Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:32 PM GMT

PDB ID	:	1BBS
Title	:	X-RAY ANALYSES OF PEPTIDE INHIBITOR COMPLEXES DEFINE THE STRUCTURAL BASIS OF SPECIFICITY FOR HUMAN AND MOUSE RENINS
Authors	:	Dhanaraj, V.; Blundell, T.L.
Deposited on	:	1992-05-21
Resolution	:	2.80 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:

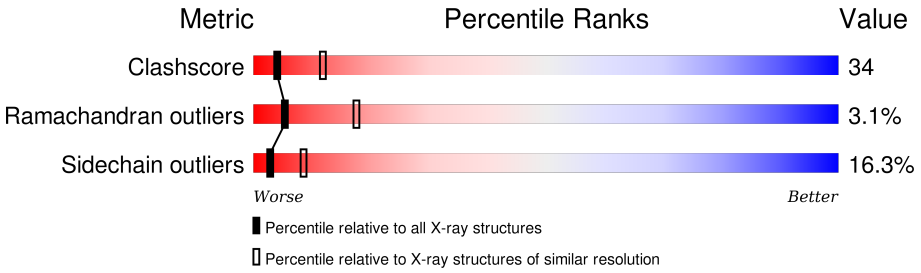
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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	340	44% 38% 13%
1	B	340	44% 39% 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5018 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 RENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2509	1609	398	488	14			
1	B	331	Total	C	N	O	S	0	0	0
			2509	1609	398	488	14			

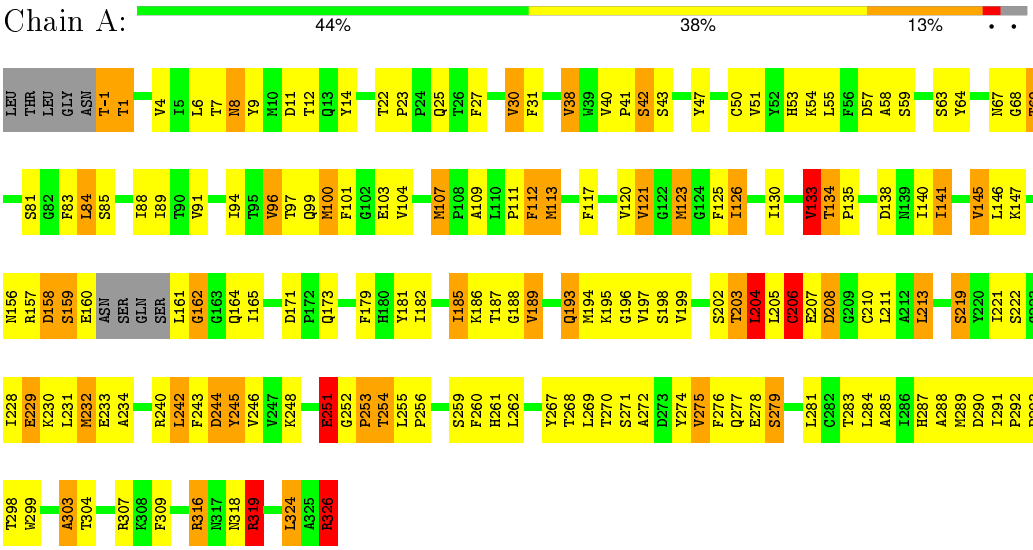
3 Residue-property plots (i)

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.

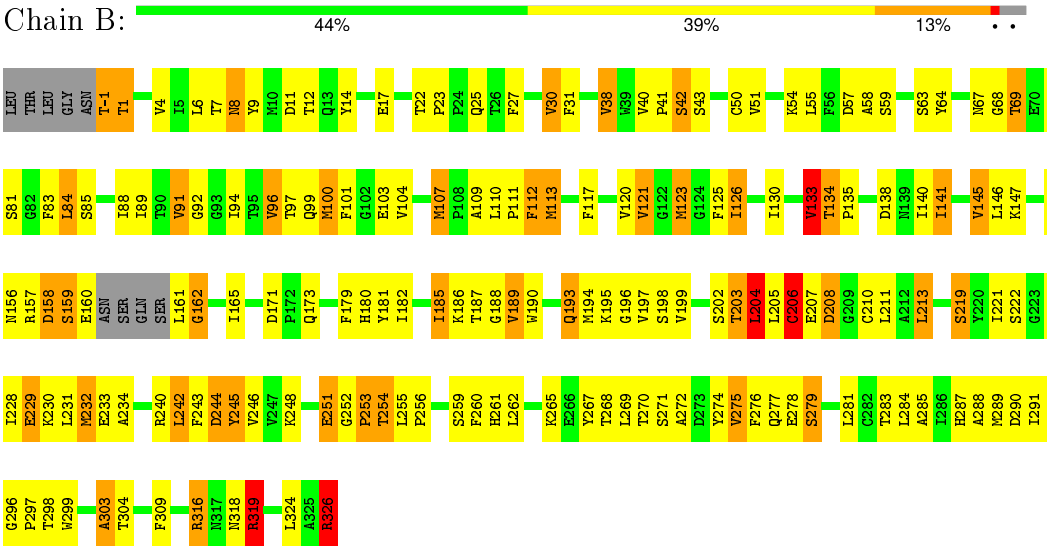
- Molecule 1: RENIN

Chain A:



- Molecule 1: RENIN

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 21 3	Depositor
Cell constants a, b, c, α, β, γ	143.10Å 143.10Å 143.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.196 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5018	wwPDB-VP
Average B, all atoms (Å^2)	0.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.94	1/2568 (0.0%)	1.57	40/3493 (1.1%)
1	B	0.94	2/2568 (0.1%)	1.57	36/3493 (1.0%)
All	All	0.94	3/5136 (0.1%)	1.57	76/6986 (1.1%)

