Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:39 PM GMT

PDB ID	:	1BTJ
Title	:	HUMAN SERUM TRANSFERRIN, RECOMBINANT N-TERMINAL LOBE, APO FORM, CRYSTAL FORM 2
Authors	:	Jeffrey, P.D.; Bewley, M.C.; Macgillivray, R.T.A.; Mason, A.B.; Woodworth, R.C.; Baker, E.N.
Deposited on	:	1998-09-01
Resolution	:	3.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.20 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	Percentile Ranks	Value
Clashscore		27
Ramachandran outliers		3.5%
Sidechain outliers		13.4%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
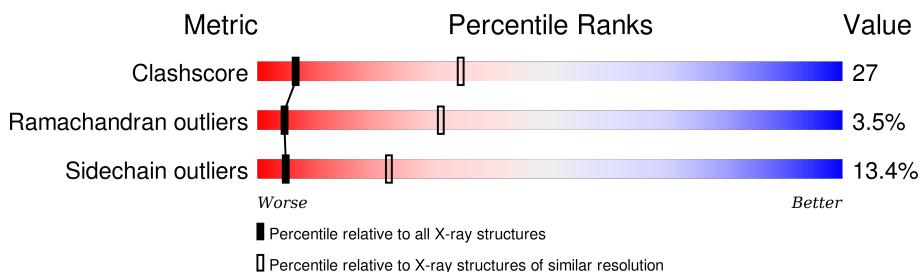
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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 <=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	337	46% 43% 9% •
1	B	337	53% 38% 5% ••
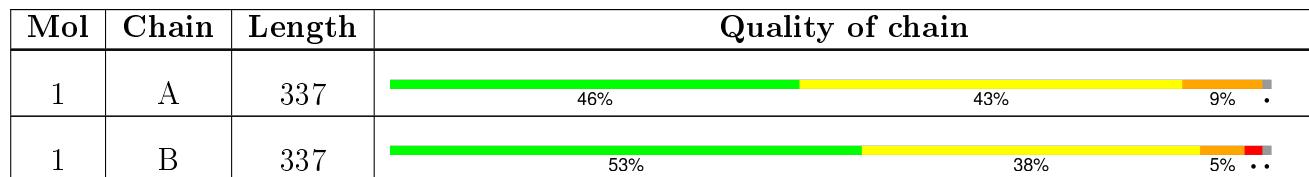
2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5154 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 PROTEIN (SERUM TRANSFERRIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2577	1630	441	485	21			
1	B	333	Total	C	N	O	S	0	0	0
			2577	1630	441	485	21			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: PROTEIN (SERUM TRANSFERRIN)

Chain A:

- Molecule 1: PROTEIN (SERUM TRANSFERRIN)

Chain B:
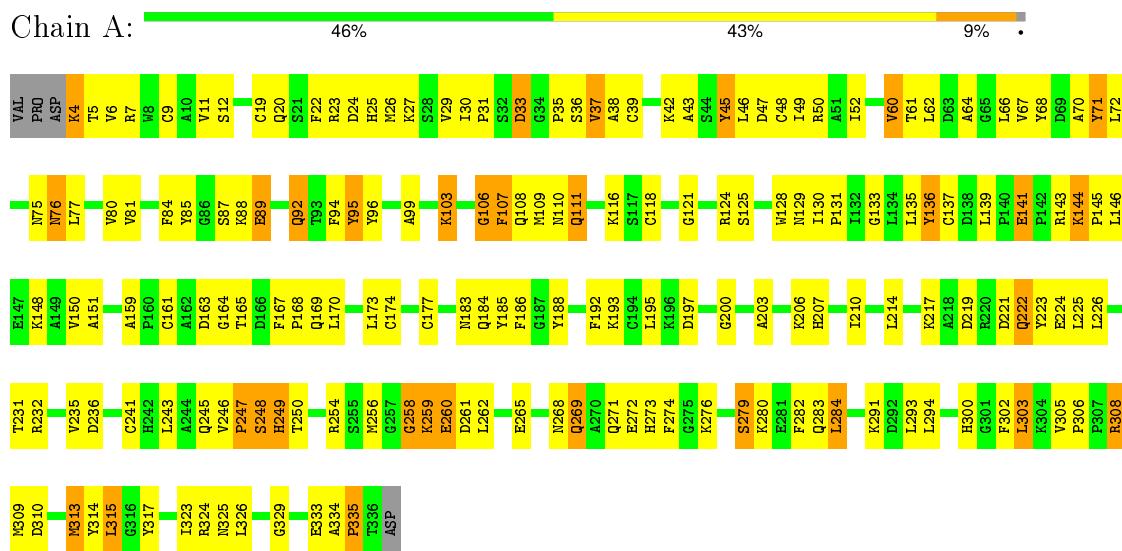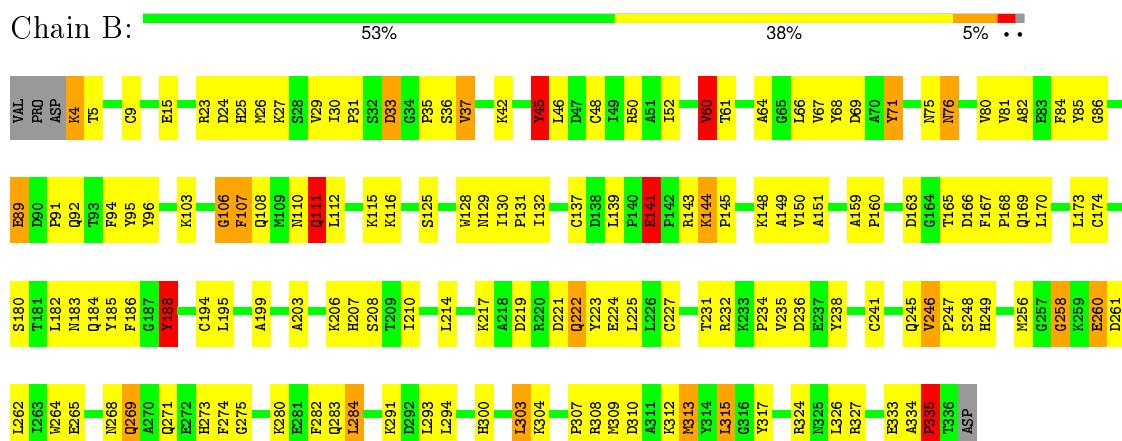
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.00Å 77.30Å 72.60Å 90.00° 104.30° 90.00°	Depositor
Resolution (Å)	6.00 – 3.20	Depositor
% Data completeness (in resolution range)	99.8 (6.00-3.20)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.217 , 0.312	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5154	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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	0.64	0/2640	0.87	1/3572 (0.0%)
1	B	0.63	0/2640	0.88	3/3572 (0.1%)
All	All	0.63	0/5280	0.87	4/7144 (0.1%)

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
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	335	PRO	N-CA-C	6.07	127.89	112.10
