Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2023 – 06:03 AM EDT

PDB ID	:	1GGP
Title	:	CRYSTAL STRUCTURE OF TRICHOSANTHES KIRILOWII LECTIN-1 AND ITS RELATION TO THE TYPE 2 RIBOSOME INACTIVATING PROTEINS
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Deposited on	:	2000-09-07
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 (1)) were used in the production of this report:

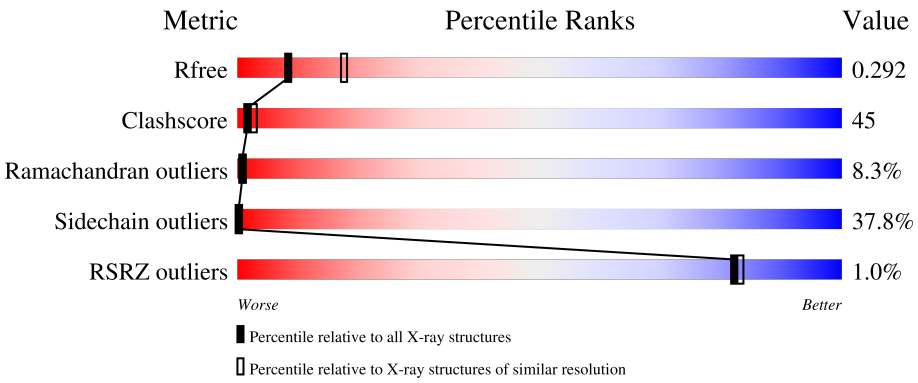
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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% 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	234	% 36% 43% 20% •
2	B	254	% 31% 44% 23% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3587 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 (LECTIN 1 A CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	234	1711	1055	299	350	7	0	0	0

- Molecule 2 is a protein called PROTEIN (LECTIN 1 B CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	254	1864	1143	327	382	12	0	0	0

- Molecule 3 is water.

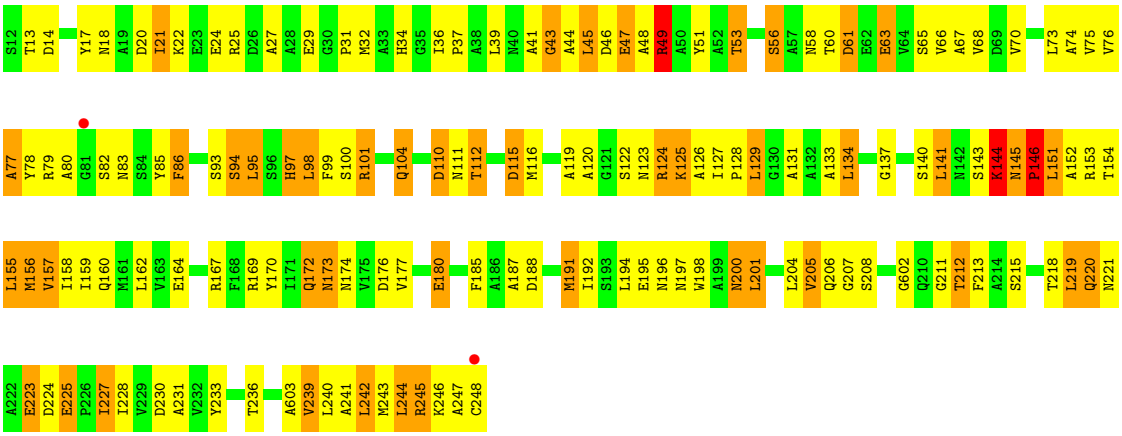
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	6	6	6	0	0
			Total	O		
3	B	6	6	6	0	0

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 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.

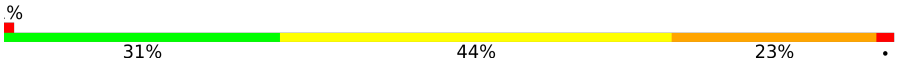
• Molecule 1: PROTEIN (LECTIN 1 A CHAIN)

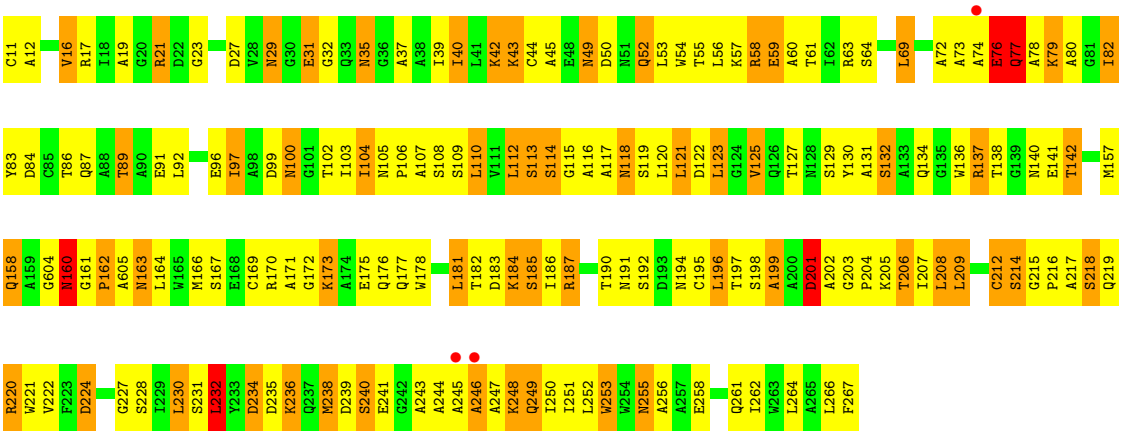
Chain A:



