Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 01:03 AM EDT

PDB ID	:	4U8H
Title	:	Crystal Structure of Mammalian Period-Cryptochrome Complex
Authors	:	Nangle, S.N.; Rosensweig, C.; Koike, N.; Tei, H.; Takahashi, J.S.; Green, C.B.; Zheng, N.
Deposited on	:	2014-08-03
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
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:

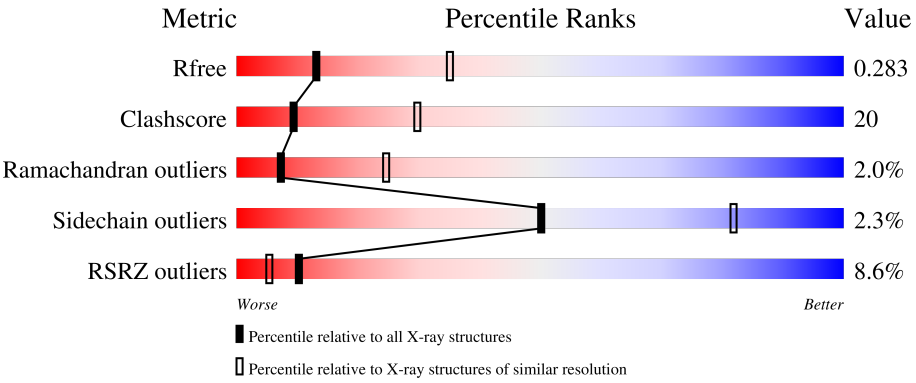
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.80 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))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 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	510	10% 65% 30%
1	C	510	6% 63% 31%
2	B	121	7% 36% 26% 35%
2	D	121	4% 36% 26% 35%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9342 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 Cryptochrome-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3992	2562	708	702	20			
1	C	490	Total	C	N	O	S	0	0	0
			3992	2562	708	702	20			

- Molecule 2 is a protein called Period circadian protein homolog 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	79	Total	C	N	O	S	0	0	0
			654	414	113	122	5			
2	D	79	Total	C	N	O	S	0	0	0
			654	414	113	122	5			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

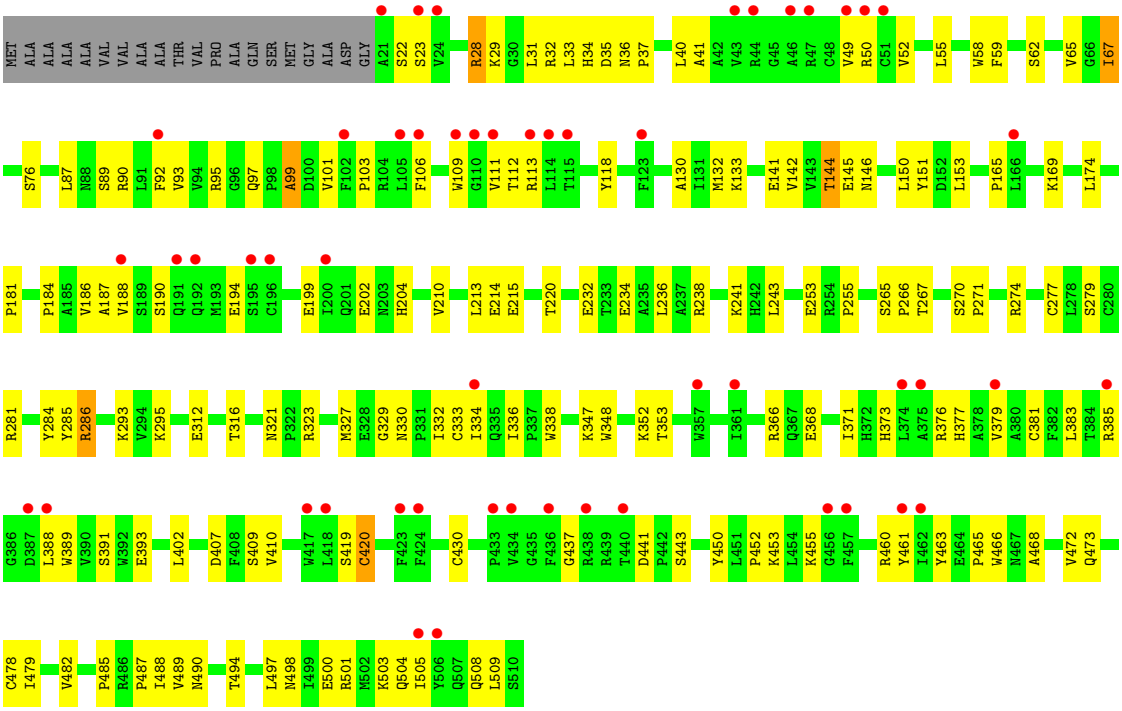
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	C	25	Total	O	0	0
			25	25		
4	B	3	Total	O	0	0
			3	3		
4	D	1	Total	O	0	0
			1	1		

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.