1	A	177	CYS	CA-CB-SG	-5.41	104.27	114.00
1	B	60	VAL	CB-CA-C	-5.19	101.53	111.40
1	B	141	GLU	N-CA-C	-5.09	97.25	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	95	TYR	Sidechain
1	B	188	TYR	Sidechain
1	B	68	TYR	Sidechain

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	2577	0	2497	141	0
1	B	2577	0	2497	136	0
All	All	5154	0	4994	277	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 (277) 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:125:SER:HA	1:A:129:ASN:HB2	1.39	1.05
1:B:85:TYR:HE1	1:B:248:SER:HG	1.02	1.00
1:B:334:ALA:HB1	1:B:335:PRO:HD2	1.47	0.97
1:B:125:SER:HA	1:B:129:ASN:HB2	1.47	0.94
1:B:145:PRO:HD2	1:B:148:LYS:HD2	1.53	0.88
1:B:268:ASN:HA	1:B:271:GLN:HE21	1.43	0.83
1:B:210:ILE:HG21	1:B:235:VAL:HG11	1.61	0.83
1:A:210:ILE:HG21	1:A:235:VAL:HG11	1.61	0.81
1:A:25:HIS:CE1	1:A:282:PHE:HB2	2.16	0.80
1:B:245:GLN:HG3	1:B:315:LEU:O	1.83	0.78
1:A:184:GLN:HG3	1:A:185:TYR:CD1	2.17	0.78
1:B:334:ALA:CB	1:B:335:PRO:HD2	2.10	0.78
1:B:64:ALA:HB2	1:B:247:PRO:HD2	1.65	0.78
1:A:145:PRO:HG2	1:A:148:LYS:HB2	1.64	0.78
1:B:108:GLN:HE22	1:B:232:ARG:HG3	1.48	0.78
1:B:24:ASP:HA	1:B:27:LYS:HE2	1.63	0.78
1:A:94:PHE:CE2	1:A:247:PRO:HG3	2.18	0.77
1:A:163:ASP:HB3	1:A:167:PHE:HD2	1.48	0.77
1:A:145:PRO:HD2	1:A:148:LYS:HD2	1.65	0.77
1:B:4:LYS:HA	1:B:4:LYS:NZ	2.00	0.76
1:B:128:TRP:HH2	1:B:150:VAL:HG21	1.51	0.76
1:A:23:ARG:HA	1:A:37:VAL:HG13	1.67	0.76
1:B:163:ASP:HB3	1:B:167:PHE:HD2	1.50	0.76
1:B:145:PRO:HG2	1:B:148:LYS:HB2	1.66	0.76
1:A:4:LYS:NZ	1:A:4:LYS:HA	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ARG:HG2	1:A:75:ASN:HD21	1.51	0.75
1:B:188:TYR:CE1	1:B:206:LYS:HB3	2.22	0.75
1:B:214:LEU:HD11	1:B:223:TYR:CE2	2.21	0.75
1:A:71:TYR:O	1:A:76:ASN:HA	1.89	0.73
1:A:48:CYS:HB3	1:A:60:VAL:HG11	1.69	0.73
1:A:68:TYR:CD2	1:A:323:ILE:HD13	2.24	0.73
1:B:94:PHE:CE2	1:B:247:PRO:HG3	2.23	0.71
1:A:25:HIS:NE2	1:A:282:PHE:HB2	2.05	0.71
1:A:268:ASN:HA	1:A:271:GLN:HE21	1.56	0.71
1:B:206:LYS:HE2	1:B:208:SER:OG	1.90	0.71
1:A:128:TRP:CH2	1:A:150:VAL:HG21	2.25	0.71