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	1	4
1	B	1	4
All	All	2	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	TYR	C-N	7.05	1.50	1.34
1	B	245	TYR	C-N	7.01	1.50	1.34
1	B	190	TRP	NE1-CE2	-5.00	1.31	1.37

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	319	ARG	NE-CZ-NH2	9.01	124.80	120.30
1	A	31	PHE	C-N-CA	8.96	144.09	121.70
1	B	31	PHE	C-N-CA	8.96	144.09	121.70
1	A	319	ARG	NE-CZ-NH2	8.95	124.77	120.30
1	B	96	VAL	CA-CB-CG2	8.72	123.98	110.90
1	A	96	VAL	CA-CB-CG2	8.71	123.96	110.90
1	B	162	GLY	O-C-N	-7.65	110.20	123.20
1	A	162	GLY	O-C-N	-7.64	110.22	123.20
1	A	123	MET	CG-SD-CE	7.59	112.35	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	123	MET	CG-SD-CE	7.58	112.33	100.20
1	B	157	ARG	NE-CZ-NH2	7.57	124.08	120.30
1	A	157	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	B	4	VAL	CA-CB-CG2	7.41	122.01	110.90
1	A	4	VAL	CA-CB-CG2	7.38	121.97	110.90
1	A	38	VAL	CA-CB-CG2	7.31	121.87	110.90
1	B	38	VAL	CA-CB-CG2	7.31	121.86	110.90
1	B	232	MET	CG-SD-CE	6.80	111.08	100.20
1	A	232	MET	CG-SD-CE	6.78	111.05	100.20
1	B	100	MET	CG-SD-CE	6.76	111.01	100.20
1	A	100	MET	CG-SD-CE	6.75	110.99	100.20
1	A	155	TYR	CB-CG-CD2	-6.54	117.08	121.00
1	B	155	TYR	CB-CG-CD2	-6.54	117.08	121.00
1	B	51	VAL	CA-CB-CG2	6.33	120.39	110.90
1	A	326	ARG	CD-NE-CZ	-6.32	114.75	123.60
1	A	51	VAL	CA-CB-CG2	6.32	120.37	110.90
1	A	275	VAL	CA-CB-CG2	6.30	120.35	110.90
1	B	326	ARG	CD-NE-CZ	-6.28	114.80	123.60
1	B	275	VAL	CA-CB-CG2	6.28	120.32	110.90
1	A	30	VAL	CA-CB-CG2	6.27	120.31	110.90
1	B	30	VAL	CA-CB-CG2	6.27	120.31	110.90
1	B	121	VAL	CA-CB-CG2	6.26	120.29	110.90
1	A	121	VAL	CA-CB-CG2	6.24	120.26	110.90
1	B	289	MET	CG-SD-CE	6.13	110.01	100.20
1	A	289	MET	CG-SD-CE	6.12	109.99	100.20
1	B	91	VAL	CA-CB-CG2	6.11	120.06	110.90
1	A	91	VAL	CA-CB-CG2	6.09	120.03	110.90
1	A	133	VAL	CA-CB-CG1	6.06	119.98	110.90
1	B	133	VAL	CA-CB-CG1	6.05	119.98	110.90
1	A	107	MET	CG-SD-CE	6.03	109.85	100.20
1	B	107	MET	CG-SD-CE	6.02	109.83	100.20
1	A	120	VAL	CA-CB-CG2	5.93	119.80	110.90
1	B	120	VAL	CA-CB-CG2	5.92	119.78	110.90
1	A	319	ARG	CD-NE-CZ	-5.88	115.38	123.60
1	B	319	ARG	CD-NE-CZ	-5.87	115.38	123.60
1	B	189	VAL	CA-CB-CG2	5.83	119.64	110.90
1	A	189	VAL	CA-CB-CG2	5.81	119.62	110.90
1	B	204	LEU	C-N-CA	-5.71	107.42	121.70
1	A	204	LEU	C-N-CA	-5.69	107.47	121.70
1	B	309	PHE	CB-CG-CD1	-5.66	116.84	120.80
1	A	309	PHE	CB-CG-CD1	-5.64	116.85	120.80
1	B	290	ASP	O-C-N	5.63	131.71	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	290	ASP	O-C-N	5.61	131.67	122.70
1	A	206	CYS	N-CA-CB	5.48	120.46	110.60
1	B	73	LEU	CA-CB-CG	-5.47	102.73	115.30
1	B	206	CYS	N-CA-CB	5.46	120.44	110.60
1	A	73	LEU	CA-CB-CG	-5.46	102.74	115.30
1	A	145	VAL	CA-CB-CG2	5.45	119.08	110.90
1	B	145	VAL	CA-CB-CG2	5.43	119.05	110.90
1	B	40	VAL	CA-CB-CG2	5.39	118.99	110.90
1	A	40	VAL	CA-CB-CG2	5.38	118.97	110.90
1	A	113	MET	CG-SD-CE	5.32	108.71	100.20
1	A	206	CYS	N-CA-C	5.32	125.37	111.00
1	B	113	MET	CG-SD-CE	5.32	108.71	100.20
1	B	206	CYS	N-CA-C	5.31	125.34	111.00
1	A	50	CYS	CA-CB-SG	-5.30	104.45	114.00
1	B	50	CYS	CA-CB-SG	-5.30	104.47	114.00
1	A	153	PHE	CB-CG-CD1	-5.18	117.17	120.80
1	B	153	PHE	CB-CG-CD1	-5.16	117.19	120.80
1	B	104	VAL	CA-CB-CG2	5.08	118.51	110.90
1	A	104	VAL	CA-CB-CG2	5.07	118.50	110.90
1	B	303	ALA	N-CA-CB	5.05	117.17	110.10
1	A	303	ALA	N-CA-CB	5.03	117.14	110.10
1	A	251	GLU	OE1-CD-OE2	-5.02	117.28	123.30
1	A	47	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	A	53	HIS	CA-CB-CG	-5.01	105.09	113.60
1	A	307	ARG	NE-CZ-NH2	5.00	122.80	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	303	ALA	CA
1	B	303	ALA	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	GLY	Mainchain
1	A	195	LYS	Mainchain
1	A	316	ARG	Sidechain
1	A	326	ARG	Sidechain
1	B	162	GLY	Mainchain
1	B	195	LYS	Mainchain
1	B	316	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	326	ARG	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	2509	0	2397	167	1
1	B	2509	0	2397	167	2
All	All	5018	0	4794	334	2

