Full wwPDB X-ray Structure Validation Report (i)

May 9, 2016 – 07:40 AM EDT

PDB ID	:	5J8R
Title	:	Crystal Structure of the Catalytic Domain of Human Protein Tyrosine Phosphatase non-receptor Type 12 - K61R mutant
Authors	:	Li, H.; Yang, F.; Xu, Y.F.; Wang, W.J.; Xiao, P.; Yu, X.; Sun, J.P.
Deposited on	:	2016-04-08
Resolution	:	2.04 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 (1)) were used in the production of this report:

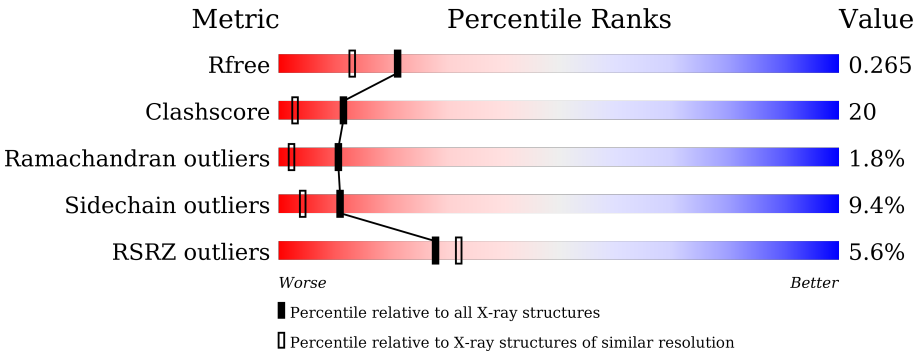
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 2.04 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}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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.

Mol	Chain	Length	Quality of chain
1	A	311	2% 69% 22% • 5%
1	B	311	2% 72% 18% • 6%
1	C	311	8% 52% 32% 7% • 8%
1	D	311	9% 49% 34% 7% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10076 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 Tyrosine-protein phosphatase non-receptor type 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	1	0
			2477	1576	434	451	16			
1	B	293	Total	C	N	O	S	0	1	0
			2453	1563	429	445	16			
1	C	286	Total	C	N	O	S	0	0	0
			2396	1531	419	430	16			
1	D	284	Total	C	N	O	S	0	0	0
			2373	1518	412	427	16			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q05209
A	-4	HIS	-	expression tag	UNP Q05209
A	-3	HIS	-	expression tag	UNP Q05209
A	-2	HIS	-	expression tag	UNP Q05209
A	-1	HIS	-	expression tag	UNP Q05209
A	0	HIS	-	expression tag	UNP Q05209
A	61	ARG	LYS	engineered mutation	UNP Q05209
B	-5	HIS	-	expression tag	UNP Q05209
B	-4	HIS	-	expression tag	UNP Q05209
B	-3	HIS	-	expression tag	UNP Q05209
B	-2	HIS	-	expression tag	UNP Q05209
B	-1	HIS	-	expression tag	UNP Q05209
B	0	HIS	-	expression tag	UNP Q05209
B	61	ARG	LYS	engineered mutation	UNP Q05209
C	-5	HIS	-	expression tag	UNP Q05209
C	-4	HIS	-	expression tag	UNP Q05209
C	-3	HIS	-	expression tag	UNP Q05209
C	-2	HIS	-	expression tag	UNP Q05209
C	-1	HIS	-	expression tag	UNP Q05209
C	0	HIS	-	expression tag	UNP Q05209
C	61	ARG	LYS	engineered mutation	UNP Q05209

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	expression tag	UNP Q05209
D	-4	HIS	-	expression tag	UNP Q05209
D	-3	HIS	-	expression tag	UNP Q05209
D	-2	HIS	-	expression tag	UNP Q05209
D	-1	HIS	-	expression tag	UNP Q05209
D	0	HIS	-	expression tag	UNP Q05209
D	61	ARG	LYS	engineered mutation	UNP Q05209