1:A:45:TYR:CD2	1:A:46:LEU:HG	2.26	0.71
1:B:210:ILE:HG21	1:B:235:VAL:CG1	2.21	0.70
1:B:23:ARG:HA	1:B:37:VAL:HG13	1.71	0.70
1:A:268:ASN:HA	1:A:271:GLN:HG2	1.74	0.69
1:B:214:LEU:HD11	1:B:223:TYR:HE2	1.57	0.69
1:A:309:MET:HG3	1:A:313:MET:HG3	1.75	0.68
1:B:45:TYR:HD2	1:B:66:LEU:HD21	1.57	0.68
1:B:128:TRP:CH2	1:B:150:VAL:HG21	2.28	0.67
1:B:96:TYR:H	1:B:207:HIS:CD2	2.12	0.67
1:B:95:TYR:CE2	1:B:246:VAL:HB	2.30	0.67
1:A:95:TYR:CE2	1:A:246:VAL:HB	2.31	0.66
1:B:225:LEU:HD13	1:B:235:VAL:HA	1.77	0.66
1:A:195:LEU:HB2	1:A:203:ALA:HB2	1.78	0.65
1:A:163:ASP:HB3	1:A:167:PHE:CD2	2.31	0.65
1:B:195:LEU:HB2	1:B:203:ALA:HB2	1.78	0.65
1:A:45:TYR:HD2	1:A:66:LEU:HD21	1.62	0.65
1:A:9:CYS:HB3	1:A:60:VAL:HG13	1.78	0.65
1:B:334:ALA:HB1	1:B:335:PRO:CD	2.26	0.63
1:A:128:TRP:HH2	1:A:150:VAL:HG21	1.63	0.63
1:B:308:ARG:HH11	1:B:308:ARG:HG3	1.64	0.63
1:B:4:LYS:HA	1:B:4:LYS:HZ3	1.62	0.63
1:A:108:GLN:HE22	1:A:232:ARG:HG3	1.64	0.63
1:A:210:ILE:HG21	1:A:235:VAL:CG1	2.27	0.62
1:A:334:ALA:HB1	1:A:335:PRO:HD2	1.81	0.62
1:B:9:CYS:HB3	1:B:60:VAL:HG13	1.80	0.62
1:B:310:ASP:O	1:B:313:MET:HG2	1.99	0.62
1:B:85:TYR:HE1	1:B:248:SER:OG	1.77	0.61
1:B:188:TYR:CZ	1:B:206:LYS:HB3	2.36	0.61
1:B:45:TYR:HD2	1:B:66:LEU:CD2	2.13	0.61
1:A:96:TYR:H	1:A:207:HIS:CD2	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ILE:HD12	1:A:269:GLN:OE1	2.00	0.61
1:B:71:TYR:O	1:B:76:ASN:HA	2.00	0.60
1:B:129:ASN:O	1:B:326:LEU:HD11	1.99	0.60
1:B:110:ASN:O	1:B:111:GLN:HG3	2.01	0.60
1:A:24:ASP:O	1:A:27:LYS:HB2	2.02	0.60
1:B:183:ASN:HB3	1:B:186:PHE:HB2	1.84	0.60
1:B:184:GLN:HG3	1:B:185:TYR:CD1	2.37	0.60
1:B:163:ASP:HB3	1:B:167:PHE:CD2	2.35	0.60
1:A:4:LYS:HZ3	1:A:4:LYS:HA	1.67	0.59
1:A:68:TYR:HD2	1:A:323:ILE:HD13	1.68	0.59
1:A:334:ALA:CB	1:A:335:PRO:HD2	2.32	0.59
1:B:210:ILE:HD13	1:B:235:VAL:HG11	1.85	0.59
1:A:31:PRO:HB2	1:A:33:ASP:OD2	2.03	0.59
1:B:112:LEU:O	1:B:115:LYS:HG2	2.03	0.59
1:A:226:LEU:HD23	1:A:232:ARG:HG2	1.86	0.58
1:A:258:GLY:O	1:A:259:LYS:HB2	2.02	0.58
1:B:165:THR:O	1:B:168:PRO:HD3	2.03	0.58
1:A:45:TYR:N	1:A:45:TYR:CD1	2.71	0.58