• Molecule 2: PROTEIN (LECTIN 1 B CHAIN)

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	44.96Å 69.87Å 180.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.70 14.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	76.2 (8.00-2.70) 77.0 (14.99-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	4.33 (at 2.69Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.225 , 0.300 0.220 , 0.292	Depositor DCC
R_{free} test set	636 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 109.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	3587	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.34	0/1737	0.63	0/2364
2	B	0.33	0/1892	0.59	0/2572
All	All	0.33	0/3629	0.61	0/4936

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	1711	0	1653	145	0
2	B	1864	0	1787	181	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
All	All	3587	0	3440	315	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 45.

All (315) 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:145:ASN:HB3	1:A:146:PRO:HD2	1.27	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:GLN:HG3	2:B:176:GLN:HG2	1.29	1.10
2:B:166:MET:HB2	2:B:245:ALA:HB1	1.39	1.03
2:B:163:ASN:HD22	2:B:164:LEU:N	1.59	0.99
2:B:163:ASN:HD22	2:B:164:LEU:H	1.07	0.98
2:B:230:LEU:HD21	2:B:235:ASP:HA	1.49	0.95
2:B:37:ALA:HB3	2:B:82:ILE:HD11	1.49	0.94
2:B:89:THR:HG23	2:B:92:LEU:HG	1.53	0.91
1:A:145:ASN:CB	1:A:146:PRO:HD2	2.03	0.88
2:B:19:ALA:HB2	2:B:142:THR:HG22	1.56	0.87
2:B:131:ALA:HA	2:B:217:ALA:HA	1.55	0.86
1:A:145:ASN:HB3	1:A:146:PRO:CD	2.05	0.86
2:B:232:LEU:HD22	2:B:232:LEU:N	1.90	0.86
1:A:46:ASP:H	1:A:49:ARG:HD2	1.40	0.86
2:B:158:GLN:NE2	2:B:173:LYS:HE2	1.90	0.85
1:A:137:GLY:HA2	1:A:154:THR:HG22	1.60	0.83
1:A:124:ARG:HH22	1:A:196:ASN:HD21	1.23	0.82
1:A:129:LEU:HD23	1:A:157:VAL:HG23	1.63	0.81
2:B:169:CYS:HA	2:B:176:GLN:HE22	1.44	0.80
2:B:220:ARG:HD2	2:B:232:LEU:HD21	1.64	0.80
2:B:100:ASN:ND2	2:B:102:THR:H	1.82	0.77
1:A:201:LEU:HD13	1:A:240:LEU:HD22	1.67	0.77
1:A:201:LEU:O	1:A:205:VAL:HG13	1.84	0.76
2:B:100:ASN:HD21	2:B:102:THR:HB	1.51	0.76
2:B:256:ALA:HB3	2:B:258:GLU:CD	2.07	0.75
2:B:164:LEU:HD12	2:B:164:LEU:O	1.86	0.75
2:B:239:ASP:O	2:B:250:ILE:HG23	1.86	0.74
2:B:253:TRP:HZ3	2:B:256:ALA:HB2	1.52	0.74
2:B:232:LEU:HD22	2:B:232:LEU:H	1.51	0.73
1:A:188:ASP:O	1:A:192:ILE:HG12	1.89	0.73
2:B:256:ALA:HB3	2:B:258:GLU:OE2	1.89	0.72
1:A:191:MET:O	1:A:195:GLU:HG3	1.89	0.72
2:B:196:LEU:HB3	2:B:221:TRP:HE1	1.55	0.71
1:A:123:ASN:O	1:A:127:ILE:HG13	1.91	0.71
2:B:173:LYS:HE3	2:B:175:GLU:HB2	1.72	0.71
2:B:57:LYS:HD2	2:B:63:ARG:HD3	1.73	0.71
1:A:66:VAL:HG13	1:A:75:VAL:HG13	1.72	0.70
2:B:258:GLU:HG2	2:B:261:GLN:HB2	1.74	0.70
2:B:253:TRP:CZ3	2:B:256:ALA:HB2	2.27	0.69
1:A:170:TYR:HB2	1:A:239:VAL:HG22	1.74	0.69
1:A:116:MET:HE3	1:A:155:LEU:HB3	1.74	0.69
1:A:46:ASP:H	1:A:49:ARG:CD	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:GLY:O	1:A:212:THR:HG23	1.93	0.68