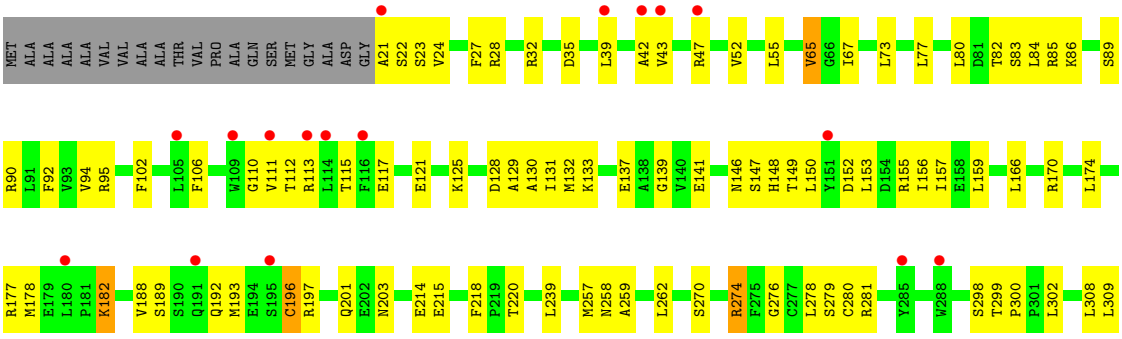
- Molecule 1: Cryptochrome-2

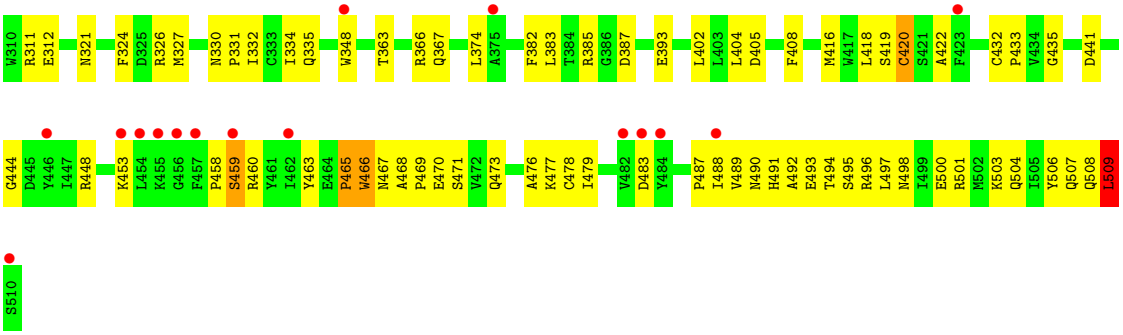
Chain A:



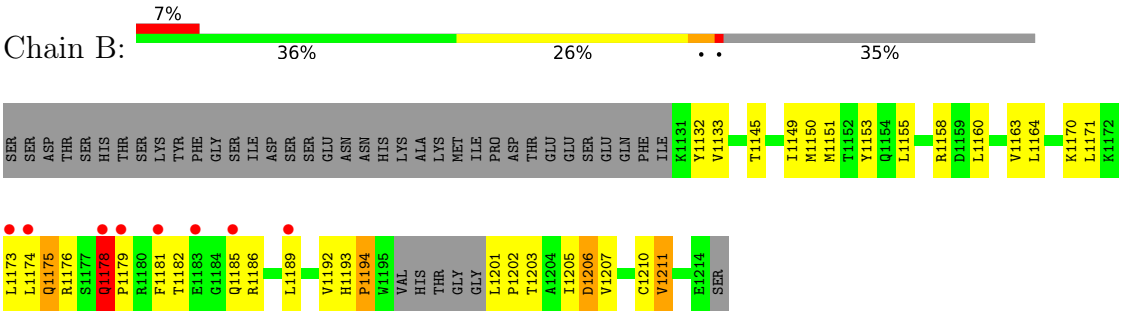
- Molecule 1: Cryptochrome-2

Chain C:

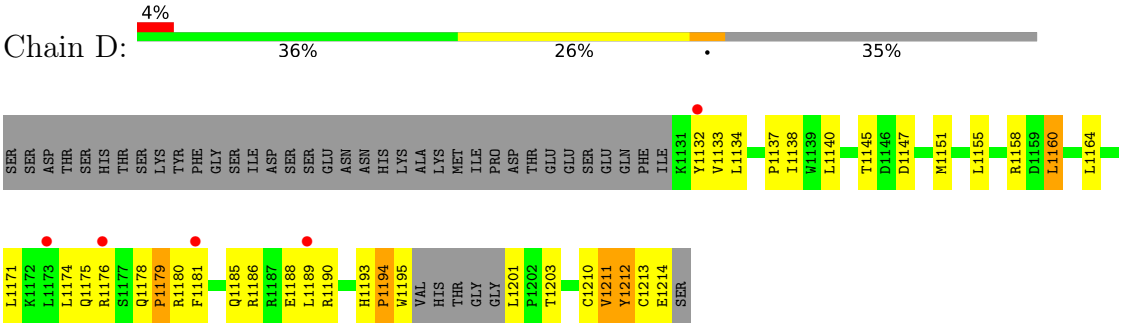




• Molecule 2: Period circadian protein homolog 2



• Molecule 2: Period circadian protein homolog 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	97.67Å 97.67Å 163.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.74 – 2.80 47.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.74-2.80) 95.4 (47.53-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.205 , 0.278 0.214 , 0.283	Depositor DCC
R_{free} test set	1881 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	75.9	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.487 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9342	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.46	0/4109	0.65	0/5576
1	C	0.48	0/4109	0.66	1/5576 (0.0%)
2	B	0.38	0/666	0.67	0/901
2	D	0.38	0/666	0.62	0/901
All	All	0.46	0/9550	0.66	1/12954 (0.0%)

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
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	509	LEU	CA-CB-CG	5.18	127.20	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1178	GLN	Peptide
2	D	1178	GLN	Peptide

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	3992	0	3921	143	1
1	C	3992	0	3920	151	0
2	B	654	0	654	54	0
2	D	654	0	653	51	1
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	19	0	0	1	0
4	B	3	0	0	0	0
4	C	25	0	0	4	0
4	D	1	0	0	0	0
All	All	9342	0	9148	364	1

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 20.