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 34.

All (334) 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:196:GLY:HA2	1:B:206:CYS:CB	1.77	1.15
1:B:196:GLY:CA	1:B:206:CYS:HB3	1.76	1.15
1:A:196:GLY:HA2	1:A:206:CYS:CB	1.77	1.15
1:A:196:GLY:CA	1:A:206:CYS:HB3	1.76	1.13
1:B:199:VAL:HG21	1:B:204:LEU:HD21	1.28	1.08
1:A:199:VAL:HG21	1:A:204:LEU:HD21	1.28	1.04
1:B:199:VAL:HB	1:B:204:LEU:HD23	1.39	1.00
1:A:270:THR:HG22	1:A:272:ALA:H	1.26	0.99
1:A:199:VAL:HB	1:A:204:LEU:HD23	1.39	0.99
1:B:270:THR:HG22	1:B:272:ALA:H	1.26	0.98
1:A:244:ASP:OD2	1:A:283:THR:HG23	1.64	0.97
1:B:89:ILE:HD12	1:B:99:GLN:HB3	1.46	0.95
1:B:244:ASP:OD2	1:B:283:THR:HG23	1.64	0.95
1:A:199:VAL:HG21	1:A:204:LEU:CD2	1.95	0.95
1:A:89:ILE:HD12	1:A:99:GLN:HB3	1.46	0.95
1:B:199:VAL:HG21	1:B:204:LEU:CD2	1.95	0.95
1:A:199:VAL:CG2	1:A:204:LEU:CD2	2.46	0.94
1:B:8:ASN:HD21	1:B:11:ASP:H	1.11	0.94
1:B:199:VAL:CG2	1:B:204:LEU:CD2	2.46	0.93
1:B:197:VAL:N	1:B:205:LEU:O	2.02	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:VAL:N	1:A:205:LEU:O	2.02	0.92
1:A:8:ASN:HD21	1:A:11:ASP:H	1.11	0.92
1:B:199:VAL:CG2	1:B:204:LEU:HD21	2.01	0.90
1:A:199:VAL:CG2	1:A:204:LEU:HD21	2.01	0.90
1:B:8:ASN:HD22	1:B:9:TYR:N	1.71	0.88
1:B:194:MET:HE1	1:B:197:VAL:HG22	1.56	0.88
1:A:194:MET:HE1	1:A:197:VAL:HG22	1.55	0.87
1:A:8:ASN:HD22	1:A:9:TYR:N	1.71	0.87
1:A:204:LEU:O	1:A:205:LEU:HD23	1.75	0.86
1:B:109:ALA:HB1	1:B:113:MET:HG3	1.56	0.86
1:B:204:LEU:O	1:B:205:LEU:HD23	1.75	0.86
1:A:109:ALA:HB1	1:A:113:MET:HG3	1.56	0.86
1:B:194:MET:HE1	1:B:260:PHE:HD1	1.42	0.85
1:B:186:LYS:HG3	1:B:187:THR:N	1.91	0.85
1:A:186:LYS:HG3	1:A:187:THR:N	1.91	0.84
1:B:8:ASN:C	1:B:8:ASN:HD22	1.80	0.84
1:B:199:VAL:CB	1:B:204:LEU:HD23	2.09	0.82
1:A:199:VAL:CB	1:A:204:LEU:HD23	2.09	0.82
1:A:8:ASN:C	1:A:8:ASN:HD22	1.80	0.82
1:B:25:GLN:HE22	1:B:57:ASP:H	1.28	0.82
1:A:244:ASP:OD2	1:A:283:THR:CG2	2.27	0.81
1:B:244:ASP:OD2	1:B:283:THR:CG2	2.27	0.81
1:A:194:MET:HE1	1:A:260:PHE:HD1	1.43	0.81
1:A:25:GLN:HE22	1:A:57:ASP:H	1.28	0.81
1:A:181:TYR:HB3	1:A:319:ARG:HD3	1.65	0.79
1:A:41:PRO:HB3	1:A:107:MET:HE3	1.64	0.79
1:A:84:LEU:HD11	1:A:133:VAL:HG11	1.66	0.77
1:B:181:TYR:HB3	1:B:319:ARG:HD3	1.65	0.77
1:A:8:ASN:HD21	1:A:11:ASP:N	1.83	0.76
1:B:84:LEU:HD11	1:B:133:VAL:HG11	1.66	0.76
1:A:199:VAL:CB	1:A:204:LEU:CD2	2.64	0.76
1:B:244:ASP:OD1	1:B:287:HIS:CE1	2.39	0.76
1:A:244:ASP:OD1	1:A:287:HIS:CE1	2.39	0.75
1:B:199:VAL:CB	1:B:204:LEU:CD2	2.64	0.75
1:A:252:GLY:N	1:A:253:PRO:HD2	2.01	0.74
1:B:252:GLY:N	1:B:253:PRO:HD2	2.00	0.74
1:B:207:GLU:O	1:B:208:ASP:HB2	1.86	0.74
1:B:8:ASN:HD21	1:B:11:ASP:N	1.83	0.74
1:A:207:GLU:O	1:A:208:ASP:HB2	1.86	0.73
1:A:27:PHE:CE1	1:A:54:LYS:HG2	2.23	0.73
1:B:27:PHE:CE1	1:B:54:LYS:HG2	2.23	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:THR:HG22	1:A:299:TRP:O	1.90	0.72
1:A:8:ASN:ND2	1:A:11:ASP:H	1.88	0.71
1:B:298:THR:HG22	1:B:299:TRP:O	1.90	0.71
1:B:89:ILE:HD12	1:B:99:GLN:CB	2.20	0.71