2:B:58:ARG:HH11	2:B:58:ARG:CG	2.06	0.68
1:A:46:ASP:HB2	1:A:49:ARG:HH11	1.58	0.68
1:A:211:GLY:O	1:A:231:ALA:HB1	1.94	0.68
1:A:46:ASP:HB2	1:A:49:ARG:NH1	2.09	0.67
2:B:212:CYS:HA	2:B:219:GLN:OE1	1.94	0.67
1:A:60:THR:O	1:A:61:ASP:HB2	1.94	0.67
1:A:172:GLN:O	1:A:176:ASP:HB2	1.93	0.67
1:A:67:ALA:CB	1:A:98:LEU:HD11	2.24	0.67
2:B:256:ALA:HB3	2:B:258:GLU:OE1	1.95	0.67
2:B:113:SER:HB2	2:B:134:GLN:HG2	1.77	0.67
1:A:156:MET:O	1:A:160:GLN:HB2	1.95	0.67
2:B:161:GLY:O	2:B:605:ALA:N	2.29	0.66
1:A:221:ASN:ND2	1:A:223:GLU:HG3	2.11	0.66
2:B:205:LYS:O	2:B:206:THR:HB	1.96	0.65
2:B:232:LEU:H	2:B:232:LEU:HD13	1.61	0.65
1:A:124:ARG:HH22	1:A:196:ASN:ND2	1.93	0.65
1:A:230:ASP:OD2	2:B:140:ASN:HB2	1.96	0.65
1:A:137:GLY:HA2	1:A:154:THR:CG2	2.27	0.64
2:B:54:TRP:CZ3	2:B:64:SER:HB2	2.33	0.64
1:A:86:PHE:CE1	1:A:104:GLN:HG3	2.33	0.64
1:A:140:SER:HB2	1:A:154:THR:HG21	1.78	0.64
2:B:73:ALA:C	2:B:76:GLU:H	2.00	0.63
2:B:137:ARG:NE	2:B:182:THR:HG22	2.13	0.63
2:B:230:LEU:CD2	2:B:235:ASP:HA	2.26	0.63
1:A:21:ILE:HD11	1:A:172:GLN:HE22	1.64	0.62
1:A:124:ARG:NH2	1:A:196:ASN:HD21	1.96	0.62
1:A:170:TYR:HB2	1:A:239:VAL:CG2	2.30	0.62
2:B:196:LEU:HB3	2:B:221:TRP:NE1	2.14	0.62
1:A:204:LEU:HD22	1:A:213:PHE:HB3	1.81	0.62
1:A:47:GLU:HB2	1:A:97:HIS:HE1	1.64	0.62
1:A:230:ASP:OD2	2:B:16:VAL:HG12	1.99	0.61
1:A:116:MET:CE	1:A:155:LEU:HB3	2.29	0.61
2:B:131:ALA:HA	2:B:217:ALA:CA	2.29	0.61
2:B:21:ARG:HD3	2:B:117:ALA:HB2	1.82	0.61
1:A:46:ASP:HB2	1:A:49:ARG:HD2	1.81	0.61
2:B:230:LEU:HD22	2:B:231:SER:N	2.16	0.61
1:A:101:ARG:O	1:A:101:ARG:HG2	2.00	0.61
2:B:116:ALA:HB3	2:B:121:LEU:CD1	2.30	0.61
2:B:77:GLN:HG3	2:B:79:LYS:NZ	2.17	0.60
2:B:83:TYR:HE1	2:B:87:GLN:HB2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ARG:NH1	1:A:49:ARG:HB3	2.17	0.59
1:A:58:ASN:CG	1:A:60:THR:H	2.05	0.59
2:B:21:ARG:HH11	2:B:117:ALA:HB2	1.65	0.59
2:B:19:ALA:HB2	2:B:142:THR:CG2	2.30	0.59
2:B:230:LEU:HD22	2:B:231:SER:H	1.68	0.59
2:B:37:ALA:CB	2:B:82:ILE:HD11	2.29	0.59
2:B:77:GLN:HG3	2:B:79:LYS:HZ3	1.67	0.59
2:B:163:ASN:ND2	2:B:164:LEU:H	1.91	0.58
1:A:151:LEU:H	1:A:151:LEU:CD2	2.16	0.58
2:B:220:ARG:HD2	2:B:232:LEU:CD2	2.33	0.58
2:B:164:LEU:HD23	2:B:209:LEU:HD21	1.86	0.58
1:A:230:ASP:CB	2:B:140:ASN:H	2.15	0.58
1:A:228:ILE:HG13	2:B:141:GLU:HG2	1.86	0.57
1:A:230:ASP:CG	2:B:16:VAL:HG12	2.24	0.57
1:A:46:ASP:N	1:A:49:ARG:HD2	2.15	0.57
1:A:236:THR:HG22	2:B:267:PHE:CD2	2.40	0.57
2:B:201:ASP:OD1	2:B:236:LYS:HE2	2.04	0.57
1:A:86:PHE:CD1	1:A:86:PHE:N	2.71	0.57
2:B:100:ASN:O	2:B:220:ARG:NH1	2.38	0.57
1:A:239:VAL:HG12	1:A:240:LEU:N	2.19	0.56
1:A:18:ASN:O	1:A:21:ILE:HD13	2.05	0.56
2:B:21:ARG:CD	2:B:117:ALA:HB2	2.35	0.56
1:A:154:THR:O	1:A:158:ILE:HG12	2.05	0.56
1:A:145:ASN:O	1:A:151:LEU:N	2.37	0.56
2:B:228:SER:HB3	2:B:261:GLN:O	2.04	0.56
2:B:201:ASP:O	2:B:203:GLY:N	2.38	0.56
2:B:97:ILE:HG23	2:B:103:ILE:HG12	1.88	0.56
1:A:58:ASN:C	1:A:61:ASP:H	2.09	0.56
2:B:163:ASN:ND2	2:B:164:LEU:N	2.42	0.56