1:A:309:MET:HA	1:A:313:MET:CE	2.34	0.57
1:A:168:PRO:HD2	1:A:169:GLN:OE1	2.04	0.57
1:A:29:VAL:HG23	1:A:30:ILE:HD13	1.86	0.57
1:A:130:ILE:N	1:A:131:PRO:HD2	2.19	0.57
1:B:151:ALA:HB2	1:B:170:LEU:CD1	2.34	0.57
1:A:85:TYR:HE1	1:A:248:SER:HG	1.46	0.57
1:B:48:CYS:HB3	1:B:60:VAL:HG11	1.87	0.57
1:A:308:ARG:HH11	1:A:308:ARG:HG3	1.69	0.57
1:B:35:PRO:HB3	1:B:262:LEU:HD12	1.86	0.57
1:A:80:VAL:HG23	1:A:81:VAL:HG23	1.87	0.57
1:B:45:TYR:CD2	1:B:66:LEU:HD21	2.39	0.56
1:B:50:ARG:HA	1:B:75:ASN:ND2	2.21	0.56
1:B:26:MET:SD	1:B:274:PHE:CE1	2.98	0.56
1:B:45:TYR:N	1:B:45:TYR:CD1	2.72	0.56
1:B:324:ARG:HB3	1:B:324:ARG:NH1	2.20	0.56
1:A:94:PHE:HA	1:A:247:PRO:HA	1.88	0.56
1:A:309:MET:HA	1:A:313:MET:HE3	1.88	0.56
1:A:45:TYR:HD1	1:A:45:TYR:H	1.53	0.55
1:B:52:ILE:CD1	1:B:60:VAL:HG22	2.37	0.55
1:B:116:LYS:HB3	1:B:173:LEU:HD21	1.87	0.55
1:A:4:LYS:HZ2	1:A:4:LYS:HA	1.72	0.55
1:B:269:GLN:OE1	1:B:273:HIS:CE1	2.60	0.55
1:B:159:ALA:CB	1:B:170:LEU:HD23	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ASN:HB3	1:A:186:PHE:HB2	1.89	0.55
1:B:227:CYS:CA	1:B:241:CYS:SG	2.95	0.54
1:B:324:ARG:CZ	1:B:324:ARG:HB3	2.38	0.54
1:B:25:HIS:CE1	1:B:282:PHE:HB2	2.43	0.54
1:A:144:LYS:HE3	1:A:144:LYS:HA	1.89	0.54
1:A:23:ARG:HA	1:A:37:VAL:CG1	2.35	0.54
1:B:219:ASP:O	1:B:222:GLN:HB2	2.08	0.54
1:B:45:TYR:CD2	1:B:46:LEU:HG	2.43	0.54
1:A:116:LYS:HB3	1:A:173:LEU:HD21	1.89	0.54
1:A:29:VAL:HG23	1:A:30:ILE:CD1	2.38	0.54
1:B:29:VAL:HG23	1:B:30:ILE:HD13	1.90	0.54
1:A:26:MET:SD	1:A:274:PHE:CE1	3.01	0.54
1:B:108:GLN:NE2	1:B:232:ARG:HG3	2.18	0.54
1:A:121:GLY:HA3	1:A:124:ARG:HD2	1.90	0.53
1:B:264:TRP:CD1	1:B:304:LYS:HD2	2.43	0.53
1:A:50:ARG:HG2	1:A:75:ASN:ND2	2.22	0.53
1:B:84:PHE:CD1	1:B:303:LEU:HD23	2.43	0.53
1:A:293:LEU:O	1:A:294:LEU:HB2	2.09	0.53
1:A:324:ARG:CZ	1:A:324:ARG:HB3	2.39	0.52
1:A:87:SER:O	1:A:88:LYS:HD3	2.09	0.52
1:B:48:CYS:HB3	1:B:60:VAL:CG1	2.40	0.52
1:A:279:SER:OG	1:A:280:LYS:N	2.43	0.52
1:B:273:HIS:HB2	1:B:274:PHE:CD1	2.46	0.51
1:A:110:ASN:O	1:A:111:GLN:HG3	2.10	0.51
1:A:42:LYS:HB3	1:A:47:ASP:HB3	1.93	0.51
1:A:30:ILE:HG23	1:A:31:PRO:HD2	1.92	0.51
