Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2023 – 03:56 PM EDT

PDB ID	:	6DD7
Title	:	Crystal structure of plant UVB photoreceptor UVR8 from in situ serial Laue diffraction
Authors	:	Ren, Z.
Deposited on	:	2018-05-09
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

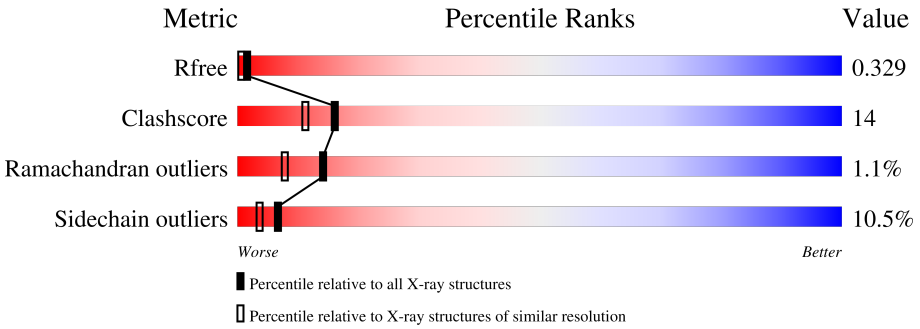
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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%

Mol	Chain	Length	Quality of chain
1	A	377	61% 31% 5% • •
1	B	377	68% 27% • •
1	C	377	70% 25% • •
1	D	377	66% 29% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12160 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 Ultraviolet-B receptor UVR8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2793	1741	505	534	13			
1	B	368	Total	C	N	O	S	0	0	0
			2793	1741	505	534	13			
1	C	368	Total	C	N	O	S	0	0	0
			2793	1741	505	534	13			
1	D	368	Total	C	N	O	S	0	0	0
			2793	1741	505	534	13			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	LEU	-	expression tag	UNP Q9FN03
A	383	GLU	-	expression tag	UNP Q9FN03
A	384	HIS	-	expression tag	UNP Q9FN03
A	385	HIS	-	expression tag	UNP Q9FN03
A	386	HIS	-	expression tag	UNP Q9FN03
A	387	HIS	-	expression tag	UNP Q9FN03
A	388	HIS	-	expression tag	UNP Q9FN03
A	389	HIS	-	expression tag	UNP Q9FN03
B	382	LEU	-	expression tag	UNP Q9FN03
B	383	GLU	-	expression tag	UNP Q9FN03
B	384	HIS	-	expression tag	UNP Q9FN03
B	385	HIS	-	expression tag	UNP Q9FN03
B	386	HIS	-	expression tag	UNP Q9FN03
B	387	HIS	-	expression tag	UNP Q9FN03
B	388	HIS	-	expression tag	UNP Q9FN03
B	389	HIS	-	expression tag	UNP Q9FN03
C	382	LEU	-	expression tag	UNP Q9FN03
C	383	GLU	-	expression tag	UNP Q9FN03
C	384	HIS	-	expression tag	UNP Q9FN03
C	385	HIS	-	expression tag	UNP Q9FN03
C	386	HIS	-	expression tag	UNP Q9FN03

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	387	HIS	-	expression tag	UNP Q9FN03
C	388	HIS	-	expression tag	UNP Q9FN03
C	389	HIS	-	expression tag	UNP Q9FN03
D	382	LEU	-	expression tag	UNP Q9FN03
D	383	GLU	-	expression tag	UNP Q9FN03
D	384	HIS	-	expression tag	UNP Q9FN03
D	385	HIS	-	expression tag	UNP Q9FN03
D	386	HIS	-	expression tag	UNP Q9FN03
D	387	HIS	-	expression tag	UNP Q9FN03
D	388	HIS	-	expression tag	UNP Q9FN03
D	389	HIS	-	expression tag	UNP Q9FN03

- Molecule 2 is water.

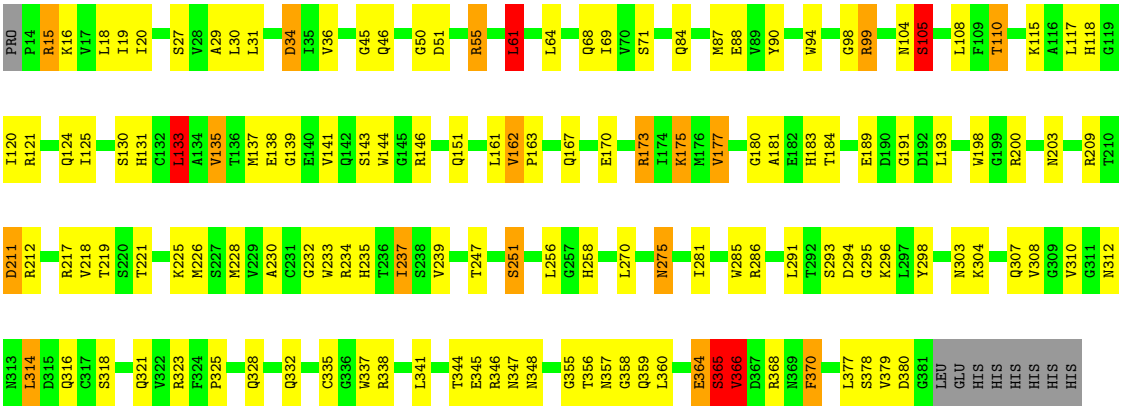
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	200	Total O 200 200	0	0
2	B	306	Total O 306 306	0	0
2	C	276	Total O 276 276	0	0
2	D	206	Total O 206 206	0	0

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.