All (364) 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)
2:B:1175:GLN:CG	2:B:1178:GLN:NE2	1.87	1.37
2:B:1175:GLN:CG	2:B:1178:GLN:HE22	1.39	1.30
2:D:1181:PHE:CZ	2:D:1189:LEU:HD12	1.68	1.28
2:D:1181:PHE:CZ	2:D:1189:LEU:CD1	2.21	1.24
1:A:109:TRP:CZ3	1:A:199:GLU:OE1	1.95	1.18
2:B:1175:GLN:HG2	2:B:1178:GLN:NE2	1.45	1.17
1:C:332:ILE:HD13	4:C:615:HOH:O	1.45	1.15
2:B:1175:GLN:CB	2:B:1178:GLN:HE21	1.61	1.13
2:D:1190:ARG:NH1	2:D:1195:TRP:HD1	1.46	1.12
1:A:109:TRP:HZ3	1:A:199:GLU:OE1	1.25	1.10
1:C:259:ALA:HB2	1:C:441:ASP:OD1	1.55	1.06
2:B:1175:GLN:HG2	2:B:1178:GLN:HE22	0.91	1.06
1:C:113:ARG:HB3	1:C:141:GLU:HG2	1.35	1.03
1:A:34:HIS:ND1	1:A:232:GLU:OE2	1.92	1.02
1:C:113:ARG:HB3	1:C:141:GLU:CG	1.90	1.01
1:C:432:CYS:HG	2:D:1212:TYR:HD2	1.02	1.01
1:C:489:VAL:CG1	2:D:1155:LEU:HD12	1.91	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1190:ARG:HH11	2:D:1195:TRP:HD1	1.07	0.99
1:A:488:ILE:CG2	2:B:1155:LEU:HD13	1.91	0.99
1:A:132:MET:SD	1:A:142:VAL:HG11	2.04	0.98
1:A:488:ILE:HG23	2:B:1155:LEU:CD1	1.94	0.97
1:C:159:LEU:O	1:C:159:LEU:HD23	1.63	0.97
2:D:1190:ARG:NH1	2:D:1195:TRP:CD1	2.34	0.94
1:C:28:ARG:NH2	1:C:117:GLU:O	2.02	0.93
2:B:1175:GLN:HB3	2:B:1178:GLN:HE21	1.30	0.92
1:C:489:VAL:HG12	2:D:1155:LEU:HD12	1.49	0.92
2:D:1181:PHE:CZ	2:D:1189:LEU:HD11	2.05	0.92
1:C:113:ARG:HD3	1:C:141:GLU:OE2	1.71	0.91
2:B:1175:GLN:CB	2:B:1178:GLN:NE2	2.25	0.89
2:B:1175:GLN:CD	2:B:1178:GLN:HE22	1.75	0.89
2:D:1181:PHE:HZ	2:D:1189:LEU:HD12	1.17	0.89
1:C:259:ALA:HB2	1:C:441:ASP:CG	1.94	0.87
1:C:432:CYS:SG	2:D:1212:TYR:CD2	2.68	0.85
1:C:385:ARG:NH1	1:C:418:LEU:O	2.09	0.85
1:C:82:THR:HG22	1:C:85:ARG:NH1	1.90	0.84
1:C:113:ARG:CB	1:C:141:GLU:CG	2.55	0.84
2:B:1175:GLN:CD	2:B:1178:GLN:NE2	2.30	0.84
1:A:488:ILE:HG22	2:B:1155:LEU:HD13	1.60	0.84
1:A:50:ARG:HD3	1:A:92:PHE:HE2	1.41	0.83
1:C:432:CYS:SG	2:D:1212:TYR:HD2	2.02	0.82
1:A:50:ARG:HH21	1:A:199:GLU:HB2	1.44	0.82
1:A:150:LEU:N	1:A:312:GLU:OE2	2.11	0.81
1:C:84:LEU:HD22	1:C:90:ARG:C	1.98	0.81
1:A:488:ILE:HG23	2:B:1155:LEU:HD13	1.54	0.81
1:C:441:ASP:O	1:C:463:TYR:OH	1.96	0.81
1:C:189:SER:OG	1:C:192:GLN:HB2	1.81	0.81
1:C:113:ARG:HB2	1:C:141:GLU:HG3	1.63	0.80
1:C:113:ARG:CB	1:C:141:GLU:HG3	2.12	0.80
1:A:87:LEU:HA	1:A:194:GLU:HG2	1.62	0.80
1:C:150:LEU:N	1:C:312:GLU:OE2	2.14	0.79
2:D:1181:PHE:CE1	2:D:1186:ARG:HG3	2.18	0.79
2:D:1181:PHE:HZ	2:D:1189:LEU:CD1	1.78	0.78
1:A:489:VAL:CG1	2:B:1155:LEU:HD22	2.13	0.78
1:C:170:ARG:NH1	2:D:1188:GLU:OE2	2.17	0.78
1:A:488:ILE:CG2	2:B:1155:LEU:CD1	2.55	0.77
1:C:23:SER:HA	1:C:111:VAL:HG13	1.67	0.76
1:A:494:THR:O	1:A:498:ASN:ND2	2.19	0.75
1:C:214:GLU:OE2	1:C:220:THR:OG1	2.02	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1181:PHE:CE1	2:D:1189:LEU:HD12	2.21	0.75
1:A:488:ILE:HG22	1:A:489:VAL:HG13	1.68	0.75
1:C:489:VAL:HG11	2:D:1155:LEU:HD12	1.69	0.75
1:A:32:ARG:HA	1:A:232:GLU:OE1	1.87	0.74
1:A:274:ARG:NE	1:A:407:ASP:OD2	2.21	0.74
1:C:117:GLU:OE1	1:C:147:SER:OG	2.04	0.74
1:C:39:LEU:HD23	1:C:188:VAL:HG21	1.70	0.73
1:A:130:ALA:HA	1:A:133:LYS:HE2	1.72	0.72
1:C:270:SER:OG	1:C:405:ASP:OD2	2.08	0.72
1:A:33:LEU:N	1:A:232:GLU:OE1	2.23	0.72
1:A:500:GLU:OE1	1:A:503:LYS:NZ	2.14	0.71
1:C:494:THR:O	1:C:498:ASN:ND2	2.23	0.71
1:A:29:LYS:HG2	1:A:274:ARG:HH12	1.56	0.70
2:D:1181:PHE:HE1	2:D:1186:ARG:HA	1.55	0.70
1:A:132:MET:CE	1:A:142:VAL:HG11	2.21	0.69
1:A:497:LEU:HD21	2:B:1163:VAL:HG21	1.72	0.69
1:A:190:SER:HA	1:A:194:GLU:HG3	1.73	0.69
1:C:106:PHE:O	1:C:110:GLY:N	2.24	0.68
1:A:113:ARG:HB3	1:A:141:GLU:HB3	1.76	0.68
1:A:32:ARG:HB2	1:A:232:GLU:CD	2.14	0.68
1:C:193:MET:HA	1:C:196:CYS:HB3	1.75	0.68
1:C:448:ARG:HH12	1:C:459:SER:HB3	1.57	0.68
1:A:37:PRO:HB2	1:A:145:GLU:HG3	1.76	0.68
1:C:113:ARG:CB	1:C:141:GLU:HG2	2.16	0.67
1:C:448:ARG:HH22	1:C:459:SER:N	1.93	0.67
1:C:84:LEU:CD2	1:C:90:ARG:CA	2.73	0.66
1:A:29:LYS:HE2	1:A:274:ARG:HH22	1.60	0.66
1:C:82:THR:HG22	1:C:85:ARG:CZ	2.24	0.66
1:C:84:LEU:CD2	1:C:90:ARG:C	2.64	0.66
2:D:1174:LEU:O	2:D:1176:ARG:N	2.28	0.66
1:A:109:TRP:CH2	1:A:199:GLU:OE1	2.50	0.65