1:B:71:TYR:OH	1:B:312:LYS:HD3	2.11	0.51
1:A:133:GLY:O	1:A:136:TYR:HB2	2.10	0.51
1:B:258:GLY:HA3	1:B:260:GLU:OE1	2.11	0.51
1:B:4:LYS:HA	1:B:4:LYS:HZ2	1.73	0.51
1:B:293:LEU:O	1:B:294:LEU:HB2	2.11	0.51
1:B:106:GLY:O	1:B:107:PHE:HB3	2.11	0.51
1:A:52:ILE:HD12	1:A:60:VAL:HG22	1.93	0.51
1:A:25:HIS:HB3	1:A:274:PHE:CE2	2.47	0.50
1:A:310:ASP:O	1:A:313:MET:HG2	2.10	0.50
1:B:309:MET:HG3	1:B:313:MET:HG3	1.93	0.50
1:A:64:ALA:O	1:A:67:VAL:HB	2.11	0.50
1:B:103:LYS:HA	1:B:224:GLU:HG3	1.93	0.50
1:A:30:ILE:CG2	1:A:31:PRO:HD2	2.41	0.50
1:A:35:PRO:HB3	1:A:262:LEU:HD12	1.93	0.50
1:A:225:LEU:HD13	1:A:235:VAL:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ASP:OD1	1:B:313:MET:SD	2.70	0.50
1:B:30:ILE:HG23	1:B:31:PRO:HD2	1.94	0.50
1:B:238:TYR:HA	1:B:241:CYS:O	2.12	0.50
1:B:96:TYR:N	1:B:207:HIS:CD2	2.80	0.50
1:B:52:ILE:HD12	1:B:60:VAL:HG22	1.94	0.49
1:A:49:ILE:CD1	1:A:70:ALA:HB2	2.41	0.49
1:B:271:GLN:O	1:B:275:GLY:N	2.44	0.49
1:A:24:ASP:HA	1:A:27:LYS:HE2	1.94	0.49
1:A:48:CYS:HB3	1:A:60:VAL:CG1	2.40	0.49
1:B:227:CYS:HA	1:B:241:CYS:SG	2.53	0.49
1:B:144:LYS:HE3	1:B:144:LYS:HA	1.93	0.49
1:A:99:ALA:HB2	1:A:243:LEU:HD11	1.94	0.49
1:B:29:VAL:HG23	1:B:30:ILE:CD1	2.43	0.48
1:A:50:ARG:HA	1:A:75:ASN:ND2	2.28	0.48
1:B:80:VAL:HG23	1:B:81:VAL:HG23	1.95	0.48
1:A:48:CYS:CB	1:A:60:VAL:HG11	2.43	0.48
1:B:269:GLN:OE1	1:B:273:HIS:HE1	1.96	0.48
1:B:141:GLU:CD	1:B:141:GLU:H	2.15	0.48
1:B:268:ASN:HA	1:B:271:GLN:HG2	1.96	0.48
1:A:168:PRO:CD	1:A:169:GLN:OE1	2.62	0.48
1:A:184:GLN:HG3	1:A:185:TYR:HD1	1.72	0.48
1:B:165:THR:HG22	1:B:166:ASP:N	2.29	0.48
1:A:174:CYS:O	1:A:174:CYS:SG	2.72	0.48
1:A:151:ALA:HB2	1:A:170:LEU:CD1	2.44	0.48
1:A:103:LYS:HA	1:A:224:GLU:HG3	1.96	0.48
1:A:43:ALA:HB3	1:A:47:ASP:OD2	2.13	0.48
1:B:188:TYR:OH	1:B:206:LYS:HB3	2.14	0.47
1:A:24:ASP:HA	1:A:27:LYS:CE	2.43	0.47
1:A:89:GLU:CD	1:A:89:GLU:N	2.68	0.47
1:A:106:GLY:O	1:A:107:PHE:HB3	2.15	0.47
1:B:30:ILE:HD12	1:B:269:GLN:OE1	2.14	0.47
1:B:82:ALA:HB3	1:B:303:LEU:HB2	1.95	0.47
1:A:11:VAL:O	1:A:12:SER:HB3	2.14	0.47
1:A:52:ILE:CD1	1:A:60:VAL:HG22	2.45	0.46