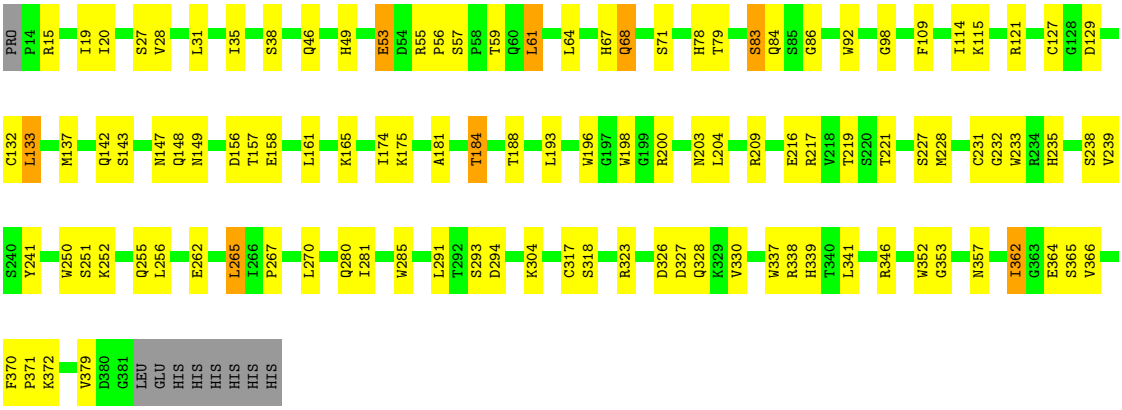
• Molecule 1: Ultraviolet-B receptor UVR8

Chain A:



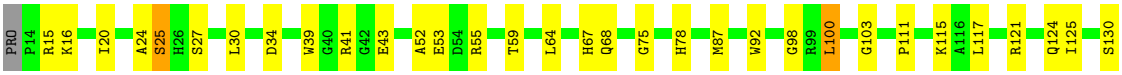
• Molecule 1: Ultraviolet-B receptor UVR8

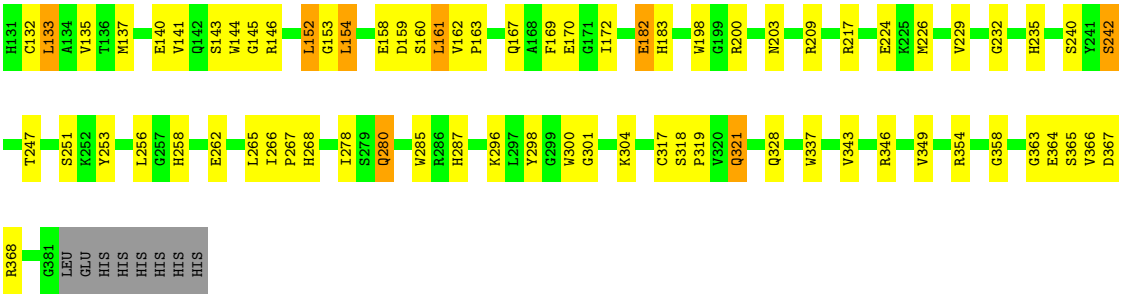
Chain B:



• Molecule 1: Ultraviolet-B receptor UVR8

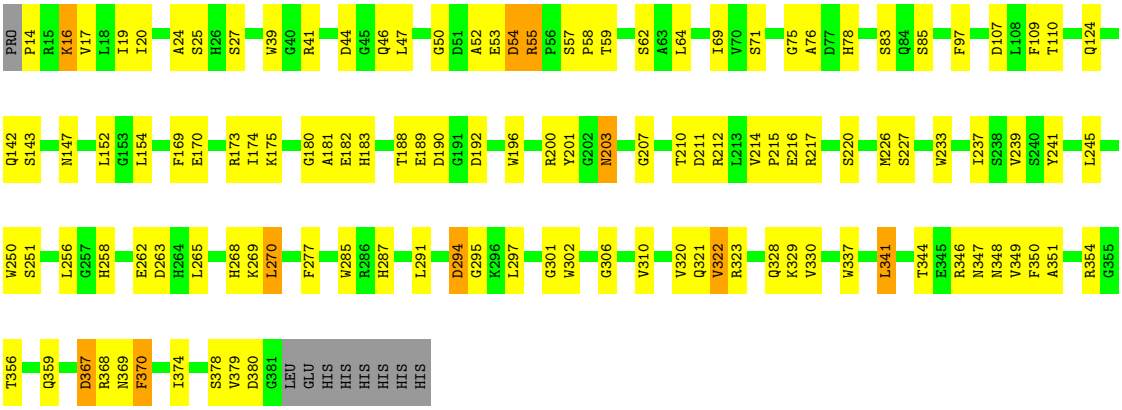
Chain C:





• Molecule 1: Ultraviolet-B receptor UVR8

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	111.20Å 80.30Å 190.00Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	47.33 – 2.00 65.02 – 1.93	Depositor EDS
% Data completeness (in resolution range)	86.6 (47.33-2.00) 79.4 (65.02-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.68 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.254 , 0.328 0.254 , 0.329	Depositor DCC
R_{free} test set	5010 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 78.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.41	EDS
Total number of atoms	12160	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5245e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.41	0/2860	0.63	2/3877 (0.1%)
1	B	0.51	1/2860 (0.0%)	0.67	0/3877
1	C	0.49	0/2860	0.67	0/3877
1	D	0.41	0/2860	0.58	0/3877
All	All	0.46	1/11440 (0.0%)	0.64	2/15508 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	CYS	CB-SG	-5.98	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133	LEU	CA-CB-CG	6.81	130.95	115.30
1	A	61	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2793	0	2670	94	0
1	B	2793	0	2670	79	0
1	C	2793	0	2670	72	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2793	0	2670	76	0
2	A	200	0	0	15	0
2	B	306	0	0	38	0
2	C	276	0	0	29	0
2	D	206	0	0	23	0
All	All	12160	0	10680	316	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 14.

All (316) 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:348:ASN:HD22	1:A:378:SER:HB2	1.29	0.95
1:D:200:ARG:NH2	2:D:404:HOH:O	2.05	0.89
1:C:145:GLY:O	2:C:401:HOH:O	1.90	0.89
1:D:76:ALA:O	2:D:401:HOH:O	1.93	0.87
1:B:98:GLY:O	2:B:401:HOH:O	1.96	0.84
1:D:182:GLU:OE2	2:D:402:HOH:O	1.95	0.83
1:C:158:GLU:O	2:C:402:HOH:O	1.98	0.81
1:A:61:LEU:HG	1:A:64:LEU:HD12	1.61	0.80
1:B:20:ILE:O	2:B:402:HOH:O	1.97	0.80
1:D:183:HIS:ND1	2:D:407:HOH:O	2.13	0.79
1:C:285:TRP:HB2	1:C:337:TRP:HA	1.65	0.79
1:A:121:ARG:HG3	1:A:137:MET:HB2	1.66	0.78
1:B:149:ASN:ND2	2:B:407:HOH:O	2.11	0.78
1:A:133:LEU:HD13	1:A:143:SER:HB3	1.66	0.77
1:B:127:CYS:O	2:B:403:HOH:O	2.01	0.77
1:B:129:ASP:O	2:B:404:HOH:O	2.02	0.76
1:C:160:SER:N	2:C:401:HOH:O	2.16	0.75
1:D:59:THR:OG1	2:D:403:HOH:O	2.03	0.75
1:A:294:ASP:OD1	2:A:401:HOH:O	2.05	0.74
1:D:192:ASP:OD1	1:D:217:ARG:NH1	2.21	0.73
1:A:304:LYS:NZ	2:A:407:HOH:O	2.20	0.73
1:C:301:GLY:O	2:C:404:HOH:O	2.07	0.72
1:A:293:SER:OG	2:A:403:HOH:O	2.07	0.72
1:A:316:GLN:OE1	2:A:402:HOH:O	2.07	0.71
1:B:364:GLU:O	1:B:366:VAL:N	2.24	0.71
1:B:366:VAL:O	2:B:405:HOH:O	2.08	0.71
1:C:183:HIS:ND1	2:C:408:HOH:O	2.25	0.70
1:B:203:ASN:ND2	2:B:415:HOH:O	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:LEU:O	2:D:405:HOH:O	2.10	0.70
1:A:275:ASN:OD1	1:A:275:ASN:N	2.23	0.69
1:A:379:VAL:O	2:A:404:HOH:O	2.11	0.69
1:B:175:LYS:NZ	1:B:227:SER:O	2.27	0.68
1:C:217:ARG:NH1	2:C:410:HOH:O	2.25	0.68
1:C:301:GLY:N	2:C:404:HOH:O	2.27	0.68
1:D:27:SER:HB2	1:D:341:LEU:HD11	1.76	0.68
1:B:67:HIS:NE2	2:B:420:HOH:O	2.28	0.67
1:D:328:GLN:HB3	1:D:346:ARG:HH11	1.60	0.66
1:C:64:LEU:O	2:C:405:HOH:O	2.12	0.66