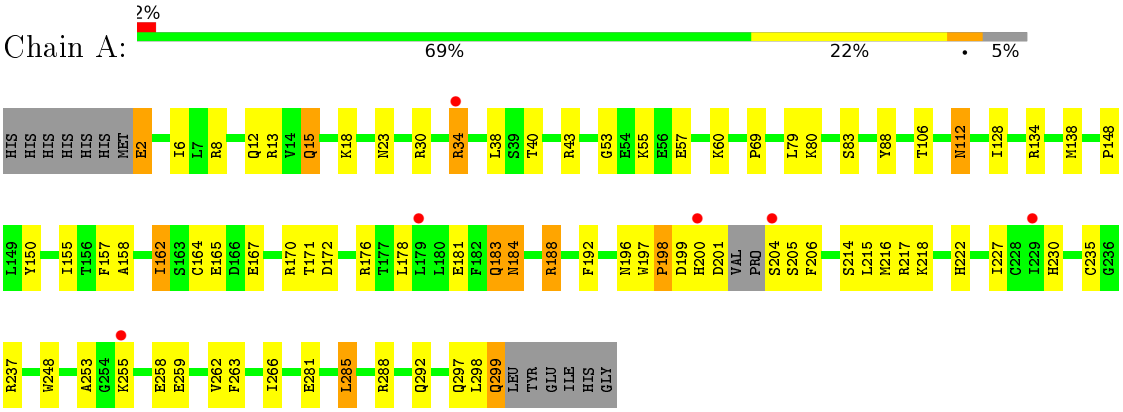
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	130	Total O 130 130	0	0
2	B	142	Total O 142 142	0	0
2	C	51	Total O 51 51	0	0
2	D	54	Total O 54 54	0	0

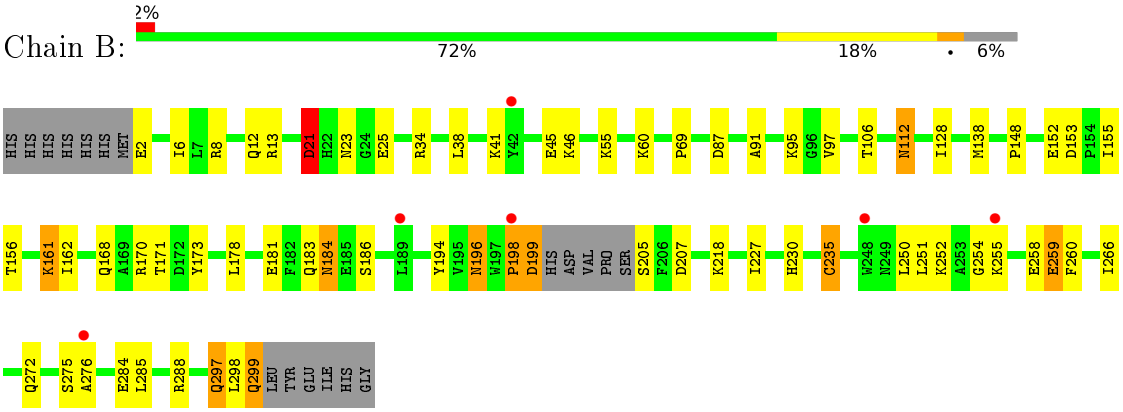
3 Residue-property plots (i)

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.

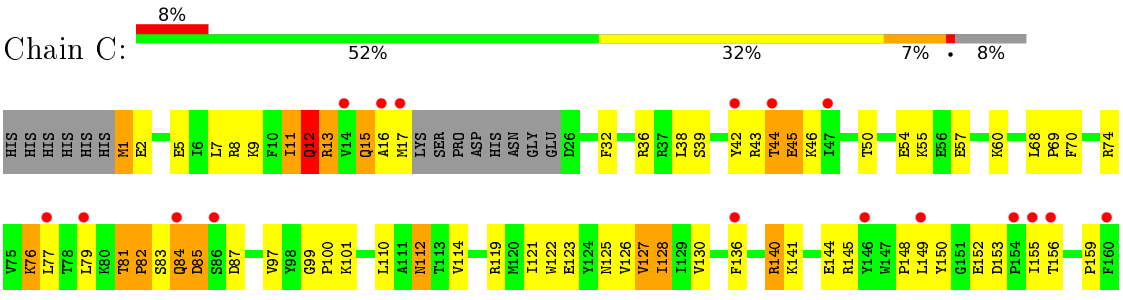
- Molecule 1: Tyrosine-protein phosphatase non-receptor type 12

