67	112.43	106.30
1	B	10	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	B	204	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	90	VAL	CA-CB-CG2	-7.47	99.70	110.90
1	A	166	ILE	CA-C-N	-7.14	101.50	117.20
1	B	62	LEU	CA-CB-CG	7.11	131.66	115.30
1	B	153	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	A	317	TRP	CE2-CD2-CG	-6.85	101.82	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	6	LYS	CB-CG-CD	-6.80	93.91	111.60
1	A	10	TRP	CE2-CD2-CG	-6.78	101.88	107.30
1	B	222	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	A	239	LEU	CA-CB-CG	6.48	130.19	115.30
1	B	119	TYR	CB-CG-CD1	-6.39	117.17	121.00
1	B	317	TRP	CG-CD1-NE1	-6.37	103.73	110.10
1	A	47	LYS	CB-CG-CD	-6.34	95.12	111.60
1	B	326	LYS	CB-CG-CD	-6.32	95.17	111.60
1	B	309	THR	CA-CB-CG2	6.21	121.10	112.40
1	B	317	TRP	CB-CG-CD1	-6.02	119.17	127.00
1	B	76	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	317	TRP	CG-CD1-NE1	-5.96	104.14	110.10
1	A	166	ILE	CB-CG1-CD1	-5.91	97.37	113.90
1	A	350	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	42	GLU	CA-CB-CG	-5.74	100.77	113.40
1	B	90	VAL	CA-CB-CG2	-5.73	102.31	110.90
1	A	76	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	153	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	B	10	TRP	CG-CD2-CE3	5.58	138.92	133.90
1	A	65	ARG	CG-CD-NE	-5.47	100.32	111.80
1	A	264	VAL	CA-CB-CG2	-5.46	102.71	110.90
1	B	317	TRP	CG-CD2-CE3	5.46	138.82	133.90
1	B	203	SER	CA-CB-OG	5.44	125.89	111.20
1	B	269	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	39	LYS	CA-CB-CG	-5.38	101.56	113.40
1	A	219	GLN	N-CA-C	5.38	125.53	111.00
1	A	218	GLN	CA-CB-CG	5.38	125.23	113.40
1	A	68	GLU	CA-CB-CG	5.38	125.22	113.40
1	B	218	GLN	CA-CB-CG	5.31	125.08	113.40
1	B	65	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	126	GLN	CG-CD-NE2	5.25	129.29	116.70
1	B	222	ARG	CB-CG-CD	-5.24	97.98	111.60
1	B	91	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	88	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	5	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	A	252	GLN	CA-CB-CG	5.15	124.73	113.40
1	A	91	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	166	ILE	CA-C-O	5.14	130.90	120.10
1	A	258	LYS	CA-CB-CG	5.12	124.65	113.40
1	A	242	LYS	CG-CD-CE	-5.08	96.66	111.90
1	A	197	VAL	CG1-CB-CG2	-5.07	102.78	110.90
1	A	10	TRP	CB-CG-CD1	-5.02	120.47	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	VAL	CA-CB-CG1	5.01	118.42	110.90

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	2686	0	2668	66	0
1	B	2686	0	2668	68	0
2	A	43	0	0	2	0
2	B	40	0	0	1	0
All	All	5455	0	5336	123	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 11.