1:B:45:TYR:HD1	1:B:45:TYR:H	1.63	0.46
1:B:151:ALA:HB2	1:B:170:LEU:HD11	1.98	0.46
1:A:139:LEU:O	1:A:143:ARG:NE	2.48	0.46
1:B:274:PHE:O	1:B:284:LEU:HB2	2.15	0.46
1:B:145:PRO:O	1:B:148:LYS:HB3	2.15	0.46
1:B:64:ALA:O	1:B:67:VAL:HB	2.15	0.46
1:A:226:LEU:CD2	1:A:232:ARG:HG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ILE:CG1	1:B:214:LEU:HD12	2.46	0.46
1:A:192:PHE:CZ	1:A:210:ILE:HG13	2.50	0.46
1:B:159:ALA:HB2	1:B:170:LEU:HD23	1.97	0.46
1:A:274:PHE:HB2	1:A:284:LEU:HG	1.98	0.46
1:B:23:ARG:HA	1:B:37:VAL:CG1	2.44	0.46
1:A:94:PHE:CE2	1:A:247:PRO:CG	2.96	0.45
1:A:52:ILE:HG22	1:A:77:LEU:HD21	1.98	0.45
1:B:42:LYS:HD3	1:B:42:LYS:HA	1.74	0.45
1:A:245:GLN:HG3	1:A:315:LEU:O	2.17	0.45
1:A:173:LEU:N	1:A:173:LEU:HD12	2.32	0.45
1:A:193:LYS:HG2	1:A:197:ASP:OD2	2.16	0.45
1:B:103:LYS:HA	1:B:224:GLU:CD	2.36	0.45
1:A:141:GLU:CD	1:A:141:GLU:H	2.19	0.45
1:A:305:VAL:HB	1:A:306:PRO:HD2	1.98	0.45
1:A:19:CYS:C	1:A:39:CYS:SG	2.95	0.45
1:A:231:THR:HG22	1:A:232:ARG:N	2.31	0.45
1:A:269:GLN:OE1	1:A:273:HIS:CE1	2.69	0.45
1:B:30:ILE:CG2	1:B:31:PRO:HD2	2.46	0.45
1:B:168:PRO:HD2	1:B:169:GLN:OE1	2.17	0.44
1:B:25:HIS:ND1	1:B:282:PHE:CD1	2.86	0.44
1:A:42:LYS:HD3	1:A:42:LYS:HA	1.68	0.44
1:B:69:ASP:OD1	1:B:327:ARG:NH1	2.50	0.44
1:B:139:LEU:O	1:B:143:ARG:NE	2.47	0.44
1:B:108:GLN:O	1:B:111:GLN:HB2	2.17	0.44
1:A:109:MET:SD	1:A:243:LEU:HD21	2.57	0.44
1:B:15:GLU:HG2	1:B:294:LEU:HD23	2.00	0.44
1:A:214:LEU:HD11	1:A:223:TYR:CE1	2.53	0.44
1:B:262:LEU:O	1:B:265:GLU:HB3	2.17	0.44
1:A:7:ARG:HA	1:A:38:ALA:HB3	1.99	0.44
1:A:20:GLN:HB3	1:A:23:ARG:NH2	2.33	0.43
1:A:325:ASN:O	1:A:329:GLY:HA2	2.19	0.43
1:A:302:PHE:C	1:A:303:LEU:HD23	2.37	0.43
1:B:308:ARG:HG3	1:B:308:ARG:NH1	2.33	0.43
1:B:48:CYS:CB	1:B:60:VAL:HG11	2.49	0.43
1:B:225:LEU:CD1	1:B:235:VAL:HG22	2.48	0.43
1:B:24:ASP:O	1:B:27:LYS:HB2	2.19	0.43
1:B:151:ALA:HB2	1:B:170:LEU:HD12	1.99	0.43
1:B:131:PRO:HG2	1:B:132:ILE:H	1.83	0.43
1:B:225:LEU:CD1	1:B:235:VAL:HA	2.44	0.43
1:A:92:GLN:H	1:A:92:GLN:CD	2.21	0.43
1:A:219:ASP:O	1:A:222:GLN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ILE:H	1:A:131:PRO:HD2	1.83	0.43