1:B:55:ARG:NE	2:B:408:HOH:O	2.23	0.66
1:A:365:SER:HA	1:A:366:VAL:HG12	1.77	0.66
1:D:78:HIS:ND1	2:D:416:HOH:O	2.29	0.65
1:D:181:ALA:HB2	1:D:233:TRP:CD1	2.31	0.65
1:A:124:GLN:HE22	1:A:177:VAL:H	1.43	0.64
1:B:53:GLU:O	2:B:408:HOH:O	2.15	0.64
1:D:152:LEU:HB3	1:D:154:LEU:HG	1.78	0.64
1:B:147:ASN:ND2	1:B:156:ASP:O	2.30	0.64
1:A:15:ARG:HH21	1:A:15:ARG:HB3	1.63	0.64
1:D:330:VAL:HA	1:D:344:THR:HA	1.79	0.63
1:B:216:GLU:HB2	2:B:469:HOH:O	1.99	0.63
1:A:94:TRP:O	1:A:99:ARG:HD2	1.98	0.62
1:B:238:SER:HB2	2:B:571:HOH:O	1.98	0.62
1:A:303:ASN:ND2	2:A:408:HOH:O	2.23	0.62
1:A:173:ARG:NH2	1:A:189:GLU:OE2	2.33	0.62
1:A:198:TRP:CZ2	1:A:200:ARG:HB2	2.35	0.62
1:A:378:SER:HB3	2:A:445:HOH:O	1.98	0.61
1:A:232:GLY:HA3	1:A:235:HIS:CE1	2.35	0.61
1:B:68:GLN:NE2	2:B:423:HOH:O	2.33	0.61
1:D:237:ILE:HG22	1:D:245:LEU:HD11	1.82	0.61
1:B:184:THR:O	2:B:410:HOH:O	2.16	0.61
1:D:354:ARG:NH1	1:D:367:ASP:OD2	2.30	0.60
1:C:103:GLY:HA3	2:C:563:HOH:O	2.01	0.60
1:D:41:ARG:NH2	1:D:44:ASP:OD2	2.34	0.60
1:D:285:TRP:HB2	1:D:337:TRP:HA	1.83	0.60
1:D:367:ASP:OD1	1:D:367:ASP:N	2.32	0.60
1:B:232:GLY:HA3	1:B:235:HIS:CE1	2.37	0.60
1:B:262:GLU:HG2	2:B:617:HOH:O	2.01	0.59
1:D:54:ASP:O	1:D:55:ARG:HD3	2.02	0.59
1:D:270:LEU:HD22	2:D:417:HOH:O	2.02	0.59
1:C:167:GLN:HB2	2:C:597:HOH:O	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:SER:OG	2:B:406:HOH:O	2.17	0.59
1:C:296:LYS:HG2	2:C:467:HOH:O	2.02	0.59
1:D:175:LYS:NZ	2:D:420:HOH:O	2.34	0.59
1:C:55:ARG:NE	2:C:418:HOH:O	2.36	0.59
1:A:193:LEU:HD22	1:A:226:MET:HG3	1.84	0.59
1:C:343:VAL:HG22	1:C:349:VAL:HG22	1.84	0.59
1:D:351:ALA:N	2:D:423:HOH:O	2.36	0.58
1:A:146:ARG:NH2	2:A:418:HOH:O	2.36	0.58
1:A:144:TRP:HB3	1:A:163:PRO:HA	1.84	0.58
1:B:304:LYS:NZ	2:B:429:HOH:O	2.36	0.58
1:D:196:TRP:HB3	1:D:215:PRO:HA	1.84	0.57
1:C:253:TYR:OH	2:C:403:HOH:O	2.06	0.57
1:B:338:ARG:NH1	2:B:424:HOH:O	2.33	0.57
1:B:98:GLY:HA3	1:B:161:LEU:HD23	1.87	0.57
1:D:180:GLY:HA3	1:D:183:HIS:CE1	2.39	0.57
1:C:268:HIS:ND1	2:C:414:HOH:O	2.32	0.57
1:B:193:LEU:HD13	2:B:571:HOH:O	2.04	0.56
1:D:323:ARG:O	2:D:409:HOH:O	2.17	0.56
1:A:19:ILE:HD11	2:A:535:HOH:O	2.05	0.56
1:D:227:SER:HB2	1:D:241:TYR:CE2	2.41	0.56
1:D:52:ALA:HB2	1:D:109:PHE:HE2	1.71	0.56
1:D:226:MET:O	2:D:410:HOH:O	2.18	0.55
1:C:169:PHE:HD1	1:C:172:ILE:HD12	1.71	0.55
1:B:328:GLN:HB3	1:B:346:ARG:HE	1.72	0.55
1:C:68:GLN:HG3	2:C:522:HOH:O	2.07	0.55
1:D:287:HIS:HA	1:D:301:GLY:HA3	1.88	0.55
1:D:39:TRP:HB3	1:D:58:PRO:HA	1.88	0.55
1:B:38:SER:OG	1:B:49:HIS:NE2	2.37	0.55
1:D:350:PHE:HB3	2:D:423:HOH:O	2.06	0.54
1:C:140:GLU:HA	2:C:424:HOH:O	2.08	0.54
1:B:227:SER:HB3	1:B:241:TYR:CE1	2.42	0.54
1:A:144:TRP:CE3	1:A:163:PRO:HB3	2.43	0.54
1:C:15:ARG:NH2	2:C:417:HOH:O	2.35	0.54
1:A:211:ASP:O	1:A:212:ARG:HD3	2.07	0.54
1:B:181:ALA:HB2	1:B:233:TRP:CD1	2.43	0.53
1:C:98:GLY:HA3	1:C:161:LEU:HD12	1.89	0.53
1:A:161:LEU:N	2:A:423:HOH:O	2.40	0.53
1:C:247:THR:HB	1:C:256:LEU:HD22	1.89	0.53
1:B:217:ARG:NH1	2:B:438:HOH:O	2.42	0.53
1:A:286:ARG:NH1	1:D:107:ASP:OD2	2.36	0.53
1:A:296:LYS:HD2	2:A:511:HOH:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:GLN:HG3	2:C:618:HOH:O	2.09	0.53