All (123) 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:29:MET:SD	1:B:151:ASP:HB3	2.01	0.98
1:B:2:HIS:HA	1:B:185:GLN:HE22	1.43	0.83
1:B:166:ILE:HG21	1:B:225:LEU:HD12	1.62	0.80
1:A:204:ARG:HH11	1:A:204:ARG:HG3	1.50	0.76
1:A:166:ILE:HD11	1:A:225:LEU:HD12	1.66	0.76
1:A:29:MET:SD	1:A:151:ASP:HB3	2.28	0.73
1:B:267:MET:HE1	1:B:317:TRP:HB2	1.77	0.65
1:B:126:GLN:O	1:B:177:LYS:HG3	1.96	0.65
1:A:79:ARG:HH11	1:B:39:LYS:HE2	1.61	0.64
1:B:155:THR:HA	1:B:158:ILE:O	1.97	0.64
1:A:98:GLU:HB3	1:A:239:LEU:HD21	1.80	0.63
1:A:65:ARG:HH11	1:A:283:GLN:HE22	1.48	0.62
1:A:95:TYR:HB3	1:A:243:ALA:HA	1.82	0.61
1:B:26:VAL:O	1:B:30:LYS:HD2	2.00	0.61
1:B:177:LYS:HB3	1:B:180:GLU:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:VAL:O	1:B:268:LYS:HG3	2.00	0.60
1:B:142:LEU:HD11	1:B:144:LEU:HD13	1.84	0.59
1:A:114:THR:O	1:B:203:SER:HB3	2.02	0.59
1:A:224:ASP:OD1	1:A:232:ALA:HB2	2.03	0.58
1:A:209:LEU:HD23	1:B:108:GLN:HG2	1.86	0.58
1:A:99:ALA:HA	1:A:239:LEU:HD11	1.83	0.58
1:B:23:THR:HG21	1:B:92:ALA:O	2.04	0.58
1:A:297:GLU:HG3	1:A:301:LEU:HG	1.86	0.57
1:B:27:ALA:HB1	1:B:89:ALA:HB1	1.87	0.57
1:B:197:VAL:HG13	1:B:203:SER:HB2	1.86	0.57
1:B:267:MET:CE	1:B:317:TRP:HB2	2.33	0.57
1:B:99:ALA:HA	1:B:239:LEU:HD21	1.87	0.57
1:B:296:LYS:H	1:B:296:LYS:NZ	2.03	0.56
1:B:155:THR:O	1:B:159:SER:HB3	2.05	0.56
1:A:166:ILE:HD11	1:A:225:LEU:HB2	1.87	0.55
1:A:134:MET:HG2	1:A:139:CYS:HB2	1.88	0.55
1:B:277:LEU:HG	1:B:281:LYS:HE2	1.89	0.55
1:B:95:TYR:HB3	1:B:243:ALA:HA	1.89	0.55
1:B:92:ALA:HA	1:B:246:SER:HB3	1.89	0.55
1:A:79:ARG:HD2	1:B:39:LYS:NZ	2.22	0.54
1:A:107:ILE:HG22	1:A:134:MET:CE	2.37	0.54
1:B:3:PHE:HA	1:B:177:LYS:O	2.09	0.53
1:A:107:ILE:HG22	1:A:134:MET:HE2	1.90	0.53
1:B:229:SER:O	1:B:233:ARG:HG2	2.09	0.53
1:A:65:ARG:HH12	1:B:357:VAL:HG23	1.73	0.52
1:B:156:ASP:O	1:B:164:PRO:HG2	2.10	0.52
1:B:327:GLY:O	1:B:350:ARG:HB3	2.09	0.51
1:A:162:GLY:O	1:A:164:PRO:HD3	2.11	0.51
1:A:133:ALA:O	1:A:137:GLN:HG2	2.11	0.51
1:B:102:ALA:HB2	1:B:209:LEU:HD12	1.93	0.51
1:B:11:GLN:HG2	1:B:137:GLN:HG3	1.93	0.50
1:A:11:GLN:HB3	1:A:12:PRO:HD3	1.94	0.49
1:A:168:PRO:O	1:A:169:LEU:HD23	2.13	0.49
1:B:149:THR:O	1:B:150:GLU:HB2	2.13	0.49
1:A:11:GLN:HG2	1:A:137:GLN:HG3	1.94	0.49
1:B:135:ALA:HA	1:B:139:CYS:O	2.13	0.48
1:A:53:ALA:HA	2:A:368:HOH:O	2.13	0.48
1:A:197:VAL:HG13	1:A:203:SER:HB2	1.95	0.48
1:B:102:ALA:CB	1:B:209:LEU:HD12	2.43	0.48
1:B:9:LEU:HD22	1:B:222:ARG:HB2	1.96	0.48
1:A:203:SER:HB3	1:B:114:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ALA:O	1:A:279:SER:HB3	2.15	0.47
1:A:282:PHE:CE1	1:B:333:PRO:HG3	2.49	0.47
1:B:163:PHE:O	1:B:226:SER:HA	2.14	0.47
1:A:27:ALA:HB1	1:A:89:ALA:HB1	1.96	0.46
1:A:204:ARG:HG3	1:A:204:ARG:NH1	2.23	0.46
1:B:78:LEU:HG	1:B:257:PRO:HD2	1.97	0.46