1:A:94:SER:O	1:A:98:LEU:HB2	2.06	0.55
1:A:124:ARG:NH1	1:A:192:ILE:HG23	2.21	0.55
2:B:234:ASP:OD1	2:B:234:ASP:N	2.40	0.55
2:B:198:SER:O	2:B:199:ALA:HB2	2.05	0.55
2:B:74:ALA:H	2:B:79:LYS:NZ	2.05	0.55
1:A:151:LEU:HD23	1:A:152:ALA:N	2.22	0.55
2:B:42:LYS:HZ3	2:B:120:LEU:HD21	1.72	0.55
2:B:118:ASN:O	2:B:121:LEU:HB3	2.07	0.55
1:A:221:ASN:ND2	1:A:225:GLU:HB2	2.22	0.54
2:B:69:LEU:HD21	2:B:80:ALA:HB1	1.90	0.54
1:A:145:ASN:HD22	1:A:146:PRO:HD2	1.72	0.54
2:B:184:LYS:HB2	2:B:220:ARG:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ILE:HG13	1:A:228:ILE:O	2.07	0.54
2:B:215:GLY:N	2:B:216:PRO:CD	2.71	0.54
1:A:39:LEU:HD11	1:A:198:TRP:HH2	1.72	0.54
2:B:73:ALA:C	2:B:76:GLU:N	2.61	0.54
2:B:248:LYS:HE3	2:B:249:GLN:NE2	2.23	0.54
2:B:54:TRP:CE3	2:B:64:SER:HB2	2.43	0.54
1:A:49:ARG:HB3	1:A:49:ARG:CZ	2.37	0.54
1:A:230:ASP:HB3	2:B:140:ASN:H	1.73	0.54
1:A:66:VAL:HG12	1:A:68:VAL:HG13	1.90	0.53
2:B:104:ILE:HD11	2:B:109:SER:HA	1.90	0.53
1:A:128:PRO:HA	1:A:185:PHE:O	2.08	0.53
2:B:74:ALA:O	2:B:76:GLU:HB2	2.07	0.53
2:B:84:ASP:HB2	2:B:87:GLN:HG2	1.88	0.53
2:B:116:ALA:H	2:B:121:LEU:HD11	1.73	0.53
1:A:145:ASN:O	1:A:146:PRO:C	2.46	0.53
2:B:232:LEU:N	2:B:232:LEU:CD2	2.62	0.53
2:B:89:THR:HG23	2:B:92:LEU:CG	2.33	0.53
1:A:41:ALA:O	1:A:44:ALA:N	2.42	0.53
1:A:131:ALA:O	1:A:134:LEU:HD12	2.09	0.53
1:A:164:GLU:HG2	1:A:195:GLU:HG2	1.90	0.52
2:B:27:ASP:O	2:B:39:ILE:HG23	2.09	0.52
2:B:197:THR:O	2:B:207:ILE:HG23	2.09	0.52
2:B:248:LYS:HE3	2:B:249:GLN:HE21	1.74	0.52
1:A:157:VAL:O	1:A:158:ILE:HD13	2.09	0.52
2:B:170:ARG:O	2:B:171:ALA:HB3	2.10	0.52
1:A:76:VAL:O	1:A:77:ALA:HB2	2.08	0.52
1:A:46:ASP:C	1:A:48:ALA:N	2.62	0.52
2:B:197:THR:HG22	2:B:198:SER:H	1.74	0.52
1:A:25:ARG:HA	1:A:242:LEU:HD21	1.92	0.51
2:B:129:SER:O	2:B:130:TYR:HB2	2.11	0.51
2:B:173:LYS:HG3	2:B:176:GLN:HG3	1.92	0.51
1:A:17:TYR:O	1:A:20:ASP:HB3	2.10	0.51
1:A:41:ALA:C	1:A:44:ALA:H	2.14	0.51
1:A:197:ASN:O	1:A:201:LEU:HB2	2.11	0.51
1:A:145:ASN:ND2	1:A:146:PRO:HD2	2.26	0.51
2:B:37:ALA:HB3	2:B:82:ILE:CD1	2.33	0.51
2:B:207:ILE:HD13	2:B:238:MET:CE	2.40	0.51
2:B:58:ARG:NH1	2:B:58:ARG:HG2	2.25	0.51
2:B:73:ALA:HA	2:B:77:GLN:O	2.11	0.51
2:B:100:ASN:HD21	2:B:102:THR:H	1.57	0.51
1:A:188:ASP:OD1	1:A:191:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:ARG:HH11	2:B:58:ARG:HG2	1.73	0.50
2:B:169:CYS:HA	2:B:176:GLN:NE2	2.21	0.50
1:A:46:ASP:C	1:A:48:ALA:H	2.15	0.50
1:A:247:ALA:O	1:A:248:CYS:HB2	2.11	0.50
2:B:181:LEU:HB3	2:B:183:ASP:OD1	2.11	0.50
2:B:216:PRO:C	2:B:218:SER:H	2.15	0.50
1:A:236:THR:HG22	2:B:267:PHE:CE2	2.47	0.50
2:B:19:ALA:HB3	2:B:182:THR:HG21	1.94	0.49
1:A:204:LEU:O	1:A:208:SER:HB3	2.13	0.49
2:B:216:PRO:HG2	2:B:219:GLN:HG3	1.94	0.49
2:B:91:GLU:HB3	2:B:107:ALA:CB	2.42	0.49
2:B:197:THR:HG22	2:B:198:SER:N	2.27	0.49
2:B:112:LEU:HD22	2:B:123:LEU:HD23	1.93	0.49
2:B:207:ILE:HD11	2:B:252:LEU:HG	1.95	0.49
1:A:80:ALA:N	1:A:83:ASN:O	2.45	0.49
2:B:19:ALA:CB	2:B:142:THR:HG22	2.38	0.49