1:B:246:VAL:CG2	1:B:281:LEU:HD23	2.21	0.71
1:A:246:VAL:CG2	1:A:281:LEU:HD23	2.21	0.71
1:A:224:SER:OG	1:A:227:SER:HB2	1.91	0.71
1:B:224:SER:OG	1:B:227:SER:HB2	1.91	0.71
1:B:199:VAL:HB	1:B:204:LEU:CD2	2.18	0.70
1:B:8:ASN:ND2	1:B:11:ASP:H	1.88	0.70
1:A:275:VAL:HG22	1:A:284:LEU:CD2	2.22	0.70
1:B:275:VAL:HG22	1:B:284:LEU:CD2	2.22	0.70
1:B:41:PRO:HB3	1:B:107:MET:HE3	1.73	0.69
1:A:89:ILE:HD12	1:A:99:GLN:CB	2.20	0.69
1:B:194:MET:HE1	1:B:260:PHE:CD1	2.26	0.69
1:A:246:VAL:HG21	1:A:281:LEU:HD23	1.76	0.68
1:B:246:VAL:HG21	1:B:281:LEU:HD23	1.76	0.68
1:A:270:THR:HG22	1:A:271:SER:N	2.09	0.68
1:A:204:LEU:O	1:A:205:LEU:CD2	2.41	0.67
1:B:204:LEU:O	1:B:205:LEU:CD2	2.41	0.67
1:A:199:VAL:HB	1:A:204:LEU:CD2	2.18	0.67
1:A:185:ILE:HD13	1:A:193:GLN:HG3	1.75	0.67
1:B:270:THR:HG22	1:B:271:SER:N	2.09	0.67
1:A:194:MET:CE	1:A:260:PHE:HD1	2.08	0.66
1:B:185:ILE:HD13	1:B:193:GLN:CG	2.26	0.66
1:B:194:MET:CE	1:B:260:PHE:HD1	2.09	0.66
1:B:185:ILE:HD13	1:B:193:GLN:HG3	1.75	0.66
1:A:185:ILE:HD13	1:A:193:GLN:CG	2.26	0.65
1:A:194:MET:HE1	1:A:260:PHE:CD1	2.28	0.65
1:B:262:LEU:HD12	1:B:267:TYR:CD2	2.32	0.64
1:A:270:THR:HG22	1:A:272:ALA:N	2.07	0.64
1:B:84:LEU:HD22	1:B:101:PHE:O	1.97	0.64
1:A:84:LEU:HD22	1:A:101:PHE:O	1.97	0.64
1:B:38:VAL:HG22	1:B:121:VAL:HG13	1.79	0.64
1:A:262:LEU:HD12	1:A:267:TYR:CD2	2.32	0.63
1:B:225:THR:O	1:B:229:GLU:HB2	1.99	0.63
1:A:38:VAL:HG22	1:A:121:VAL:HG13	1.79	0.62
1:B:270:THR:HG22	1:B:272:ALA:N	2.06	0.62
1:B:204:LEU:HD12	1:B:204:LEU:O	2.00	0.62
1:A:204:LEU:HD12	1:A:204:LEU:O	2.00	0.62
1:A:270:THR:CG2	1:A:271:SER:N	2.63	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:THR:O	1:A:229:GLU:HB2	1.99	0.61
1:B:232:MET:HG3	1:B:245:TYR:CD1	2.36	0.61
1:B:194:MET:CE	1:B:197:VAL:HG22	2.28	0.61
1:B:270:THR:CG2	1:B:271:SER:N	2.63	0.61
1:B:159:SER:O	1:B:160:GLU:CB	2.49	0.61
1:A:194:MET:CE	1:A:197:VAL:HG22	2.28	0.60
1:A:248:LYS:O	1:A:251:GLU:HG3	2.01	0.60
1:B:244:ASP:OD1	1:B:287:HIS:HE1	1.82	0.60
1:A:232:MET:HG3	1:A:245:TYR:CD1	2.35	0.60
1:B:278:GLU:O	1:B:279:SER:HB3	2.01	0.60
1:B:248:LYS:O	1:B:251:GLU:HG3	2.00	0.60
1:A:198:SER:OG	1:A:261:HIS:HE1	1.85	0.60
1:B:196:GLY:HA2	1:B:206:CYS:HB3	0.83	0.60
1:B:228:ILE:HG21	1:B:288:ALA:HB2	1.84	0.60
1:A:196:GLY:HA2	1:A:206:CYS:HB3	0.83	0.59
1:A:228:ILE:HG21	1:A:288:ALA:HB2	1.84	0.59
1:A:159:SER:O	1:A:160:GLU:CB	2.49	0.59
1:A:278:GLU:O	1:A:279:SER:HB3	2.01	0.59
1:B:-1:THR:HG23	1:B:1:THR:N	2.18	0.59
1:A:8:ASN:ND2	1:A:8:ASN:C	2.51	0.59
1:A:244:ASP:OD1	1:A:287:HIS:HE1	1.82	0.58
1:A:41:PRO:HB2	1:A:55:LEU:HD23	1.86	0.58
1:B:198:SER:OG	1:B:261:HIS:HE1	1.85	0.58
1:B:41:PRO:HB2	1:B:55:LEU:HD23	1.86	0.58
1:B:41:PRO:HB3	1:B:107:MET:CE	2.34	0.58
1:B:207:GLU:O	1:B:208:ASP:CB	2.52	0.57
1:A:-1:THR:HG23	1:A:1:THR:N	2.18	0.57
1:A:101:PHE:CD1	1:A:101:PHE:N	2.71	0.57
1:A:126:ILE:HD12	1:A:135:PRO:HD2	1.86	0.57
1:A:207:GLU:O	1:A:208:ASP:CB	2.52	0.57
1:B:101:PHE:CD1	1:B:101:PHE:N	2.71	0.57