2:D:1138:ILE:HD12	2:D:1138:ILE:H	1.62	0.65
1:A:270:SER:OG	1:A:271:PRO:HD3	1.96	0.65
1:C:492:ALA:O	2:D:1214:GLU:OE2	2.15	0.65
2:D:1194:PRO:HG2	2:D:1203:THR:HG21	1.78	0.65
1:C:504:GLN:NE2	2:D:1164:LEU:O	2.30	0.64
1:C:490:ASN:ND2	1:C:493:GLU:OE1	2.31	0.64
1:A:330:ASN:HD22	1:A:333:CYS:HB2	1.63	0.64
1:C:476:ALA:O	1:C:478:CYS:N	2.30	0.64
1:A:22:SER:O	1:A:112:THR:N	2.30	0.64
1:C:65:VAL:HG13	1:C:402:LEU:HD21	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HD12	1:A:312:GLU:HG3	1.78	0.64
1:A:23:SER:H	1:A:49:VAL:HG12	1.62	0.63
1:C:435:GLY:HA3	2:D:1212:TYR:CG	2.34	0.63
1:C:159:LEU:HD11	1:C:177:ARG:HH11	1.62	0.63
1:C:117:GLU:CD	1:C:147:SER:OG	2.36	0.63
2:B:1174:LEU:O	2:B:1176:ARG:N	2.25	0.63
1:A:488:ILE:HG23	2:B:1155:LEU:HD11	1.81	0.63
1:A:55:LEU:O	1:A:95:ARG:HA	2.00	0.62
1:C:102:PHE:CD2	1:C:131:ILE:HD11	2.35	0.62
1:A:214:GLU:OE2	1:A:220:THR:OG1	2.15	0.62
1:A:385:ARG:CZ	1:A:430:CYS:SG	2.88	0.62
1:A:29:LYS:CE	1:A:274:ARG:HH22	2.12	0.62
1:C:55:LEU:O	1:C:95:ARG:HA	2.00	0.61
1:A:32:ARG:CA	1:A:232:GLU:OE1	2.48	0.61
1:C:458:PRO:O	1:C:460:ARG:N	2.25	0.61
1:C:506:TYR:HA	1:C:509:LEU:HG	1.82	0.61
2:D:1210:CYS:O	2:D:1213:CYS:O	2.19	0.60
1:C:465:PRO:O	1:C:467:ASN:N	2.31	0.60
1:C:42:ALA:HB2	1:C:115:THR:OG1	2.01	0.60
1:A:67:ILE:HD12	1:A:213:LEU:HD22	1.83	0.59
1:C:146:ASN:O	1:C:281:ARG:NH2	2.35	0.59
1:C:448:ARG:HH22	1:C:459:SER:H	1.50	0.59
1:A:274:ARG:HE	1:A:407:ASP:CG	2.05	0.58
1:A:489:VAL:HG12	2:B:1155:LEU:HB2	1.86	0.58
1:C:382:PHE:HD1	1:C:433:PRO:HG3	1.68	0.58
1:A:391:SER:OG	1:A:393:GLU:HG2	2.04	0.58
1:C:497:LEU:O	1:C:501:ARG:HG3	2.03	0.58
1:C:148:HIS:O	1:C:311:ARG:NH2	2.37	0.58
1:C:453:LYS:NZ	1:C:483:ASP:OD1	2.28	0.58
1:A:253:GLU:O	1:A:255:PRO:HD3	2.04	0.57
2:D:1211:VAL:O	2:D:1213:CYS:N	2.38	0.57
2:B:1205:ILE:O	2:B:1207:VAL:N	2.36	0.57
1:A:29:LYS:NZ	1:A:274:ARG:HH22	2.02	0.57
1:C:84:LEU:HD22	1:C:90:ARG:CA	2.33	0.57
1:C:334:ILE:HD13	2:D:1179:PRO:HG2	1.87	0.57
1:C:488:ILE:HG22	1:C:489:VAL:HG13	1.86	0.57
1:A:312:GLU:HG2	4:A:2103:HOH:O	2.05	0.57
1:A:338:TRP:HA	1:A:389:TRP:CD1	2.40	0.57
1:A:371:ILE:HG13	1:A:376:ARG:HG3	1.86	0.56
1:C:52:VAL:HG22	1:C:92:PHE:HB2	1.86	0.56
1:C:159:LEU:O	1:C:159:LEU:CD2	2.47	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ARG:HE	1:A:407:ASP:CB	2.18	0.56
1:A:505:ILE:O	1:A:509:LEU:HB2	2.05	0.56
1:C:156:ILE:HG12	1:C:178:MET:SD	2.45	0.56
2:B:1145:THR:HA	2:B:1150:MET:HE3	1.87	0.56
1:A:190:SER:O	1:A:194:GLU:N	2.31	0.56
1:A:489:VAL:HG12	2:B:1155:LEU:HD22	1.85	0.56
1:C:95:ARG:NH2	1:C:215:GLU:OE2	2.30	0.56
1:A:241:LYS:HB3	1:A:267:THR:HG22	1.89	0.55
1:A:500:GLU:HG3	2:B:1160:LEU:HD11	1.87	0.55
1:A:452:PRO:HB3	1:A:455:LYS:HE3	1.88	0.55
2:D:1181:PHE:HE1	2:D:1186:ARG:HG3	1.68	0.55
1:A:232:GLU:HG3	1:A:277:CYS:O	2.07	0.55
1:C:84:LEU:CD2	1:C:90:ARG:N	2.70	0.55
1:A:132:MET:CE	1:A:142:VAL:CG1	2.83	0.55
1:A:169:LYS:HD2	2:B:1192:VAL:HG22	1.87	0.55
1:C:146:ASN:HD21	1:C:152:ASP:HA	1.72	0.55
1:C:153:LEU:HD12	1:C:153:LEU:H	1.71	0.55
1:C:332:ILE:HG23	4:C:604:HOH:O	2.05	0.55
1:C:468:ALA:HB3	1:C:473:GLN:HE21	1.71	0.55
1:A:65:VAL:CG1	1:A:402:LEU:HD21	2.38	0.54
2:D:1190:ARG:HH12	2:D:1195:TRP:HD1	1.49	0.54
1:C:83:SER:HA	1:C:86:LYS:HD3	1.89	0.54
1:C:24:VAL:HG23	1:C:111:VAL:HG21	1.88	0.54
1:C:363:THR:O	1:C:367:GLN:HG3	2.06	0.54
1:C:21:ALA:N	1:C:47:ARG:H	2.05	0.53
1:C:201:GLN:OE1	1:C:203:ASN:ND2	2.38	0.53
1:A:132:MET:HE1	1:A:142:VAL:CG1	2.39	0.53
1:C:432:CYS:SG	1:C:435:GLY:N	2.78	0.53
1:A:321:ASN:ND2	1:A:330:ASN:OD1	2.32	0.53
1:A:461:TYR:HE2	1:A:472:VAL:HG21	1.74	0.53
2:D:1211:VAL:C	2:D:1213:CYS:N	2.62	0.52
2:D:1176:ARG:O	2:D:1180:ARG:NH2	2.43	0.52
1:A:40:LEU:HD21	1:A:187:ALA:HA	1.92	0.52
1:A:295:LYS:HD2	2:D:1133:VAL:HG21	1.92	0.52
1:A:274:ARG:HE	1:A:407:ASP:HB3	1.75	0.52
1:C:189:SER:N	1:C:192:GLN:OE1	2.42	0.52
1:C:21:ALA:HB1	1:C:112:THR:HG21	1.92	0.52
1:A:32:ARG:HB2	1:A:232:GLU:OE2	2.10	0.51
1:C:321:ASN:ND2	1:C:330:ASN:OD1	2.29	0.51
2:D:1211:VAL:C	2:D:1213:CYS:H	2.12	0.51