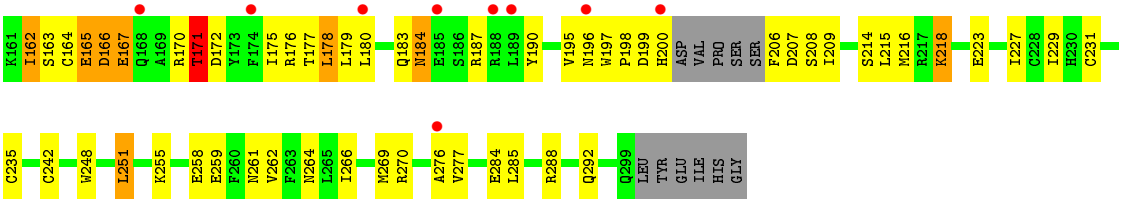


- Molecule 1: Tyrosine-protein phosphatase non-receptor type 12



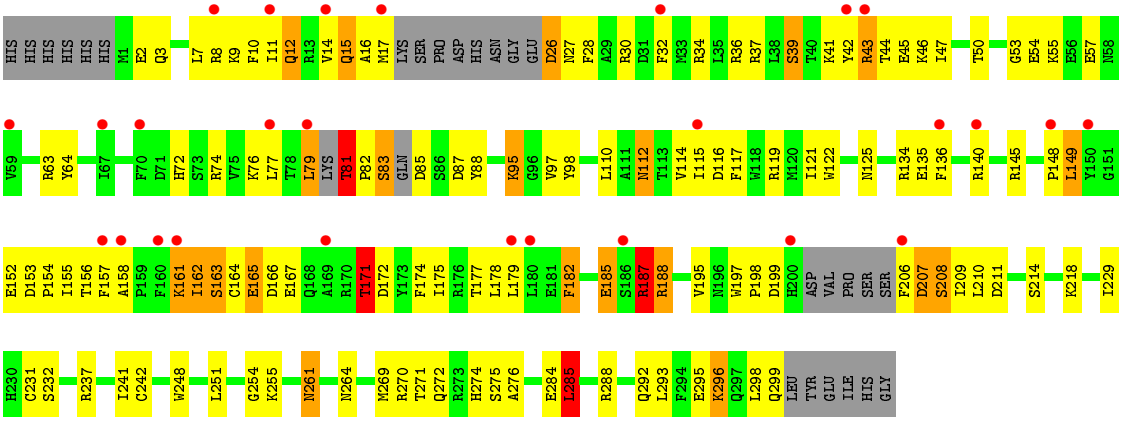
- Molecule 1: Tyrosine-protein phosphatase non-receptor type 12





• Molecule 1: Tyrosine-protein phosphatase non-receptor type 12

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	129.94Å 129.94Å 278.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.79 – 2.04 37.79 – 2.04	Depositor EDS
% Data completeness (in resolution range)	90.3 (37.79-2.04) 90.4 (37.79-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.84 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.239 , 0.275 0.231 , 0.265	Depositor DCC
R_{free} test set	5005 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.457 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10076	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.54	0/2536	0.59	0/3422
1	B	0.46	0/2511	0.59	0/3388
1	C	0.51	0/2452	0.59	0/3307
1	D	0.48	0/2427	0.56	2/3272 (0.1%)
All	All	0.50	0/9926	0.59	2/13389 (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
1	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	81	THR	C-N-CD	5.96	140.92	128.40
1	D	285	LEU	CA-CB-CG	5.41	127.74	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	184	ASN	Peptide

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	2477	0	2420	79	0
1	B	2453	0	2404	56	0
1	C	2396	0	2358	125	0
1	D	2373	0	2326	135	0
2	A	130	0	0	10	0
2	B	142	0	0	9	0
2	C	51	0	0	8	0
2	D	54	0	0	9	0
All	All	10076	0	9508	392	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 20.