1:A:41:PRO:HB3	1:A:107:MET:CE	2.34	0.56
1:A:109:ALA:CB	1:A:113:MET:HG3	2.34	0.56
1:B:126:ILE:HD12	1:B:135:PRO:HD2	1.86	0.56
1:A:155:TYR:CD2	1:A:303:ALA:HB2	2.41	0.56
1:A:251:GLU:O	1:A:252:GLY:C	2.42	0.56
1:B:155:TYR:CD2	1:B:303:ALA:HB2	2.41	0.56
1:A:206:CYS:SG	1:A:210:CYS:N	2.79	0.56
1:A:94:ILE:HD13	1:A:140:ILE:CG2	2.35	0.56
1:B:94:ILE:HD13	1:B:140:ILE:CG2	2.35	0.56
1:B:8:ASN:C	1:B:8:ASN:ND2	2.51	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:CYS:SG	1:B:210:CYS:N	2.79	0.55
1:A:68:GLY:O	1:A:83:PHE:HB2	2.07	0.55
1:B:68:GLY:O	1:B:83:PHE:HB2	2.07	0.55
1:B:84:LEU:HD13	1:B:100:MET:HE2	1.88	0.54
1:A:242:LEU:HG	1:A:243:PHE:HD2	1.72	0.54
1:B:251:GLU:O	1:B:252:GLY:C	2.42	0.54
1:A:293:PRO:HA	1:A:294:PRO:C	2.28	0.54
1:B:293:PRO:HA	1:B:294:PRO:C	2.28	0.54
1:A:41:PRO:CB	1:A:107:MET:HE3	2.35	0.53
1:A:58:ALA:HB1	1:A:64:TYR:CG	2.44	0.53
1:B:58:ALA:HB1	1:B:64:TYR:CG	2.44	0.53
1:A:88:ILE:O	1:A:88:ILE:HG13	2.09	0.53
1:A:-1:THR:HB	1:A:145:VAL:O	2.09	0.53
1:B:182:ILE:HD13	1:B:262:LEU:HB3	1.91	0.53
1:A:199:VAL:CB	1:A:204:LEU:HD21	2.37	0.53
1:A:221:ILE:HG13	1:A:304:THR:HB	1.91	0.53
1:B:271:SER:HA	1:B:274:TYR:CE2	2.44	0.52
1:B:242:LEU:HG	1:B:243:PHE:HD2	1.72	0.52
1:B:-1:THR:HB	1:B:145:VAL:O	2.09	0.52
1:B:204:LEU:O	1:B:205:LEU:CG	2.58	0.52
1:A:94:ILE:HD13	1:A:140:ILE:HG21	1.90	0.52
1:B:94:ILE:HD13	1:B:140:ILE:HG21	1.90	0.52
1:A:109:ALA:HB1	1:A:113:MET:CG	2.36	0.52
1:B:109:ALA:CB	1:B:113:MET:HG3	2.34	0.52
1:A:204:LEU:O	1:A:205:LEU:CG	2.57	0.52
1:B:109:ALA:HB1	1:B:113:MET:CG	2.36	0.52
1:B:199:VAL:HG23	1:B:204:LEU:HG	1.92	0.52
1:A:199:VAL:HG23	1:A:204:LEU:HG	1.92	0.52
1:A:271:SER:HA	1:A:274:TYR:CE2	2.44	0.51
1:A:58:ALA:HB1	1:A:64:TYR:CD2	2.45	0.51
1:B:58:ALA:HB1	1:B:64:TYR:CD2	2.45	0.51
1:A:199:VAL:HG11	1:A:234:ALA:CB	2.40	0.51
1:B:126:ILE:HD12	1:B:134:THR:HA	1.93	0.51
1:A:182:ILE:HD13	1:A:262:LEU:HB3	1.92	0.51
1:A:181:TYR:CB	1:A:319:ARG:HD3	2.38	0.51
1:B:221:ILE:HG13	1:B:304:THR:HB	1.92	0.51
1:B:41:PRO:HG3	1:B:107:MET:HE3	1.92	0.51
1:A:186:LYS:HG3	1:A:187:THR:H	1.74	0.51
1:A:246:VAL:HG23	1:A:281:LEU:HD23	1.93	0.50
1:A:6:LEU:HD21	1:A:165:ILE:HG13	1.94	0.50
1:B:199:VAL:HG11	1:B:234:ALA:CB	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ILE:HG13	1:B:88:ILE:O	2.09	0.50
1:B:41:PRO:CB	1:B:107:MET:HE3	2.41	0.50
1:B:6:LEU:HD21	1:B:165:ILE:HG13	1.93	0.50
1:B:275:VAL:HG22	1:B:284:LEU:HD22	1.94	0.50
1:A:298:THR:HG22	1:A:299:TRP:N	2.27	0.50
1:B:30:VAL:HG23	1:B:117:PHE:CD2	2.47	0.50
1:A:84:LEU:HD13	1:A:100:MET:HE2	1.94	0.50
1:B:171:ASP:OD1	1:B:171:ASP:C	2.48	0.50
1:A:126:ILE:HD12	1:A:134:THR:HA	1.93	0.50
1:A:199:VAL:HG21	1:A:204:LEU:CG	2.42	0.49
1:B:181:TYR:CB	1:B:319:ARG:HD3	2.38	0.49
1:A:30:VAL:HG23	1:A:117:PHE:CD2	2.47	0.49
1:B:298:THR:HG22	1:B:299:TRP:N	2.27	0.49
1:A:255:LEU:HB3	1:A:256:PRO:HD2	1.94	0.49
1:B:199:VAL:CG2	1:B:204:LEU:CG	2.90	0.49
1:A:202:SER:C	1:A:204:LEU:H	2.16	0.49