1:A:437:GLY:HA3	1:A:463:TYR:HE2	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:SER:OG	1:C:192:GLN:CB	2.54	0.51
1:C:444:GLY:O	1:C:448:ARG:HG3	2.09	0.51
2:D:1181:PHE:CE1	2:D:1186:ARG:HA	2.41	0.51
1:A:65:VAL:HG22	1:A:366:ARG:CZ	2.40	0.51
1:A:508:GLN:O	2:B:1175:GLN:NE2	2.39	0.51
1:C:280:CYS:HB2	1:C:308:LEU:HD22	1.92	0.51
1:C:196:CYS:C	1:C:197:ARG:HG2	2.31	0.51
1:C:504:GLN:O	1:C:508:GLN:HB2	2.10	0.51
1:A:441:ASP:OD1	1:A:443:SER:OG	2.24	0.50
1:A:265:SER:HG	1:A:267:THR:HG1	1.60	0.50
1:C:130:ALA:HA	1:C:133:LYS:HD3	1.92	0.50
1:C:153:LEU:O	1:C:157:ILE:HG13	2.11	0.50
2:D:1147:ASP:O	2:D:1151:MET:HG2	2.11	0.50
1:A:385:ARG:NH1	1:A:430:CYS:SG	2.85	0.50
1:C:432:CYS:HB2	2:D:1212:TYR:HB3	1.94	0.50
1:A:89:SER:OG	1:A:90:ARG:N	2.45	0.50
1:A:334:ILE:HG22	1:A:336:ILE:HG13	1.94	0.50
2:B:1210:CYS:SG	2:B:1211:VAL:N	2.82	0.50
2:D:1189:LEU:O	2:D:1193:HIS:N	2.36	0.49
1:C:159:LEU:CD2	1:C:174:LEU:HD22	2.43	0.49
1:C:496:ARG:HB3	2:D:1214:GLU:OE2	2.13	0.49
1:A:468:ALA:O	1:A:473:GLN:NE2	2.46	0.49
1:C:125:LYS:O	1:C:129:ALA:N	2.44	0.49
2:B:1193:HIS:ND1	2:B:1201:LEU:HD21	2.28	0.49
1:A:504:GLN:NE2	2:B:1164:LEU:HG	2.28	0.49
1:C:52:VAL:HG13	1:C:94:VAL:HG23	1.95	0.49
1:A:441:ASP:O	1:A:463:TYR:OH	2.18	0.49
2:D:1160:LEU:O	2:D:1164:LEU:HB2	2.13	0.49
2:D:1181:PHE:CE2	2:D:1189:LEU:HD11	2.48	0.49
1:A:327:MET:HE1	1:A:338:TRP:HE1	1.78	0.49
1:C:149:THR:HB	1:C:312:GLU:OE2	2.11	0.49
2:B:1175:GLN:CA	2:B:1178:GLN:HE21	2.22	0.49
2:B:1194:PRO:HB2	2:B:1201:LEU:N	2.27	0.49
1:C:302:LEU:HD22	1:C:309:LEU:HD11	1.95	0.49
1:C:348:TRP:CD2	1:C:383:LEU:HD13	2.48	0.48
1:C:332:ILE:CG2	4:C:604:HOH:O	2.60	0.48
1:C:239:LEU:HD22	1:C:278:LEU:HD11	1.95	0.48
1:C:159:LEU:HD22	1:C:174:LEU:HD22	1.95	0.48
2:D:1181:PHE:HB2	2:D:1185:GLN:CD	2.34	0.48
1:A:37:PRO:HB2	1:A:145:GLU:CG	2.42	0.48
1:A:181:PRO:O	1:A:285:TYR:OH	2.15	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:LYS:HE2	1:A:488:ILE:HG12	1.95	0.48
2:B:1181:PHE:HB2	2:B:1186:ARG:HG3	1.96	0.48
1:C:52:VAL:HG13	1:C:92:PHE:O	2.14	0.47
1:C:274:ARG:HD2	1:C:404:LEU:O	2.14	0.47
1:C:332:ILE:O	1:C:332:ILE:HG22	2.13	0.47
1:C:32:ARG:HD3	1:C:276:GLY:O	2.14	0.47
1:C:84:LEU:HD23	1:C:84:LEU:O	2.13	0.47
1:A:151:TYR:CE1	1:A:181:PRO:HD3	2.49	0.47
1:C:65:VAL:HG22	1:C:366:ARG:NE	2.29	0.47
1:A:202:GLU:C	1:A:204:HIS:H	2.17	0.47
1:A:368:GLU:OE2	1:A:450:TYR:OH	2.28	0.47
2:B:1132:TYR:CD1	2:B:1133:VAL:N	2.83	0.47
1:C:419:SER:O	1:C:420:CYS:HB2	2.15	0.47
2:B:1189:LEU:O	2:B:1193:HIS:N	2.42	0.47
1:A:327:MET:HE1	1:A:338:TRP:NE1	2.30	0.47
1:C:159:LEU:HD11	1:C:177:ARG:NH1	2.30	0.47
1:C:479:ILE:H	1:C:483:ASP:HB3	1.79	0.47
2:B:1160:LEU:O	2:B:1164:LEU:HB2	2.15	0.47
1:A:35:ASP:OD2	1:A:279:SER:OG	2.24	0.47
1:C:150:LEU:HD12	1:C:312:GLU:HG3	1.96	0.47
1:A:29:LYS:HG2	1:A:274:ARG:NH1	2.27	0.46
1:A:274:ARG:NH1	1:A:274:ARG:O	2.34	0.46
1:C:469:PRO:C	1:C:471:SER:H	2.19	0.46
1:A:31:LEU:HD13	1:A:76:SER:HB3	1.97	0.46
1:A:373:HIS:HA	1:A:376:ARG:HD2	1.96	0.46
1:A:437:GLY:HA3	1:A:463:TYR:CE2	2.51	0.46
1:A:243:LEU:HD12	1:A:286:ARG:HH21	1.80	0.46
1:C:27:PHE:C	1:C:28:ARG:HG3	2.36	0.46
2:B:1175:GLN:HB3	2:B:1178:GLN:NE2	2.09	0.46
1:A:461:TYR:CE2	1:A:472:VAL:HG21	2.50	0.46
1:A:485:PRO:HA	2:B:1151:MET:O	2.16	0.46
1:A:353:THR:HA	1:A:488:ILE:HG13	1.98	0.45
1:C:332:ILE:CG2	1:C:332:ILE:O	2.64	0.45
1:C:416:MET:HB3	1:C:422:ALA:HB2	1.98	0.45
2:B:1201:LEU:HD23	2:B:1201:LEU:HA	1.44	0.45
2:D:1193:HIS:ND1	2:D:1201:LEU:HD21	2.31	0.45
1:C:259:ALA:O	1:C:262:LEU:HB2	2.17	0.45
2:B:1170:LYS:O	2:B:1173:LEU:HB2	2.17	0.45
1:C:166:LEU:HA	4:C:615:HOH:O	2.17	0.45
1:A:327:MET:HE2	1:A:334:ILE:O	2.17	0.45
1:C:155:ARG:HB3	1:C:178:MET:HE3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:PRO:HD2	1:C:491:HIS:CE1	2.50	0.45
1:A:234:GLU:O	1:A:238:ARG:HG3	2.17	0.45
1:C:35:ASP:OD2	1:C:279:SER:OG	2.31	0.45
1:C:463:TYR:C	1:C:465:PRO:HD3	2.37	0.45
1:C:331:PRO:O	2:D:1179:PRO:HB3	2.17	0.45
1:A:489:VAL:HG11	2:B:1155:LEU:HD22	1.97	0.45
1:C:67:ILE:H	1:C:67:ILE:HG13	1.37	0.45
1:C:496:ARG:O	1:C:500:GLU:HG2	2.17	0.45
1:A:58:TRP:HB3	1:A:59:PHE:CE2	2.52	0.45