1:B:166:ILE:HG23	1:B:222:ARG:HD3	1.98	0.46
1:A:108:GLN:O	1:A:111:HIS:HB3	2.16	0.46
1:B:258:LYS:O	1:B:258:LYS:HE3	2.16	0.46
1:A:181:CYS:SG	1:A:183:LEU:HB2	2.56	0.45
1:B:284:LEU:HD21	1:B:305:TYR:OH	2.16	0.45
1:A:9:LEU:HA	1:A:222:ARG:NH1	2.32	0.45
1:B:7:TYR:HA	1:B:10:TRP:NE1	2.31	0.45
1:A:3:PHE:HB2	2:A:392:HOH:O	2.16	0.45
1:B:7:TYR:CZ	1:B:11:GLN:HG3	2.52	0.45
1:B:328:ALA:HB1	1:B:342:LEU:HD11	1.99	0.45
1:B:65:ARG:NE	1:B:283:GLN:NE2	2.65	0.45
1:A:135:ALA:HA	1:A:139:CYS:O	2.17	0.44
1:B:120:CYS:HA	1:B:181:CYS:HB2	1.99	0.44
1:A:111:HIS:HB2	1:A:134:MET:CE	2.47	0.44
1:B:277:LEU:HD13	1:B:302:LYS:HG2	1.99	0.44
1:B:71:LEU:HD22	1:B:270:LEU:HD21	1.99	0.44
1:A:303:THR:HG23	1:A:308:LYS:HG3	1.99	0.44
1:B:61:ALA:O	1:B:65:ARG:HG3	2.18	0.44
1:B:65:ARG:HE	1:B:283:GLN:NE2	2.15	0.44
1:B:73:THR:HG22	1:B:76:ARG:NH2	2.33	0.44
1:B:111:HIS:HA	1:B:131:ASN:HD21	1.83	0.44
1:A:25:GLY:HA2	1:A:148:LEU:HB3	1.99	0.44
1:A:6:LYS:HD3	1:A:173:GLN:O	2.18	0.43
1:A:108:GLN:HG2	1:B:209:LEU:HD23	2.00	0.43
1:A:267:MET:SD	1:A:317:TRP:CE3	3.12	0.43
1:B:13:GLU:OE2	1:B:222:ARG:HG3	2.18	0.43
1:A:111:HIS:HA	1:A:131:ASN:OD1	2.18	0.43
1:A:118:THR:HG21	1:B:192:ALA:HB2	2.01	0.43
1:A:310:GLU:O	1:A:312:ASN:N	2.52	0.43
1:B:270:LEU:HA	1:B:273:LYS:HD2	2.01	0.43
1:A:307:GLY:HA3	1:A:310:GLU:O	2.19	0.43
1:A:29:MET:SD	1:A:151:ASP:CB	3.04	0.43
1:B:2:HIS:CA	1:B:185:GLN:HE22	2.24	0.42
1:B:118:THR:HB	1:B:180:GLU:HA	2.01	0.42
1:A:65:ARG:HH11	1:A:283:GLN:NE2	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:HB	1:A:180:GLU:O	2.18	0.42
1:A:318:ASN:HA	1:A:321:LYS:HG2	1.99	0.42
1:B:1:THR:HA	1:B:218:GLN:OE1	2.19	0.42
1:A:186:ALA:HB2	1:A:217:ALA:HB2	2.00	0.42
1:A:7:TYR:CZ	1:A:11:GLN:HG3	2.54	0.42
1:A:198:GLN:HG2	2:B:387:HOH:O	2.19	0.42
1:A:14:CYS:O	1:A:17:THR:HB	2.19	0.42
1:B:342:LEU:HD12	1:B:342:LEU:HA	1.88	0.42
1:A:3:PHE:HA	1:A:177:LYS:O	2.19	0.42
1:A:120:CYS:HA	1:A:181:CYS:HB2	2.02	0.42
1:B:296:LYS:H	1:B:296:LYS:HZ2	1.66	0.41
1:A:236:ALA:O	1:A:241:GLY:HA3	2.21	0.41
1:B:43:LEU:HD21	1:B:343:ASN:HD22	1.85	0.41
1:A:326:LYS:HG2	1:A:336:GLU:HG2	2.03	0.41
1:A:3:PHE:O	1:A:181:CYS:HB3	2.20	0.41
1:A:166:ILE:CD1	1:A:225:LEU:HB2	2.49	0.41
1:B:11:GLN:HB3	1:B:12:PRO:HD3	2.02	0.41
1:B:177:LYS:HD2	1:B:180:GLU:OE2	2.21	0.41
1:A:10:TRP:CG	1:A:121:LEU:HD22	2.57	0.40
1:A:65:ARG:HD2	1:A:283:GLN:HE22	1.87	0.40
1:A:161:LYS:HD3	1:A:161:LYS:HA	1.81	0.40
1:A:7:TYR:HA	1:A:10:TRP:CD1	2.56	0.40
1:A:79:ARG:NH1	1:B:39:LYS:HG3	2.36	0.40
1:A:87:ASP:HB2	1:B:28:LYS:HZ1	1.86	0.40
1:A:166:ILE:O	1:A:166:ILE:HG13	2.22	0.40
1:B:134:MET:HG2	1:B:139:CYS: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	356/358 (99%)	318 (89%)	32 (9%)	6 (2%)	9 23
1	B	356/358 (99%)	336 (94%)	14 (4%)	6 (2%)	9 23
All	All	712/716 (99%)	654 (92%)	46 (6%)	12 (2%)	9 23