1:B:199:VAL:HG21	1:B:204:LEU:CG	2.42	0.49
1:A:199:VAL:CG2	1:A:204:LEU:CG	2.90	0.49
1:A:171:ASP:C	1:A:171:ASP:OD1	2.48	0.48
1:B:133:VAL:CG2	1:B:133:VAL:O	2.62	0.48
1:B:125:PHE:CB	1:B:188:GLY:HA2	2.43	0.48
1:A:125:PHE:CB	1:A:188:GLY:HA2	2.43	0.48
1:B:202:SER:C	1:B:204:LEU:H	2.16	0.48
1:B:255:LEU:HD12	1:B:275:VAL:HG21	1.95	0.48
1:B:246:VAL:HG23	1:B:281:LEU:HD23	1.93	0.48
1:B:199:VAL:CB	1:B:204:LEU:HD21	2.37	0.48
1:B:255:LEU:HB3	1:B:256:PRO:HD2	1.94	0.48
1:B:185:ILE:HD12	1:B:211:LEU:CD2	2.43	0.48
1:B:42:SER:HB2	1:B:103:GLU:HG2	1.96	0.47
1:A:12:THR:O	1:A:219:SER:HB3	2.14	0.47
1:A:255:LEU:HD12	1:A:275:VAL:HG21	1.95	0.47
1:A:232:MET:HG3	1:A:245:TYR:CE1	2.49	0.47
1:B:291:ILE:O	1:B:296:GLY:HA3	2.15	0.47
1:A:185:ILE:HD12	1:A:211:LEU:CD2	2.43	0.47
1:A:153:PHE:CZ	1:A:165:ILE:HD13	2.50	0.47
1:B:41:PRO:CG	1:B:107:MET:HE3	2.44	0.47
1:A:291:ILE:O	1:A:296:GLY:HA3	2.15	0.47
1:B:153:PHE:CZ	1:B:165:ILE:HD13	2.50	0.47
1:B:205:LEU:HD11	1:B:227:SER:O	2.15	0.47
1:A:275:VAL:HG22	1:A:284:LEU:HD22	1.94	0.47
1:B:296:GLY:HA2	1:B:298:THR:OG1	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:SER:HB2	1:A:103:GLU:HG2	1.96	0.47
1:A:205:LEU:HD11	1:A:227:SER:O	2.15	0.47
1:A:296:GLY:HA2	1:A:298:THR:OG1	2.15	0.47
1:A:155:TYR:HD2	1:A:303:ALA:HB2	1.80	0.46
1:B:12:THR:O	1:B:219:SER:HB3	2.14	0.46
1:A:133:VAL:O	1:A:133:VAL:CG2	2.62	0.46
1:B:232:MET:HG3	1:B:245:TYR:CE1	2.49	0.46
1:B:71:LEU:HD23	1:B:71:LEU:HA	1.79	0.46
1:A:41:PRO:HG2	1:A:54:LYS:O	2.16	0.46
1:A:231:LEU:HD12	1:A:231:LEU:O	2.16	0.46
1:B:271:SER:O	1:B:275:VAL:HB	2.15	0.46
1:B:186:LYS:HG3	1:B:187:THR:H	1.74	0.46
1:B:155:TYR:HD2	1:B:303:ALA:HB2	1.80	0.46
1:B:231:LEU:O	1:B:231:LEU:HD12	2.16	0.46
1:A:271:SER:O	1:A:275:VAL:HB	2.15	0.45
1:B:41:PRO:HG2	1:B:54:LYS:O	2.16	0.45
1:B:262:LEU:HB2	1:B:267:TYR:CE2	2.52	0.45
1:A:262:LEU:HB2	1:A:267:TYR:CE2	2.52	0.45
1:B:240:ARG:O	1:B:242:LEU:C	2.55	0.45
1:B:111:PRO:HD2	1:B:112:PHE:H	1.82	0.45
1:A:276:PHE:HB2	1:A:283:THR:O	2.17	0.45
1:A:64:TYR:CD1	1:A:64:TYR:C	2.90	0.45
1:A:94:ILE:CD1	1:A:140:ILE:HG21	2.47	0.45
1:B:230:LYS:O	1:B:233:GLU:HB3	2.17	0.45
1:B:194:MET:HG2	1:B:262:LEU:HD23	1.99	0.45
1:A:194:MET:HG2	1:A:262:LEU:HD23	1.99	0.45
1:A:99:GLN:HG3	1:A:100:MET:N	2.32	0.45
1:A:198:SER:HA	1:A:203:THR:HA	1.99	0.45
1:B:99:GLN:HG3	1:B:100:MET:N	2.32	0.44
1:B:94:ILE:CD1	1:B:140:ILE:HG21	2.47	0.44
1:B:199:VAL:CG2	1:B:204:LEU:HG	2.47	0.44
1:A:133:VAL:HG22	1:A:133:VAL:O	2.18	0.44
1:B:268:THR:HG22	1:B:269:LEU:N	2.32	0.44
1:A:324:LEU:HA	1:A:324:LEU:HD23	1.62	0.44
1:B:255:LEU:HD12	1:B:275:VAL:CG2	2.47	0.44
1:B:276:PHE:HB2	1:B:283:THR:O	2.17	0.44
1:B:135:PRO:HG2	1:B:138:ASP:OD1	2.17	0.44
1:A:111:PRO:HD2	1:A:112:PHE:H	1.82	0.44
1:A:135:PRO:HG2	1:A:138:ASP:OD1	2.18	0.44
1:B:133:VAL:O	1:B:133:VAL:HG22	2.18	0.44
1:A:268:THR:HG22	1:A:269:LEU:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ARG:O	1:A:242:LEU:C	2.55	0.44
1:A:204:LEU:O	1:A:205:LEU:HG	2.18	0.44