2:B:116:ALA:O	2:B:121:LEU:HD13	2.13	0.49
1:A:245:ARG:HH12	1:A:247:ALA:HB2	1.77	0.49
1:A:207:GLY:HA2	1:A:248:CYS:HB3	1.94	0.48
1:A:218:THR:HA	1:A:227:ILE:O	2.13	0.48
2:B:84:ASP:CB	2:B:87:GLN:HG2	2.44	0.48
1:A:155:LEU:O	1:A:159:ILE:HG13	2.13	0.48
2:B:49:ASN:N	2:B:49:ASN:ND2	2.59	0.48
1:A:51:TYR:HE2	1:A:97:HIS:HE2	1.62	0.48
2:B:186:ILE:HB	2:B:196:LEU:HB2	1.96	0.48
1:A:37:PRO:HG2	1:A:241:ALA:O	2.14	0.48
2:B:239:ASP:OD1	2:B:240:SER:N	2.42	0.47
2:B:216:PRO:HD2	2:B:219:GLN:HG3	1.95	0.47
2:B:42:LYS:HD3	2:B:43:LYS:N	2.29	0.47
1:A:169:ARG:NH2	2:B:227:GLY:HA2	2.30	0.47
2:B:108:SER:O	2:B:109:SER:CB	2.63	0.47
2:B:112:LEU:HD22	2:B:123:LEU:CD2	2.45	0.47
1:A:144:LYS:O	1:A:145:ASN:O	2.32	0.47
1:A:221:ASN:HA	2:B:267:PHE:HD1	1.80	0.47
2:B:99:ASP:O	2:B:222:VAL:HG21	2.15	0.47
2:B:604:GLY:H	2:B:164:LEU:HA	1.80	0.47
2:B:181:LEU:HD13	2:B:187:ARG:HG3	1.96	0.47
2:B:209:LEU:N	2:B:209:LEU:HD12	2.30	0.47
1:A:68:VAL:HA	1:A:74:ALA:O	2.15	0.47
2:B:55:THR:O	2:B:55:THR:HG22	2.13	0.47
2:B:59:GLU:HG2	2:B:61:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:LEU:HD13	2:B:230:LEU:C	2.35	0.47
2:B:604:GLY:O	2:B:160:ASN:ND2	2.48	0.46
1:A:144:LYS:O	1:A:151:LEU:HB3	2.16	0.46
2:B:241:GLU:HG2	2:B:251:ILE:HG23	1.97	0.46
1:A:56:SER:O	1:A:63:GLU:HA	2.15	0.46
2:B:43:LYS:NZ	2:B:44:CYS:H	2.13	0.46
2:B:108:SER:O	2:B:109:SER:HB3	2.14	0.46
1:A:86:PHE:N	1:A:86:PHE:HD1	2.13	0.46
1:A:244:LEU:HD13	1:A:246:LYS:HD2	1.98	0.46
2:B:45:ALA:CB	2:B:49:ASN:HD21	2.28	0.46
2:B:42:LYS:HD3	2:B:43:LYS:H	1.81	0.46
2:B:166:MET:O	2:B:246:ALA:HA	2.16	0.46
1:A:112:THR:OG1	1:A:115:ASP:HB2	2.16	0.45
1:A:157:VAL:O	1:A:157:VAL:HG13	2.16	0.45
1:A:18:ASN:HA	1:A:21:ILE:CD1	2.47	0.45
1:A:141:LEU:CD2	1:A:151:LEU:HB2	2.46	0.45
2:B:83:TYR:CE1	2:B:87:GLN:HB2	2.49	0.45
2:B:224:ASP:OD1	2:B:230:LEU:HB3	2.16	0.45
2:B:241:GLU:HG3	2:B:249:GLN:HG2	1.97	0.45
2:B:42:LYS:NZ	2:B:120:LEU:HD21	2.31	0.45
2:B:43:LYS:HD2	2:B:43:LYS:HA	1.56	0.45
2:B:49:ASN:HB2	2:B:52:GLN:HB2	1.99	0.45
2:B:158:GLN:HE22	2:B:173:LYS:HE2	1.74	0.45
2:B:197:THR:OG1	2:B:219:GLN:NE2	2.48	0.45
1:A:145:ASN:CB	1:A:146:PRO:CD	2.77	0.45
1:A:152:ALA:O	1:A:155:LEU:HB2	2.17	0.45
1:A:200:ASN:O	1:A:201:LEU:C	2.55	0.45
2:B:59:GLU:O	2:B:60:ALA:HB3	2.16	0.45
2:B:78:ALA:CB	2:B:125:VAL:HG12	2.47	0.45
1:A:43:GLY:C	1:A:45:LEU:H	2.20	0.45
1:A:53:THR:HA	1:A:66:VAL:O	2.17	0.45
1:A:151:LEU:H	1:A:151:LEU:HD22	1.80	0.45
1:A:169:ARG:CZ	1:A:603:ALA:O	2.65	0.45
2:B:77:GLN:HE21	2:B:77:GLN:HB2	1.60	0.45
2:B:104:ILE:HG12	2:B:110:LEU:O	2.16	0.45
1:A:177:VAL:O	1:A:180:GLU:HB3	2.17	0.44
1:A:220:GLN:HE21	1:A:220:GLN:HB2	1.60	0.44
2:B:158:GLN:NE2	2:B:173:LYS:CE	2.72	0.44
1:A:116:MET:HB2	1:A:156:MET:HE1	1.99	0.44
1:A:164:GLU:CG	1:A:195:GLU:HG2	2.47	0.44
2:B:123:LEU:HD21	2:B:136:TRP:CH2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ALA:C	1:A:44:ALA:N	2.70	0.44
2:B:183:ASP:OD2	2:B:185:SER:HB3	2.18	0.44
2:B:186:ILE:O	2:B:195:CYS:HB2	2.17	0.44