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	150	GLU
1	A	289	GLY
1	A	311	SER
1	B	126	GLN
1	B	230	GLY
1	B	233	ARG
1	B	298	ASP
1	B	171	ASN
1	A	227	ASP
1	A	310	GLU
1	A	56	PRO
1	A	164	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	A	283/283 (100%)	236 (83%)	47 (17%)	2 5
1	B	283/283 (100%)	240 (85%)	43 (15%)	3 7
All	All	566/566 (100%)	476 (84%)	90 (16%)	2 6

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	PRO
1	A	15	GLU
1	A	29	MET
1	A	32	ASN

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Mol	Chain	Res	Type
1	A	57	GLU
1	A	58	SER
1	A	59	LYS
1	A	62	LEU
1	A	68	GLU
1	A	76	ARG
1	A	78	LEU
1	A	84	ASN
1	A	88	ARG
1	A	90	VAL
1	A	98	GLU
1	A	126	GLN
1	A	128	SER
1	A	144	LEU
1	A	145	PRO
1	A	146	GLU
1	A	151	ASP
1	A	165	LYS
1	A	167	SER
1	A	170	THR
1	A	171	ASN
1	A	203	SER
1	A	204	ARG
1	A	205	ILE
1	A	215	SER
1	A	231	THR
1	A	233	ARG
1	A	234	ASN
1	A	237	ASP
1	A	239	LEU
1	A	248	THR
1	A	250	LEU
1	A	265	GLU
1	A	269	LEU
1	A	283	GLN
1	A	290	LYS
1	A	291	LYS
1	A	293	SER
1	A	302	LYS
1	A	312	ASN
1	A	331	GLU
1	A	349	GLN

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Mol	Chain	Res	Type
1	A	357	VAL
1	B	9	LEU
1	B	11	GLN
1	B	28	LYS
1	B	29	MET
1	B	30	LYS
1	B	32	ASN
1	B	39	LYS
1	B	57	GLU
1	B	59	LYS
1	B	67	LEU
1	B	88	ARG
1	B	90	VAL
1	B	103	LEU
1	B	131	ASN
1	B	144	LEU
1	B	146	GLU
1	B	151	ASP
1	B	152	SER
1	B	155	THR
1	B	171	ASN
1	B	177	LYS
1	B	185	GLN
1	B	188	SER
1	B	191	GLN
1	B	203	SER
1	B	204	ARG
1	B	219	GLN
1	B	231	THR
1	B	233	ARG
1	B	234	ASN
1	B	248	THR
1	B	252	GLN
1	B	258	LYS
1	B	269	LEU
1	B	270	LEU
1	B	273	LYS
1	B	296	LYS
1	B	297	GLU
1	B	300	ASN
1	B	311	SER
1	B	314	GLU

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Mol	Chain	Res	Type
1	B	319	LYS
1	B	357	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	185	GLN
1	A	283	GLN
1	A	318	ASN
1	A	343	ASN
1	B	11	GLN
1	B	131	ASN
1	B	137	GLN
1	B	255	GLN
1	B	283	GLN
1	B	343	ASN

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 monosaccharides 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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.