1:A:41:PRO:HG3	1:A:107:MET:HE3	2.00	0.44
1:A:255:LEU:HD12	1:A:275:VAL:CG2	2.47	0.44
1:A:41:PRO:CG	1:A:107:MET:HE3	2.48	0.44
1:A:198:SER:OG	1:A:261:HIS:CE1	2.70	0.43
1:B:292:PRO:HA	1:B:293:PRO:HD3	1.71	0.43
1:B:64:TYR:CD1	1:B:64:TYR:C	2.90	0.43
1:A:225:THR:HA	1:A:288:ALA:HB1	2.01	0.43
1:A:230:LYS:O	1:A:233:GLU:HB3	2.17	0.43
1:A:199:VAL:CG2	1:A:204:LEU:HG	2.47	0.43
1:A:185:ILE:CD1	1:A:211:LEU:HD23	2.48	0.43
1:B:141:ILE:HD13	1:B:146:LEU:HD12	2.01	0.43
1:B:199:VAL:CG2	1:B:204:LEU:HD23	2.35	0.43
1:B:202:SER:C	1:B:204:LEU:N	2.71	0.43
1:A:202:SER:C	1:A:204:LEU:N	2.71	0.43
1:B:225:THR:HA	1:B:288:ALA:HB1	2.01	0.43
1:B:198:SER:HA	1:B:203:THR:HA	1.99	0.43
1:A:42:SER:HB2	1:A:103:GLU:CG	2.49	0.43
1:B:198:SER:OG	1:B:261:HIS:CE1	2.70	0.43
1:B:204:LEU:O	1:B:205:LEU:HG	2.18	0.42
1:B:242:LEU:HG	1:B:243:PHE:CD2	2.53	0.42
1:A:291:ILE:HA	1:A:292:PRO:HD3	1.87	0.42
1:B:185:ILE:CD1	1:B:211:LEU:HD23	2.48	0.42
1:A:242:LEU:HG	1:A:243:PHE:CD2	2.53	0.42
1:B:125:PHE:CG	1:B:188:GLY:HA2	2.54	0.42
1:A:125:PHE:CG	1:A:188:GLY:HA2	2.54	0.42
1:B:213:LEU:HB2	1:B:298:THR:HG21	2.01	0.42
1:A:141:ILE:HD13	1:A:146:LEU:HD12	2.01	0.42
1:A:7:THR:O	1:A:14:TYR:HA	2.20	0.42
1:B:180:HIS:CE1	1:B:265:LYS:HZ3	2.38	0.42
1:A:41:PRO:CG	1:A:107:MET:CE	2.98	0.42
1:B:22:THR:HA	1:B:23:PRO:C	2.40	0.42
1:A:252:GLY:C	1:A:254:THR:H	2.23	0.42
1:B:42:SER:HB2	1:B:103:GLU:CG	2.49	0.42
1:A:71:LEU:CD2	1:A:130:ILE:HG22	2.50	0.42
1:B:319:ARG:HD2	1:B:319:ARG:HH11	1.59	0.42
1:A:213:LEU:HB2	1:A:298:THR:HG21	2.00	0.42
1:A:134:THR:HA	1:A:135:PRO:HD2	1.55	0.42
1:B:252:GLY:C	1:B:254:THR:H	2.23	0.41
1:A:185:ILE:HD13	1:A:193:GLN:HG2	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:CD1	1:A:146:LEU:HD12	2.50	0.41
1:A:147:LYS:O	1:A:147:LYS:HG3	2.19	0.41
1:B:41:PRO:CB	1:B:107:MET:CE	2.97	0.41
1:B:185:ILE:HD13	1:B:193:GLN:HG2	2.00	0.41
1:A:285:ALA:HB1	1:A:304:THR:OG1	2.21	0.41
1:B:7:THR:O	1:B:14:TYR:HA	2.20	0.41
1:A:30:VAL:HG23	1:A:117:PHE:CG	2.56	0.41
1:B:30:VAL:HG23	1:B:117:PHE:CG	2.55	0.41
1:A:164:GLN:HG2	1:A:164:GLN:O	2.16	0.41
1:B:41:PRO:CG	1:B:107:MET:CE	2.97	0.41
1:B:285:ALA:HB1	1:B:304:THR:OG1	2.21	0.41
1:B:188:GLY:O	1:B:189:VAL:HG22	2.21	0.41
1:A:22:THR:HA	1:A:23:PRO:C	2.40	0.41
1:B:141:ILE:CD1	1:B:146:LEU:HD12	2.50	0.41
1:A:188:GLY:O	1:A:189:VAL:HG22	2.21	0.41
1:B:71:LEU:CD2	1:B:130:ILE:HG22	2.50	0.41
1:A:22:THR:CA	1:A:23:PRO:C	2.90	0.41
1:B:147:LYS:O	1:B:147:LYS:HG3	2.19	0.41
1:B:96:VAL:CG1	1:B:96:VAL:O	2.69	0.41
1:B:292:PRO:O	1:B:292:PRO:HD2	2.21	0.40
1:B:22:THR:CA	1:B:23:PRO:C	2.90	0.40
1:A:96:VAL:CG1	1:A:96:VAL:O	2.69	0.40
1:A:203:THR:O	1:A:203:THR:OG1	2.33	0.40
1:A:155:TYR:CE2	1:A:303:ALA:HB2	2.56	0.40
1:B:91:VAL:O	1:B:92:GLY:C	2.60	0.40
1:A:292:PRO:HD2	1:A:292:PRO:O	2.21	0.40
1:A:205:LEU:HA	1:A:205:LEU:HD23	1.92	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LEU:CD2	1:B:254:THR:CG2[5_555]	1.86	0.34
1:A:270:THR:OG1	1:B:17:GLU:OE2[5_555]	1.93	0.27