1:A:108:GLN:NE2	1:A:232:ARG:HG3	2.31	0.43
1:A:35:PRO:HD3	1:A:265:GLU:OE2	2.19	0.43
1:A:248:SER:OG	1:A:249:HIS:N	2.52	0.43
1:A:85:TYR:HE1	1:A:248:SER:OG	2.01	0.42
1:A:118:CYS:SG	1:A:200:GLY:HA3	2.59	0.42
1:A:269:GLN:NE2	1:A:272:GLU:OE1	2.52	0.42
1:A:164:GLY:O	1:A:168:PRO:HA	2.18	0.42
1:A:131:PRO:O	1:A:135:LEU:HG	2.20	0.42
1:A:260:GLU:H	1:A:260:GLU:CD	2.21	0.42
1:B:86:GLY:O	1:B:300:HIS:CD2	2.72	0.42
1:B:194:CYS:O	1:B:199:ALA:HB3	2.20	0.42
1:A:96:TYR:N	1:A:207:HIS:CD2	2.87	0.42
1:A:84:PHE:CD1	1:A:303:LEU:HD23	2.55	0.42
1:B:46:LEU:O	1:B:50:ARG:HG3	2.18	0.42
1:A:151:ALA:HB2	1:A:170:LEU:HD11	2.02	0.42
1:B:231:THR:HG22	1:B:232:ARG:N	2.34	0.42
1:B:89:GLU:C	1:B:91:PRO:HD3	2.40	0.41
1:B:174:CYS:SG	1:B:174:CYS:O	2.78	0.41
1:A:129:ASN:O	1:A:326:LEU:HD11	2.20	0.41
1:A:22:PHE:HA	1:A:282:PHE:CZ	2.55	0.41
1:B:103:LYS:HA	1:B:224:GLU:CG	2.49	0.41
1:A:188:TYR:CE1	1:A:206:LYS:HB3	2.55	0.41
1:A:247:PRO:CG	1:A:314:TYR:CE1	3.04	0.41
1:A:23:ARG:HG2	1:A:24:ASP:N	2.36	0.41
1:A:45:TYR:O	1:A:48:CYS:HB2	2.20	0.41
1:B:130:ILE:N	1:B:131:PRO:HD2	2.35	0.41
1:B:227:CYS:SG	1:B:241:CYS:CB	3.08	0.41
1:A:313:MET:HG2	1:A:313:MET:H	1.66	0.41
1:B:52:ILE:HD11	1:B:60:VAL:HG22	2.02	0.41
1:B:246:VAL:HA	1:B:247:PRO:HD3	1.90	0.41
1:B:110:ASN:O	1:B:111:GLN:CG	2.68	0.41
1:A:146:LEU:O	1:A:150:VAL:HG22	2.20	0.41
1:B:273:HIS:CB	1:B:274:PHE:CD1	3.04	0.41
1:A:173:LEU:CD1	1:A:173:LEU:N	2.84	0.41
1:B:107:PHE:C	1:B:107:PHE:CD1	2.94	0.41
1:A:159:ALA:CB	1:A:170:LEU:HD23	2.51	0.41
1:A:325:ASN:O	1:A:329:GLY:N	2.53	0.41
1:A:309:MET:HA	1:A:313:MET:HE2	2.02	0.40
1:B:31:PRO:HB2	1:B:33:ASP:OD2	2.21	0.40
1:B:280:LYS:HB2	1:B:280:LYS:HE3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:CB	1:A:314:TYR:HE1	2.33	0.40
1:B:25:HIS:CE1	1:B:282:PHE:CD1	3.09	0.40
1:B:180:SER:OG	1:B:182:LEU:HB2	2.20	0.40
1:A:144:LYS:HA	1:A:145:PRO:HA	1.91	0.40
1:A:77:LEU:HD23	1:A:254:ARG:HA	2.03	0.40
1:B:143:ARG:HA	1:B:149:ALA:HB2	2.02	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	331/337 (98%)	280 (85%)	36 (11%)	15 (4%)	3	24