1:A:39:LEU:HD11	1:A:198:TRP:CH2	2.52	0.44
1:A:98:LEU:HB3	1:A:99:PHE:H	1.67	0.44
2:B:56:LEU:HD11	2:B:97:ILE:HD11	2.00	0.44
2:B:241:GLU:HG2	2:B:251:ILE:CG2	2.48	0.44
1:A:125:LYS:HG3	1:A:187:ALA:O	2.18	0.43
1:A:125:LYS:HD3	1:A:192:ILE:HG13	2.00	0.43
1:A:211:GLY:HA3	1:A:233:TYR:CE2	2.52	0.43
2:B:100:ASN:HB2	2:B:232:LEU:HD12	2.00	0.43
2:B:184:LYS:O	2:B:220:ARG:HA	2.18	0.43
2:B:58:ARG:CG	2:B:58:ARG:NH1	2.71	0.43
1:A:58:ASN:OD1	1:A:60:THR:N	2.51	0.43
1:A:78:TYR:CE1	1:A:141:LEU:HD13	2.53	0.43
1:A:86:PHE:HD1	1:A:86:PHE:H	1.65	0.43
2:B:164:LEU:HD23	2:B:209:LEU:HD11	2.00	0.43
2:B:55:THR:HG22	2:B:57:LYS:HG3	2.00	0.43
1:A:29:GLU:O	1:A:29:GLU:HG3	2.18	0.43
1:A:116:MET:HB2	1:A:156:MET:CE	2.48	0.43
1:A:173:ASN:HB3	2:B:266:LEU:HD13	2.00	0.43
1:A:219:LEU:O	1:A:227:ILE:HB	2.19	0.43
1:A:95:LEU:N	1:A:95:LEU:CD2	2.82	0.42
1:A:144:LYS:O	1:A:151:LEU:HD13	2.19	0.42
1:A:110:ASP:OD1	1:A:110:ASP:N	2.52	0.42
2:B:605:ALA:O	2:B:208:LEU:HB2	2.19	0.42
2:B:164:LEU:HD22	2:B:178:TRP:CH2	2.53	0.42
2:B:207:ILE:HD13	2:B:238:MET:HE3	2.00	0.42
1:A:58:ASN:CG	1:A:60:THR:N	2.71	0.42
1:A:221:ASN:HD21	1:A:225:GLU:HB2	1.83	0.42
2:B:40:ILE:HG22	2:B:122:ASP:HA	2.02	0.42
2:B:72:ALA:O	2:B:78:ALA:HA	2.19	0.42
2:B:100:ASN:HD21	2:B:102:THR:CB	2.28	0.42
1:A:206:GLN:HE22	1:A:245:ARG:HA	1.84	0.42
1:A:29:GLU:HB3	1:A:242:LEU:HD11	2.01	0.42
2:B:42:LYS:HZ3	2:B:120:LEU:CD2	2.32	0.41
2:B:104:ILE:HG23	2:B:106:PRO:HD3	2.02	0.41
2:B:132:SER:HA	2:B:220:ARG:HG3	2.02	0.41
2:B:232:LEU:N	2:B:232:LEU:HD13	2.33	0.41
1:A:129:LEU:N	1:A:185:PHE:O	2.49	0.41
2:B:45:ALA:HB1	2:B:49:ASN:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:GLY:O	2:B:162:PRO:C	2.58	0.41
2:B:214:SER:C	2:B:216:PRO:HD3	2.41	0.41
1:A:188:ASP:OD1	1:A:188:ASP:N	2.53	0.41
2:B:82:ILE:H	2:B:82:ILE:HG13	1.58	0.41
2:B:105:ASN:HA	2:B:106:PRO:HD2	1.84	0.41
1:A:170:TYR:CB	1:A:239:VAL:HG22	2.47	0.41
2:B:110:LEU:HD12	2:B:110:LEU:HA	1.88	0.41
1:A:239:VAL:CG1	1:A:240:LEU:N	2.84	0.41
2:B:77:GLN:HB2	2:B:78:ALA:H	1.65	0.41
1:A:120:ALA:HB1	1:A:153:ARG:HG3	2.02	0.41
2:B:84:ASP:HB2	2:B:87:GLN:CG	2.50	0.41
1:A:21:ILE:CD1	1:A:172:GLN:NE2	2.84	0.41
2:B:230:LEU:CD1	2:B:232:LEU:HD13	2.51	0.41
1:A:172:GLN:HG3	1:A:173:ASN:N	2.32	0.41
1:A:201:LEU:O	1:A:205:VAL:CG1	2.62	0.41
1:A:85:TYR:CD1	1:A:85:TYR:N	2.89	0.41
1:A:211:GLY:O	1:A:233:TYR:CE2	2.74	0.41
1:A:173:ASN:O	1:A:177:VAL:HG23	2.20	0.40
2:B:59:GLU:CD	2:B:61:THR:OG1	2.59	0.40
1:A:60:THR:O	1:A:61:ASP:CB	2.68	0.40
1:A:123:ASN:O	1:A:126:ALA:N	2.49	0.40
2:B:91:GLU:H	2:B:91:GLU:HG3	1.65	0.40
2:B:114:SER:O	2:B:115:GLY:C	2.60	0.40
1:A:21:ILE:CD1	1:A:172:GLN:HE22	2.32	0.40
2:B:23:GLY:O	2:B:43:LYS:NZ	2.54	0.40
2:B:232:LEU:H	2:B:232:LEU:CD2	2.17	0.40
2:B:267:PHE:O	2:B:267:PHE:CD1	2.75	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	232/234 (99%)	185 (80%)	32 (14%)	15 (6%)	1 2
2	B	252/254 (99%)	197 (78%)	30 (12%)	25 (10%)	0 0
All	All	484/488 (99%)	382 (79%)	62 (13%)	40 (8%)	1 1