1:D:17:VAL:HG21	1:D:349:VAL:HG21	1.91	0.53
1:B:19:ILE:HD12	1:B:71:SER:HA	1.92	0.52
1:B:78:HIS:HB2	1:B:92:TRP:O	2.09	0.52
1:B:323:ARG:HG3	1:B:323:ARG:HH11	1.75	0.52
1:A:84:GLN:OE1	2:A:406:HOH:O	2.19	0.52
1:C:132:CYS:C	1:C:133:LEU:HD22	2.29	0.52
1:C:30:LEU:HD11	1:C:34:ASP:HA	1.90	0.52
1:A:338:ARG:NH2	2:A:405:HOH:O	2.16	0.52
1:C:280:GLN:NE2	2:C:420:HOH:O	2.37	0.52
1:C:232:GLY:HA3	1:C:235:HIS:CE1	2.45	0.52
1:D:370:PHE:HD1	1:D:370:PHE:H	1.58	0.52
1:C:43:GLU:HA	1:C:52:ALA:HB1	1.91	0.52
1:D:258:HIS:N	2:D:421:HOH:O	2.35	0.51
1:A:193:LEU:HG	1:A:218:VAL:HG21	1.93	0.51
1:C:280:GLN:HG2	2:C:521:HOH:O	2.10	0.51
1:D:188:THR:OG1	1:D:190:ASP:OD2	2.27	0.51
1:A:87:MET:HE3	1:A:121:ARG:HB3	1.93	0.51
1:A:19:ILE:HA	1:A:332:GLN:OE1	2.11	0.50
1:C:247:THR:OG1	1:C:258:HIS:NE2	2.44	0.50
1:D:220:SER:HB3	2:D:547:HOH:O	2.11	0.50
1:D:263:ASP:OD2	2:D:411:HOH:O	2.19	0.50
1:A:15:ARG:HB3	1:A:15:ARG:NH2	2.26	0.50
1:A:181:ALA:HB2	1:A:233:TRP:CD1	2.47	0.50
1:A:303:ASN:OD1	1:A:308:VAL:N	2.34	0.50
1:D:210:THR:HG22	1:D:211:ASP:O	2.12	0.50
1:A:291:LEU:HD11	1:A:295:GLY:HA2	1.93	0.50
1:A:124:GLN:NE2	1:A:177:VAL:O	2.45	0.49
1:C:55:ARG:NH1	1:C:59:THR:HG21	2.26	0.49
1:A:124:GLN:HG2	1:A:125:ILE:N	2.27	0.49
1:A:16:LYS:HG3	1:A:347:ASN:OD1	2.11	0.49
1:D:297:LEU:HD23	1:D:322:VAL:HG21	1.94	0.49
1:D:356:THR:HG23	2:D:466:HOH:O	2.11	0.49
1:B:232:GLY:N	1:B:235:HIS:O	2.39	0.49
1:C:121:ARG:NH2	2:C:432:HOH:O	2.45	0.49
1:A:365:SER:HA	1:A:366:VAL:CB	2.42	0.49
1:B:46:GLN:O	1:B:79:THR:OG1	2.29	0.49
1:A:139:GLY:HA3	1:A:173:ARG:NH1	2.28	0.49
1:B:227:SER:HB3	1:B:241:TYR:HE1	1.78	0.49
1:A:298:TYR:CE1	1:A:321:GLN:HB3	2.48	0.49
1:A:356:THR:C	1:A:358:GLY:H	2.16	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLY:HA3	1:A:161:LEU:HA	1.95	0.48
1:C:182:GLU:HB2	1:C:198:TRP:HB2	1.95	0.48
1:A:173:ARG:CZ	1:A:173:ARG:HB3	2.44	0.48
1:A:105:SER:O	2:D:408:HOH:O	2.20	0.48
1:B:291:LEU:CD1	1:B:330:VAL:HB	2.43	0.48
1:B:323:ARG:HG2	2:B:560:HOH:O	2.12	0.48
1:A:365:SER:HA	1:A:366:VAL:CG1	2.42	0.48
1:B:217:ARG:NE	2:B:433:HOH:O	2.39	0.48
1:C:298:TYR:CE2	1:C:321:GLN:HB2	2.49	0.48
1:D:251:SER:HB3	1:D:262:GLU:O	2.13	0.48
1:D:295:GLY:HA3	1:D:329:LYS:HB3	1.95	0.48
1:B:61:LEU:HD13	1:B:64:LEU:HD12	1.95	0.48
1:A:348:ASN:HA	1:A:378:SER:HB2	1.96	0.48
1:A:34:ASP:CG	1:A:68:GLN:HA	2.33	0.47
1:A:310:VAL:HG23	1:A:312:ASN:ND2	2.28	0.47
1:B:231:CYS:HB2	2:B:439:HOH:O	2.14	0.47
1:A:233:TRP:HB2	1:A:285:TRP:HA	1.96	0.47
1:B:285:TRP:HB2	1:B:337:TRP:HA	1.96	0.47
1:A:247:THR:OG1	1:A:258:HIS:NE2	2.47	0.47
1:B:28:VAL:HG21	1:B:79:THR:CG2	2.45	0.47
1:B:364:GLU:HA	2:B:567:HOH:O	2.13	0.47
1:A:348:ASN:HD22	1:A:378:SER:CB	2.13	0.47
1:B:67:HIS:O	1:B:83:SER:OG	2.32	0.47
1:D:203:ASN:OD1	1:D:203:ASN:N	2.39	0.47
1:C:266:ILE:HB	1:C:267:PRO:HD2	1.97	0.47
1:D:19:ILE:HD12	1:D:71:SER:HA	1.96	0.47
1:C:121:ARG:NH1	2:C:436:HOH:O	2.47	0.47
1:D:14:PRO:N	1:D:16:LYS:HE3	2.30	0.46
1:A:234:ARG:HH21	1:D:97:PHE:HZ	1.62	0.46
1:B:270:LEU:HD12	1:B:270:LEU:HA	1.68	0.46
1:B:148:GLN:HE22	1:C:200:ARG:NH1	2.13	0.46