1:A:348:TRP:CG	1:A:383:LEU:HD13	2.52	0.45
1:A:479:ILE:O	1:A:482:VAL:HG22	2.17	0.44
1:A:34:HIS:CE1	1:A:236:LEU:HD21	2.52	0.44
1:A:50:ARG:HD3	1:A:92:PHE:CE2	2.33	0.44
1:A:95:ARG:NH2	1:A:215:GLU:OE2	2.49	0.44
1:C:155:ARG:HD2	1:C:178:MET:CE	2.47	0.44
1:A:36:ASN:H	1:A:187:ALA:CB	2.31	0.44
1:A:419:SER:O	1:A:420:CYS:HB2	2.17	0.44
2:B:1132:TYR:HD1	2:B:1133:VAL:H	1.65	0.44
2:D:1140:LEU:HD23	2:D:1140:LEU:HA	1.77	0.44
1:A:118:TYR:HB3	1:A:146:ASN:HA	1.99	0.44
1:A:153:LEU:HD23	1:A:316:THR:OG1	2.18	0.44
1:A:352:LYS:HD3	2:B:1150:MET:HB3	2.00	0.44
1:A:388:LEU:HD22	2:B:1155:LEU:HD21	1.99	0.44
2:D:1137:PRO:HD2	2:D:1140:LEU:HD12	2.00	0.44
2:D:1171:LEU:HA	2:D:1174:LEU:HD12	2.00	0.43
1:A:106:PHE:HA	1:A:111:VAL:HG22	2.00	0.43
1:A:323:ARG:HH11	1:A:329:GLY:HA3	1.82	0.43
1:A:488:ILE:CG2	2:B:1155:LEU:HD11	2.42	0.43
1:C:258:ASN:OD1	1:C:258:ASN:N	2.51	0.43
2:B:1149:ILE:HA	2:B:1153:TYR:HB2	2.00	0.43
1:A:41:ALA:O	1:A:113:ARG:NH2	2.49	0.43
1:C:80:LEU:HD23	1:C:80:LEU:HA	1.80	0.43
2:B:1175:GLN:OE1	2:B:1178:GLN:NE2	2.52	0.43
1:A:453:LYS:O	1:A:478:CYS:SG	2.69	0.43
2:B:1202:PRO:O	2:B:1206:ASP:N	2.48	0.43
1:A:132:MET:HE3	1:A:142:VAL:HB	1.99	0.43
1:A:274:ARG:HD2	1:A:274:ARG:HA	1.45	0.43
1:A:50:ARG:NH2	1:A:199:GLU:HB2	2.22	0.43
1:A:184:PRO:HD3	1:A:285:TYR:HD2	1.84	0.43
1:C:43:VAL:HG21	1:C:193:MET:HG3	2.01	0.43
1:A:103:PRO:O	1:A:106:PHE:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1201:LEU:HA	2:D:1201:LEU:HD23	1.59	0.43
1:A:409:SER:OG	1:A:410:VAL:N	2.52	0.42
1:C:491:HIS:O	1:C:495:SER:N	2.47	0.42
1:A:489:VAL:HB	1:A:494:THR:HG21	2.01	0.42
1:C:95:ARG:HH21	1:C:215:GLU:CD	2.21	0.42
1:C:159:LEU:CD2	1:C:174:LEU:CD2	2.96	0.42
1:A:465:PRO:HD2	1:A:466:TRP:CZ3	2.54	0.42
1:C:121:GLU:OE2	1:C:408:PHE:HB3	2.19	0.42
1:C:128:ASP:O	1:C:132:MET:HG3	2.18	0.42
1:C:490:ASN:O	1:C:491:HIS:HB3	2.19	0.42
2:B:1175:GLN:CA	2:B:1178:GLN:NE2	2.82	0.42
1:A:497:LEU:HD23	1:A:501:ARG:HD2	2.00	0.42
2:B:1181:PHE:HB3	2:B:1185:GLN:HB2	2.01	0.42
1:A:93:VAL:HG21	1:A:210:VAL:HA	2.02	0.42
1:A:97:GLN:O	1:A:99:ALA:N	2.53	0.42
2:D:1132:TYR:CD1	2:D:1133:VAL:N	2.88	0.42
1:C:67:ILE:HG12	1:C:218:PHE:CD1	2.55	0.42
1:C:137:GLU:C	1:C:139:GLY:H	2.23	0.42
1:C:155:ARG:HD2	1:C:178:MET:HE2	2.00	0.42
2:B:1193:HIS:HB3	2:B:1201:LEU:HD21	2.02	0.42
1:A:97:GLN:O	1:A:101:VAL:HG22	2.20	0.41
1:C:503:LYS:O	1:C:507:GLN:N	2.38	0.41
2:B:1193:HIS:HA	2:B:1194:PRO:HD2	1.76	0.41
1:A:286:ARG:HE	1:A:286:ARG:HB3	1.49	0.41
1:C:478:CYS:HA	1:C:483:ASP:OD2	2.20	0.41
2:B:1158:ARG:HD3	2:B:1163:VAL:HG11	2.02	0.41
1:C:299:THR:HA	1:C:300:PRO:HD2	1.91	0.41
2:D:1181:PHE:CE1	2:D:1189:LEU:CD1	2.89	0.41
1:A:165:PRO:HG3	1:A:174:LEU:CD1	2.51	0.41
1:C:24:VAL:CG2	1:C:111:VAL:HG21	2.50	0.41
1:C:84:LEU:CD2	1:C:90:ARG:O	2.69	0.41
1:C:257:MET:HG3	1:C:374:LEU:HD12	2.01	0.41
1:C:327:MET:HG2	1:C:335:GLN:OE1	2.21	0.41
1:A:281:ARG:O	1:A:284:TYR:HB3	2.20	0.41
1:A:509:LEU:HD12	2:B:1178:GLN:OE1	2.21	0.41
1:C:22:SER:O	1:C:111:VAL:HG13	2.20	0.41
1:C:84:LEU:HD23	1:C:89:SER:C	2.41	0.41
1:C:182:LYS:O	1:C:281:ARG:HD3	2.20	0.41
1:C:466:TRP:CE3	1:C:487:PRO:HG3	2.56	0.41
1:A:50:ARG:NH2	1:A:199:GLU:O	2.49	0.41
1:A:144:THR:O	1:A:144:THR:OG1	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:SER:HA	1:A:266:PRO:HD3	1.91	0.41
1:A:347:LYS:HE3	1:A:352:LYS:O	2.21	0.41
1:A:503:LYS:HB2	1:A:503:LYS:HE2	1.93	0.41
2:B:1175:GLN:HA	2:B:1178:GLN:NE2	2.36	0.41
2:D:1190:ARG:HD2	2:D:1195:TRP:HA	2.03	0.41
1:A:32:ARG:CB	1:A:232:GLU:CD	2.87	0.41
1:C:73:LEU:O	1:C:77:LEU:HG	2.21	0.41
2:B:1171:LEU:HD23	2:B:1171:LEU:HA	1.92	0.41
1:A:466:TRP:CE3	1:A:487:PRO:HG3	2.56	0.40
1:C:321:ASN:O	1:C:324:PHE:HB2	2.21	0.40
1:C:458:PRO:HB2	1:C:460:ARG:HG3	2.03	0.40
1:A:29:LYS:HE2	1:A:274:ARG:NH2	2.31	0.40
1:A:89:SER:O	1:A:90:ARG:HG3	2.22	0.40
1:C:326:ARG:HA	1:C:393:GLU:HG2	2.02	0.40
1:A:28:ARG:HD3	1:A:28:ARG:N	2.37	0.40
1:C:65:VAL:HG22	1:C:366:ARG:CZ	2.52	0.40
1:C:84:LEU:CD2	1:C:90:ARG:HA	2.51	0.40
1:C:84:LEU:HD21	1:C:90:ARG:O	2.21	0.40
2:D:1193:HIS:O	2:D:1195:TRP:N	2.52	0.40