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	146	PRO
2	B	76	GLU
2	B	160	ASN
2	B	162	PRO
2	B	199	ALA
2	B	204	PRO
2	B	246	ALA
2	B	255	ASN
1	A	31	PRO
1	A	43	GLY
1	A	49	ARG
1	A	133	ALA
1	A	143	SER
1	A	144	LYS
2	B	29	ASN
2	B	201	ASP
2	B	202	ALA
2	B	247	ALA
1	A	61	ASP
2	B	12	ALA
2	B	77	GLN
2	B	206	THR
2	B	212	CYS
2	B	243	ALA
1	A	77	ALA
1	A	93	SER
1	A	180	GLU
2	B	172	GLY
2	B	191	ASN
1	A	27	ALA
1	A	119	ALA
2	B	232	LEU
2	B	244	ALA
2	B	31	GLU

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Mol	Chain	Res	Type
2	B	32	GLY
2	B	35	ASN
2	B	192	SER
2	B	16	VAL
1	A	157	VAL

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	175/175 (100%)	110 (63%)	65 (37%)	0 0
2	B	190/190 (100%)	117 (62%)	73 (38%)	0 0
All	All	365/365 (100%)	227 (62%)	138 (38%)	0 0

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	14	ASP
1	A	21	ILE
1	A	22	LYS
1	A	24	GLU
1	A	32	MET
1	A	34	HIS
1	A	36	ILE
1	A	45	LEU
1	A	47	GLU
1	A	49	ARG
1	A	53	THR
1	A	56	SER
1	A	63	GLU
1	A	65	SER
1	A	70	VAL
1	A	73	LEU
1	A	79	ARG