1:B:265:LEU:HD22	2:B:662:HOH:O	2.16	0.46
1:A:325:PRO:O	1:A:328:GLN:HG3	2.15	0.46
1:B:109:PHE:CZ	1:C:304:LYS:HE2	2.50	0.46
1:C:226:MET:HA	1:C:240:SER:HA	1.96	0.46
1:A:230:ALA:HB2	1:A:281:ILE:HG13	1.98	0.46
1:B:255:GLN:N	2:B:406:HOH:O	2.49	0.46
1:D:169:PHE:CE1	1:D:174:ILE:HD11	2.50	0.46
1:A:110:THR:HG23	2:A:449:HOH:O	2.15	0.46
1:A:370:PHE:HD1	1:A:370:PHE:H	1.63	0.46
1:B:339:HIS:HA	1:B:353:GLY:HA3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:SER:HB3	1:A:341:LEU:HD11	1.98	0.46
1:C:146:ARG:HA	1:C:159:ASP:OD1	2.16	0.46
1:D:322:VAL:HB	2:D:563:HOH:O	2.15	0.46
1:A:237:ILE:HG23	1:A:247:THR:HG22	1.98	0.46
1:D:16:LYS:HG2	1:D:347:ASN:CG	2.37	0.46
1:C:27:SER:HB2	1:C:39:TRP:CE2	2.51	0.45
1:D:210:THR:HB	1:D:212:ARG:HH12	1.80	0.45
1:C:24:ALA:HA	1:C:337:TRP:CG	2.51	0.45
1:B:133:LEU:HD13	1:B:143:SER:HB3	1.98	0.45
1:B:291:LEU:HD11	1:B:330:VAL:HB	1.98	0.45
1:B:317:CYS:HB3	2:B:564:HOH:O	2.14	0.45
1:A:64:LEU:HD22	1:A:69:ILE:HD11	1.98	0.45
1:A:16:LYS:HD2	1:A:18:LEU:CD2	2.47	0.45
1:D:258:HIS:HE1	1:D:268:HIS:O	2.00	0.45
1:C:287:HIS:HA	1:C:301:GLY:HA3	1.99	0.45
1:D:173:ARG:O	1:D:189:GLU:HG2	2.17	0.45
1:B:84:GLN:N	2:B:442:HOH:O	2.50	0.45
1:A:46:GLN:OE1	1:A:46:GLN:N	2.33	0.44
1:A:104:ASN:O	1:A:161:LEU:HD22	2.17	0.44
1:A:203:ASN:HB3	1:A:234:ARG:O	2.17	0.44
1:C:167:GLN:HB3	2:C:444:HOH:O	2.17	0.44
1:D:16:LYS:HG2	1:D:347:ASN:ND2	2.31	0.44
1:A:365:SER:OG	1:A:366:VAL:O	2.20	0.44
1:B:114:ILE:HA	2:B:456:HOH:O	2.16	0.44
1:C:92:TRP:CE3	1:C:111:PRO:HG3	2.53	0.44
1:C:135:VAL:HG22	1:C:141:VAL:HG22	2.00	0.44
1:D:227:SER:HB2	1:D:241:TYR:CD2	2.52	0.44
1:A:50:GLY:HA2	1:A:110:THR:HG22	2.00	0.44
1:C:130:SER:OG	1:C:146:ARG:HB3	2.16	0.44
1:D:50:GLY:HA2	1:D:110:THR:HG23	1.99	0.44
1:B:133:LEU:HD21	1:B:184:THR:HG21	1.99	0.44
1:B:174:ILE:HA	1:B:188:THR:HA	1.99	0.44
1:B:304:LYS:HE2	2:B:537:HOH:O	2.18	0.44
1:C:152:LEU:HB3	1:C:154:LEU:HD22	1.99	0.44
1:A:87:MET:CE	1:A:121:ARG:HB3	2.48	0.44
1:B:209:ARG:NH2	2:B:448:HOH:O	2.49	0.44
1:C:285:TRP:HB2	1:C:337:TRP:CA	2.43	0.44
1:D:251:SER:HB2	1:D:256:LEU:HG	1.99	0.44
1:B:372:LYS:NZ	2:B:447:HOH:O	2.48	0.44
1:C:100:LEU:HB2	2:C:497:HOH:O	2.17	0.44
1:C:209:ARG:NH1	1:C:265:LEU:HD11	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:HD13	1:A:36:VAL:HG22	2.00	0.44
1:B:352:TRP:HB3	1:B:371:PRO:HA	2.00	0.44
1:C:25:SER:HB2	1:C:41:ARG:HB3	1.99	0.44
1:C:183:HIS:CG	1:C:203:ASN:HD22	2.36	0.44
1:C:133:LEU:HD13	1:C:143:SER:CB	2.47	0.43
1:D:69:ILE:HD13	1:D:83:SER:HB2	1.99	0.43
1:B:31:LEU:HB2	1:B:35:ILE:HB	2.00	0.43
1:A:131:HIS:CD2	1:A:151:GLN:HB2	2.53	0.43
1:A:314:LEU:HD12	1:A:314:LEU:HA	1.88	0.43
1:C:367:ASP:O	1:C:368:ARG:HD3	2.17	0.43
1:C:287:HIS:HB2	1:C:300:TRP:O	2.18	0.43
1:A:358:GLY:O	1:A:360:LEU:N	2.52	0.43
1:D:207:GLY:HA2	1:D:265:LEU:HB2	1.99	0.43
1:B:142:GLN:HG2	1:B:165:LYS:HA	2.00	0.43
1:D:201:TYR:CD2	1:D:250:TRP:CG	3.06	0.43
1:D:201:TYR:HD2	1:D:250:TRP:HB2	1.84	0.43
1:A:175:LYS:HB3	1:A:189:GLU:HG2	2.00	0.43
1:D:20:ILE:HD12	1:D:341:LEU:HB2	2.01	0.43
1:A:135:VAL:HG13	1:A:141:VAL:HG22	1.99	0.42
1:B:55:ARG:HA	1:B:55:ARG:HD3	1.79	0.42