All (1) 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:A:460:ARG:NH1	2:D:1213:CYS:CB[3_655]	2.12	0.08

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	488/510 (96%)	438 (90%)	46 (9%)	4 (1%)	19 49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	488/510 (96%)	437 (90%)	44 (9%)	7 (1%)	11 34
2	B	75/121 (62%)	61 (81%)	8 (11%)	6 (8%)	1 2
2	D	75/121 (62%)	63 (84%)	6 (8%)	6 (8%)	1 2
All	All	1126/1262 (89%)	999 (89%)	104 (9%)	23 (2%)	7 24

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	VAL
1	C	466	TRP
1	C	477	LYS
2	B	1178	GLN
2	B	1179	PRO
2	B	1211	VAL
2	D	1179	PRO
1	A	99	ALA
1	C	459	SER
1	C	465	PRO
2	D	1175	GLN
2	D	1212	TYR
1	A	420	CYS
1	C	387	ASP
1	C	470	GLU
2	B	1175	GLN
2	B	1194	PRO
2	B	1206	ASP
2	D	1160	LEU
2	D	1194	PRO
1	C	420	CYS
2	D	1211	VAL
1	A	186	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	422/432 (98%)	410 (97%)	12 (3%)	43	77
1	C	422/432 (98%)	416 (99%)	6 (1%)	67	90
2	B	74/112 (66%)	72 (97%)	2 (3%)	44	78
2	D	74/112 (66%)	71 (96%)	3 (4%)	30	64
All	All	992/1088 (91%)	969 (98%)	23 (2%)	50	82