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Mol	Chain	Res	Type
1	A	82	SER
1	A	86	PHE
1	A	94	SER
1	A	95	LEU
1	A	97	HIS
1	A	98	LEU
1	A	100	SER
1	A	101	ARG
1	A	104	GLN
1	A	110	ASP
1	A	111	ASN
1	A	112	THR
1	A	115	ASP
1	A	122	SER
1	A	124	ARG
1	A	125	LYS
1	A	129	LEU
1	A	134	LEU
1	A	141	LEU
1	A	144	LYS
1	A	146	PRO
1	A	151	LEU
1	A	155	LEU
1	A	156	MET
1	A	162	LEU
1	A	167	ARG
1	A	172	GLN
1	A	173	ASN
1	A	174	ASN
1	A	191	MET
1	A	194	LEU
1	A	200	ASN
1	A	201	LEU
1	A	205	VAL
1	A	212	THR
1	A	215	SER
1	A	219	LEU
1	A	220	GLN
1	A	223	GLU
1	A	224	ASP
1	A	225	GLU
1	A	227	ILE

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Mol	Chain	Res	Type
1	A	239	VAL
1	A	242	LEU
1	A	243	MET
1	A	244	LEU
1	A	245	ARG
2	B	11	CYS
2	B	17	ARG
2	B	21	ARG
2	B	29	ASN
2	B	31	GLU
2	B	35	ASN
2	B	40	ILE
2	B	42	LYS
2	B	43	LYS
2	B	49	ASN
2	B	50	ASP
2	B	52	GLN
2	B	53	LEU
2	B	58	ARG
2	B	59	GLU
2	B	69	LEU
2	B	76	GLU
2	B	77	GLN
2	B	79	LYS
2	B	82	ILE
2	B	86	THR
2	B	89	THR
2	B	96	GLU
2	B	97	ILE
2	B	100	ASN
2	B	104	ILE
2	B	110	LEU
2	B	112	LEU
2	B	113	SER
2	B	114	SER
2	B	118	ASN
2	B	119	SER
2	B	121	LEU
2	B	123	LEU
2	B	125	VAL
2	B	127	THR
2	B	132	SER

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Mol	Chain	Res	Type
2	B	137	ARG
2	B	138	THR
2	B	142	THR
2	B	157	MET
2	B	158	GLN
2	B	160	ASN
2	B	163	ASN
2	B	167	SER
2	B	173	LYS
2	B	177	GLN
2	B	181	LEU
2	B	184	LYS
2	B	185	SER
2	B	187	ARG
2	B	190	THR
2	B	194	ASN
2	B	196	LEU
2	B	201	ASP
2	B	208	LEU
2	B	209	LEU
2	B	214	SER
2	B	218	SER
2	B	220	ARG
2	B	224	ASP
2	B	230	LEU
2	B	232	LEU
2	B	234	ASP
2	B	236	LYS
2	B	238	MET
2	B	240	SER
2	B	248	LYS
2	B	249	GLN
2	B	253	TRP
2	B	255	ASN
2	B	262	ILE
2	B	264	LEU

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

Mol	Chain	Res	Type
1	A	18	ASN
1	A	87	HIS

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Mol	Chain	Res	Type
1	A	145	ASN
1	A	160	GLN
1	A	172	GLN
1	A	173	ASN
1	A	174	ASN
1	A	206	GLN
1	A	220	GLN
2	B	29	ASN
2	B	35	ASN
2	B	49	ASN
2	B	52	GLN
2	B	77	GLN
2	B	100	ASN
2	B	118	ASN
2	B	140	ASN
2	B	158	GLN
2	B	160	ASN
2	B	163	ASN
2	B	176	GLN
2	B	194	ASN
2	B	249	GLN
2	B	255	ASN
2	B	260	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)

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	234/234 (100%)	-0.52	2 (0%)	84	85	2, 13, 46, 76	0
2	B	254/254 (100%)	-0.40	3 (1%)	79	80	2, 14, 53, 83	0
All	All	488/488 (100%)	-0.46	5 (1%)	82	83	2, 14, 50, 83	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	245	ALA	4.5
1	A	248	CYS	3.8
2	B	74	ALA	3.5
1	A	81	GLY	2.6
2	B	246	ALA	2.5

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 monosaccharides 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.