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.84	0.42
1:A:30:LEU:O	1:A:31:LEU:HD23	2.19	0.42
1:A:88:GLU:HG3	1:A:118:HIS:HB2	2.01	0.42
1:A:348:ASN:HD21	1:A:380:ASP:H	1.67	0.42
1:B:362:ILE:H	1:B:362:ILE:HG13	1.70	0.42
1:C:24:ALA:HA	1:C:337:TRP:CD1	2.55	0.42
1:A:298:TYR:HA	1:A:321:GLN:HA	2.01	0.42
1:B:250:TRP:CZ2	1:B:252:LYS:HD2	2.53	0.42
1:B:251:SER:HB2	1:B:256:LEU:CD1	2.49	0.42
1:D:47:LEU:HD12	2:D:462:HOH:O	2.19	0.42
1:D:321:GLN:O	2:D:413:HOH:O	2.21	0.42
1:B:198:TRP:CH2	1:B:200:ARG:HB2	2.55	0.42
1:D:143:SER:OG	1:D:154:LEU:HD21	2.20	0.42
1:A:180:GLY:HA3	1:A:183:HIS:CE1	2.54	0.42
1:B:327:ASP:HA	2:B:545:HOH:O	2.19	0.42
1:D:239:VAL:HG22	1:D:245:LEU:HD13	2.01	0.42
1:A:191:GLY:HA3	1:A:225:LYS:HB3	2.02	0.42
1:B:147:ASN:O	1:B:157:THR:HA	2.19	0.42
1:D:251:SER:HB2	1:D:256:LEU:CG	2.50	0.42
1:D:306:GLY:HA3	1:D:369:ASN:HB3	2.01	0.42
1:C:278:ILE:HD13	1:C:278:ILE:HA	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ARG:HG2	1:A:55:ARG:HH11	1.85	0.42
1:C:133:LEU:HD13	1:C:143:SER:HB2	2.02	0.42
1:C:224:GLU:OE1	1:C:242:SER:HB3	2.20	0.42
1:B:219:THR:N	2:B:440:HOH:O	2.42	0.41
1:D:75:GLY:HA3	1:D:78:HIS:CE1	2.55	0.41
1:D:227:SER:HB2	1:D:241:TYR:HE2	1.84	0.41
1:A:117:LEU:HA	1:A:120:ILE:HD12	2.02	0.41
1:A:162:VAL:HG22	1:A:163:PRO:HD2	2.02	0.41
1:B:221:THR:HG22	1:B:267:PRO:HG2	2.02	0.41
1:C:75:GLY:HA3	1:C:78:HIS:CE1	2.55	0.41
1:D:348:ASN:OD1	1:D:378:SER:HB3	2.21	0.41
1:C:124:GLN:HG2	1:C:125:ILE:N	2.36	0.41
1:B:28:VAL:HG21	1:B:79:THR:HG23	2.03	0.41
1:C:153:GLY:O	2:C:406:HOH:O	2.22	0.41
1:C:358:GLY:HA2	2:C:528:HOH:O	2.19	0.41
1:A:234:ARG:N	2:A:432:HOH:O	2.54	0.41
1:A:20:ILE:HG22	1:A:29:ALA:HB2	2.02	0.41
1:A:104:ASN:OD1	1:A:105:SER:N	2.53	0.41
1:A:200:ARG:O	1:A:209:ARG:HD3	2.21	0.41
1:A:285:TRP:HB2	1:A:337:TRP:HA	2.01	0.41
1:B:158:GLU:HA	2:B:544:HOH:O	2.21	0.41
1:A:251:SER:HB2	1:A:256:LEU:HG	2.02	0.41
1:B:196:TRP:N	2:B:410:HOH:O	2.41	0.41
1:C:209:ARG:NH2	1:D:262:GLU:HB3	2.36	0.41
1:D:294:ASP:HB3	2:D:551:HOH:O	2.21	0.41
1:A:303:ASN:OD1	1:A:307:GLN:N	2.54	0.41
1:D:147:ASN:CG	1:D:152:LEU:HB2	2.42	0.41
1:B:55:ARG:HA	1:B:56:PRO:HD3	1.90	0.41
1:C:34:ASP:HB3	2:C:435:HOH:O	2.21	0.41
1:C:328:GLN:H	1:C:328:GLN:HG2	1.66	0.41
1:B:115:LYS:HD3	2:B:627:HOH:O	2.20	0.40
1:C:117:LEU:HD23	1:C:117:LEU:HA	1.84	0.40
1:C:67:HIS:HB2	2:C:405:HOH:O	2.21	0.40
1:A:355:GLY:HA3	1:A:360:LEU:HD12	2.02	0.40
1:B:204:LEU:HD12	2:B:418:HOH:O	2.20	0.40
1:C:144:TRP:CE3	1:C:163:PRO:HG3	2.56	0.40
1:C:154:LEU:HD12	1:C:154:LEU:HA	1.77	0.40
1:D:54:ASP:OD1	2:D:414:HOH:O	2.22	0.40
1:D:170:GLU:OE1	1:D:170:GLU:HA	2.21	0.40
1:A:45:GLY:N	1:A:46:GLN:OE1	2.54	0.40
1:B:228:MET:HB2	1:B:239:VAL:HB	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:PRO:CG	2:C:645:HOH:O	2.69	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	366/377 (97%)	336 (92%)	23 (6%)	7 (2%)	8 3
1	B	366/377 (97%)	337 (92%)	26 (7%)	3 (1%)	19 13
1	C	366/377 (97%)	343 (94%)	19 (5%)	4 (1%)	14 8
1	D	366/377 (97%)	335 (92%)	29 (8%)	2 (0%)	29 23
All	All	1464/1508 (97%)	1351 (92%)	97 (7%)	16 (1%)	14 8