1	B	331/337 (98%)	280 (85%)	43 (13%)	8 (2%)	7	43
All	All	662/674 (98%)	560 (85%)	79 (12%)	23 (4%)	4	31

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	GLY
1	A	335	PRO
1	B	258	GLY
1	B	335	PRO
1	A	106	GLY
1	A	111	GLN
1	A	276	LYS
1	B	106	GLY
1	B	111	GLN
1	A	107	PHE
1	A	136	TYR
1	A	241	CYS

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Mol	Chain	Res	Type
1	B	76	ASN
1	B	107	PHE
1	A	72	LEU
1	A	76	ASN
1	A	137	CYS
1	A	248	SER
1	A	279	SER
1	A	259	LYS
1	A	308	ARG
1	B	45	TYR
1	B	137	CYS

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	277/281 (99%)	239 (86%)	38 (14%)	4	21
1	B	277/281 (99%)	241 (87%)	36 (13%)	5	24
All	All	554/562 (99%)	480 (87%)	74 (13%)	5	22

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	THR
1	A	6	VAL
1	A	33	ASP
1	A	36	SER
1	A	37	VAL
1	A	45	TYR
1	A	60	VAL
1	A	61	THR
1	A	62	LEU
1	A	71	TYR
1	A	89	GLU

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Mol	Chain	Res	Type
1	A	92	GLN
1	A	103	LYS
1	A	141	GLU
1	A	144	LYS
1	A	161	CYS
1	A	165	THR
1	A	217	LYS
1	A	221	ASP
1	A	222	GLN
1	A	236	ASP
1	A	247	PRO
1	A	249	HIS
1	A	250	THR
1	A	256	MET
1	A	260	GLU
1	A	261	ASP
1	A	269	GLN
1	A	283	GLN
1	A	284	LEU
1	A	291	LYS
1	A	300	HIS
1	A	303	LEU
1	A	313	MET
1	A	315	LEU
1	A	317	TYR
1	A	333	GLU
1	B	4	LYS
1	B	5	THR
1	B	33	ASP
1	B	36	SER
1	B	37	VAL
1	B	45	TYR
1	B	60	VAL
1	B	61	THR
1	B	71	TYR
1	B	89	GLU
1	B	92	GLN
1	B	111	GLN
1	B	141	GLU
1	B	144	LYS
1	B	160	PRO
1	B	188	TYR

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Mol	Chain	Res	Type
1	B	217	LYS
1	B	221	ASP
1	B	222	GLN
1	B	234	PRO
1	B	236	ASP
1	B	246	VAL
1	B	249	HIS
1	B	256	MET
1	B	260	GLU
1	B	261	ASP
1	B	269	GLN
1	B	283	GLN
1	B	284	LEU
1	B	291	LYS
1	B	303	LEU
1	B	307	PRO
1	B	313	MET
1	B	315	LEU
1	B	317	TYR
1	B	333	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	75	ASN
1	A	108	GLN
1	A	172	GLN
1	A	207	HIS
1	A	271	GLN
1	A	273	HIS
1	A	283	GLN
1	A	300	HIS
1	B	20	GLN
1	B	108	GLN
1	B	249	HIS
1	B	271	GLN
1	B	273	HIS

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.