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	52	VAL
1	A	62	SER
1	A	67	ILE
1	A	144	THR
1	A	286	ARG
1	A	293	LYS
1	A	332	ILE
1	A	377	HIS
1	A	379	VAL
1	A	381	CYS
1	A	490	ASN
1	C	65	VAL
1	C	182	LYS
1	C	196	CYS
1	C	274	ARG
1	C	298	SER
1	C	509	LEU
2	B	1182	THR
2	B	1203	THR
2	D	1134	LEU
2	D	1145	THR
2	D	1158	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	473	GLN
1	C	429	HIS
1	C	473	GLN
2	B	1178	GLN
2	D	1168	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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, 95^{th} 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	490/510 (96%)	0.47	52 (10%) 6 3	46, 84, 156, 230	0
1	C	490/510 (96%)	0.38	33 (6%) 17 10	48, 84, 166, 228	0
2	B	79/121 (65%)	0.53	8 (10%) 7 4	58, 122, 149, 185	0
2	D	79/121 (65%)	0.19	5 (6%) 20 12	54, 121, 145, 158	0
All	All	1138/1262 (90%)	0.42	98 (8%) 10 5	46, 89, 159, 230	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	ARG	11.2
1	A	49	VAL	9.1
1	C	456	GLY	8.1
1	A	109	TRP	6.9
1	A	46	ALA	6.2
1	C	114	LEU	5.4
2	D	1181	PHE	5.2
1	C	191	GLN	5.2
1	A	191	GLN	5.0
2	B	1173	LEU	4.9
1	A	114	LEU	4.7
1	C	482	VAL	4.6
1	C	21	ALA	4.6
1	A	423	PHE	4.6
1	C	457	PHE	4.6
1	C	423	PHE	4.4
2	B	1178	GLN	4.4
1	A	44	ARG	4.3
2	B	1183	GLU	4.3
1	A	461	TYR	4.2
1	C	47	ARG	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	483	ASP	4.0
2	B	1181	PHE	4.0
1	A	43	VAL	4.0
1	C	462	ILE	3.9
1	A	105	LEU	3.8
2	B	1179	PRO	3.8
1	A	113	ARG	3.7
1	C	113	ARG	3.7
1	A	24	VAL	3.6
1	C	484	TYR	3.6
1	A	357	TRP	3.6
1	C	446	TYR	3.4
1	A	374	LEU	3.4
1	A	192	GLN	3.4
1	C	195	SER	3.3
1	A	200	ILE	3.2
1	A	23	SER	3.2
1	A	506	TYR	3.1
1	A	106	PHE	3.1
1	A	379	VAL	3.1
1	C	109	TRP	3.0
1	C	288	TRP	3.0
1	A	440	THR	2.9
1	A	462	ILE	2.8
1	C	43	VAL	2.8
1	A	92	PHE	2.8
1	C	488	ILE	2.8
1	A	110	GLY	2.8
1	C	454	LEU	2.8
1	A	47	ARG	2.8
2	B	1174	LEU	2.7
1	A	195	SER	2.7
1	C	453	LYS	2.7
1	C	42	ALA	2.7
1	A	385	ARG	2.7
1	C	459	SER	2.6
1	C	105	LEU	2.6
1	A	21	ALA	2.6
1	C	116	PHE	2.6
1	A	102	PHE	2.5
1	A	111	VAL	2.5
2	D	1173	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	39	LEU	2.5
1	C	348	TRP	2.4
1	C	151	TYR	2.4
1	A	505	ILE	2.4
1	A	51	CYS	2.4
1	A	418	LEU	2.4
1	A	388	LEU	2.3
1	A	123	PHE	2.3
1	A	457	PHE	2.3
1	C	375	ALA	2.3
1	A	196	CYS	2.3
1	A	166	LEU	2.3
1	A	188	VAL	2.3
1	A	434	VAL	2.3
1	A	417	TRP	2.3
1	C	455	LYS	2.3
1	A	375	ALA	2.3
2	B	1185	GLN	2.3
1	A	334	ILE	2.3
1	A	424	PHE	2.2
1	A	433	PRO	2.2
1	A	456	GLY	2.2
2	D	1132	TYR	2.2
1	A	436	PHE	2.1
1	A	361	ILE	2.1
1	A	438	ARG	2.1
2	D	1176	ARG	2.1
2	D	1189	LEU	2.1
1	C	285	TYR	2.1
2	B	1189	LEU	2.0
1	A	115	THR	2.0
1	A	387	ASP	2.0
1	C	510	SER	2.0
1	C	180	LEU	2.0
1	C	111	VAL	2.0

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	A	2000	1/1	0.96	0.05	115,115,115,115	0
3	ZN	D	2000	1/1	0.98	0.11	112,112,112,112	0

6.5 Other polymers (i)

There are no such residues in this entry.