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	364	GLU
1	B	365	SER
1	C	364	GLU
1	C	365	SER
1	A	105	SER
1	A	366	VAL
1	C	363	GLY
1	D	24	ALA
1	B	15	ARG
1	B	86	GLY
1	C	366	VAL
1	A	357	ASN
1	A	359	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	380	ASP
1	A	365	SER

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	291/300 (97%)	247 (85%)	44 (15%)	3 1
1	B	291/300 (97%)	268 (92%)	23 (8%)	12 8
1	C	291/300 (97%)	266 (91%)	25 (9%)	10 6
1	D	291/300 (97%)	261 (90%)	30 (10%)	7 4
All	All	1164/1200 (97%)	1042 (90%)	122 (10%)	7 4

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	34	ASP
1	A	51	ASP
1	A	55	ARG
1	A	61	LEU
1	A	71	SER
1	A	90	TYR
1	A	105	SER
1	A	108	LEU
1	A	110	THR
1	A	115	LYS
1	A	130	SER
1	A	133	LEU
1	A	135	VAL
1	A	138	GLU
1	A	162	VAL
1	A	167	GLN
1	A	170	GLU
1	A	173	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	175	LYS
1	A	177	VAL
1	A	184	THR
1	A	211	ASP
1	A	217	ARG
1	A	219	THR
1	A	221	THR
1	A	228	MET
1	A	237	ILE
1	A	239	VAL
1	A	251	SER
1	A	270	LEU
1	A	275	ASN
1	A	314	LEU
1	A	318	SER
1	A	323	ARG
1	A	335	CYS
1	A	344	THR
1	A	345	GLU
1	A	346	ARG
1	A	364	GLU
1	A	365	SER
1	A	366	VAL
1	A	368	ARG
1	A	370	PHE
1	B	27	SER
1	B	53	GLU
1	B	57	SER
1	B	59	THR
1	B	61	LEU
1	B	68	GLN
1	B	83	SER
1	B	121	ARG
1	B	133	LEU
1	B	137	MET
1	B	184	THR
1	B	265	LEU
1	B	280	GLN
1	B	281	ILE
1	B	293	SER
1	B	294	ASP
1	B	318	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	326	ASP
1	B	341	LEU
1	B	357	ASN
1	B	362	ILE
1	B	370	PHE
1	B	379	VAL
1	C	16	LYS
1	C	20	ILE
1	C	25	SER
1	C	53	GLU
1	C	87	MET
1	C	100	LEU
1	C	115	LYS
1	C	133	LEU
1	C	137	MET
1	C	152	LEU
1	C	154	LEU
1	C	161	LEU
1	C	162	VAL
1	C	170	GLU
1	C	182	GLU
1	C	229	VAL
1	C	242	SER
1	C	251	SER
1	C	262	GLU
1	C	280	GLN
1	C	317	CYS
1	C	318	SER
1	C	321	GLN
1	C	346	ARG
1	C	354	ARG
1	D	16	LYS
1	D	25	SER
1	D	46	GLN
1	D	53	GLU
1	D	54	ASP
1	D	55	ARG
1	D	57	SER
1	D	62	SER
1	D	85	SER
1	D	124	GLN
1	D	142	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	203	ASN
1	D	214	VAL
1	D	216	GLU
1	D	269	LYS
1	D	270	LEU
1	D	277	PHE
1	D	291	LEU
1	D	294	ASP
1	D	302	TRP
1	D	310	VAL
1	D	320	VAL
1	D	322	VAL
1	D	341	LEU
1	D	359	GLN
1	D	367	ASP
1	D	368	ARG
1	D	370	PHE
1	D	374	ILE
1	D	379	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	ASN
1	B	67	HIS
1	C	203	ASN
1	D	235	HIS
1	D	264	HIS
1	D	268	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 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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.