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	327/340 (96%)	290 (89%)	27 (8%)	10 (3%)	5	17
1	B	327/340 (96%)	290 (89%)	27 (8%)	10 (3%)	5	17
All	All	654/680 (96%)	580 (89%)	54 (8%)	20 (3%)	5	17

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASP
1	A	206	CYS
1	B	158	ASP
1	B	206	CYS
1	A	242	LEU
1	B	242	LEU
1	A	69	THR
1	A	112	PHE
1	A	208	ASP
1	A	279	SER
1	B	69	THR
1	B	112	PHE
1	B	208	ASP
1	B	279	SER
1	A	67	ASN
1	A	126	ILE
1	B	67	ASN
1	B	126	ILE
1	A	253	PRO
1	B	253	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	270/290 (93%)	226 (84%)	44 (16%)	3 8
1	B	270/290 (93%)	226 (84%)	44 (16%)	3 8
All	All	540/580 (93%)	452 (84%)	88 (16%)	3 8

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	THR
1	A	1	THR
1	A	8	ASN
1	A	42	SER
1	A	43	SER
1	A	59	SER
1	A	63	SER
1	A	69	THR
1	A	81	SER
1	A	84	LEU
1	A	85	SER
1	A	97	THR
1	A	123	MET
1	A	133	VAL
1	A	134	THR
1	A	141	ILE
1	A	152	SER
1	A	156	ASN
1	A	158	ASP
1	A	159	SER
1	A	161	LEU
1	A	173	GLN
1	A	179	PHE
1	A	185	ILE
1	A	193	GLN
1	A	203	THR
1	A	204	LEU
1	A	213	LEU
1	A	219	SER
1	A	222	SER
1	A	226	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	227	SER
1	A	229	GLU
1	A	244	ASP
1	A	251	GLU
1	A	254	THR
1	A	259	SER
1	A	277	GLN
1	A	297	PRO
1	A	316	ARG
1	A	318	ASN
1	A	319	ARG
1	A	324	LEU
1	A	326	ARG
1	B	-1	THR
1	B	1	THR
1	B	8	ASN
1	B	42	SER
1	B	43	SER
1	B	59	SER
1	B	63	SER
1	B	69	THR
1	B	81	SER
1	B	84	LEU
1	B	85	SER
1	B	97	THR
1	B	123	MET
1	B	133	VAL
1	B	134	THR
1	B	141	ILE
1	B	152	SER
1	B	156	ASN
1	B	158	ASP
1	B	159	SER
1	B	161	LEU
1	B	173	GLN
1	B	179	PHE
1	B	185	ILE
1	B	193	GLN
1	B	203	THR
1	B	204	LEU
1	B	213	LEU
1	B	219	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	222	SER
1	B	226	SER
1	B	227	SER
1	B	229	GLU
1	B	244	ASP
1	B	251	GLU
1	B	254	THR
1	B	259	SER
1	B	277	GLN
1	B	297	PRO
1	B	316	ARG
1	B	318	ASN
1	B	319	ARG
1	B	324	LEU
1	B	326	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	25	GLN
1	A	99	GLN
1	A	128	GLN
1	A	139	ASN
1	A	156	ASN
1	A	164	GLN
1	A	174	HIS
1	A	178	ASN
1	A	261	HIS
1	A	317	ASN
1	B	8	ASN
1	B	25	GLN
1	B	99	GLN
1	B	128	GLN
1	B	139	ASN
1	B	143	GLN
1	B	156	ASN
1	B	164	GLN
1	B	174	HIS
1	B	178	ASN
1	B	261	HIS
1	B	317	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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