All (392) 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:C:165:GLU:OE2	1:C:179:LEU:HD11	1.18	1.30
1:C:13:ARG:HH21	1:C:17:MET:HG3	1.11	1.12
1:C:165:GLU:OE2	1:C:179:LEU:CD1	2.00	1.07
1:B:299:GLN:OE1	1:B:299:GLN:HA	1.60	1.01
1:B:155:ILE:C	1:B:161:LYS:HZ3	1.62	1.01
1:B:161:LYS:HE2	1:B:161:LYS:HA	1.42	1.01
1:C:171:THR:HG22	1:C:172:ASP:H	1.27	0.96
1:C:13:ARG:NH2	1:C:17:MET:HG3	1.82	0.95
1:D:171:THR:HG22	1:D:172:ASP:H	1.31	0.93
1:D:9:LYS:HB2	2:D:402:HOH:O	1.68	0.92
1:B:183:GLN:O	1:B:184:ASN:ND2	2.02	0.90
1:B:21:ASP:HB3	1:B:23:ASN:H	1.41	0.86
1:B:21:ASP:HB2	1:B:25:GLU:H	1.41	0.86
1:C:69:PRO:HA	2:C:419:HOH:O	1.77	0.83
1:D:81:THR:HB	1:D:82:PRO:CD	2.11	0.81
1:D:171:THR:CG2	1:D:172:ASP:H	1.94	0.80
1:A:204:SER:HB3	1:A:292:GLN:OE1	1.81	0.79
1:B:259:GLU:CD	1:B:259:GLU:H	1.84	0.79
1:D:83:SER:O	1:D:85:ASP:N	2.15	0.79
1:C:171:THR:HG22	1:C:172:ASP:N	1.97	0.78
1:C:171:THR:CG2	1:C:172:ASP:N	2.46	0.78
1:D:171:THR:CG2	1:D:172:ASP:N	2.47	0.77
1:D:148:PRO:HG3	1:D:163:SER:HA	1.65	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:ASN:HD21	1:C:264:ASN:ND2	1.83	0.76
1:B:254:GLY:O	2:B:401:HOH:O	2.03	0.76
1:D:145:ARG:NH2	1:D:149:LEU:HG	2.01	0.76
1:A:183:GLN:O	1:A:184:ASN:ND2	2.16	0.75
1:D:149:LEU:HD12	1:D:152:GLU:OE1	1.87	0.75
1:A:198:PRO:O	1:A:200:HIS:N	2.20	0.74
1:B:156:THR:N	1:B:161:LYS:HZ3	1.84	0.74
1:C:112:ASN:HD22	1:C:112:ASN:H	1.35	0.74
1:B:162:ILE:HD11	1:B:178:LEU:HB3	1.70	0.73
1:C:50:THR:HG22	1:C:70:PHE:HA	1.70	0.73
1:D:11:ILE:HD13	1:D:295:GLU:HB2	1.70	0.73
1:D:135:GLU:HG2	1:D:136:PHE:CD1	2.24	0.73
1:C:261:ASN:HD21	1:C:264:ASN:HD22	1.37	0.72
1:C:1:MET:HG3	2:C:447:HOH:O	1.88	0.72
1:D:206:PHE:CE1	1:D:285:LEU:HD13	2.25	0.72
1:D:165:GLU:OE2	1:D:179:LEU:HD11	1.90	0.71
1:C:197:TRP:CD1	1:C:199:ASP:HB3	2.25	0.71
1:D:148:PRO:HG2	1:D:164:CYS:N	2.05	0.71
1:A:204:SER:HA	1:A:205:SER:HB2	1.72	0.70
1:A:299:GLN:OE1	1:A:299:GLN:HA	1.90	0.70
1:C:84:GLN:HA	1:C:84:GLN:HE21	1.55	0.70
1:D:148:PRO:HB3	1:D:155:ILE:HG13	1.73	0.70
1:B:161:LYS:CE	1:B:161:LYS:HA	2.20	0.70
1:B:260:PHE:O	2:B:402:HOH:O	2.10	0.70
1:D:206:PHE:CE2	1:D:288:ARG:HB3	2.26	0.70
1:D:148:PRO:HG2	1:D:164:CYS:H	1.57	0.70
1:D:261:ASN:ND2	1:D:264:ASN:HB2	2.06	0.69
1:D:83:SER:O	1:D:85:ASP:HB3	1.92	0.69
1:A:204:SER:N	1:A:205:SER:OG	2.25	0.69
1:D:10:PHE:N	2:D:402:HOH:O	2.23	0.69
1:A:183:GLN:HE22	1:C:101:LYS:HD2	1.58	0.69
1:C:214:SER:HB3	1:C:248:TRP:CH2	2.28	0.68
1:D:177:THR:CG2	1:D:188:ARG:HD3	2.23	0.68
1:D:43:ARG:HH11	1:D:43:ARG:CG	2.06	0.68
1:C:44:THR:CB	1:C:45:GLU:HB2	2.24	0.68
1:C:54:GLU:HG2	1:C:68:LEU:CD1	2.23	0.68
1:C:148:PRO:HB3	1:C:155:ILE:HG13	1.76	0.68
1:D:125:ASN:OD1	2:D:401:HOH:O	2.11	0.68
1:D:36:ARG:HG2	1:D:36:ARG:HH11	1.60	0.67
1:C:261:ASN:ND2	1:C:264:ASN:HD22	1.93	0.67
1:C:82:PRO:HD3	1:C:159:PRO:HG3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:SER:HA	1:A:205:SER:CB	2.25	0.66
1:D:179:LEU:HD12	1:D:179:LEU:N	2.11	0.66
1:D:206:PHE:HD2	1:D:292:GLN:OE1	1.78	0.66
1:C:44:THR:H	1:C:45:GLU:C	2.00	0.65
1:B:161:LYS:CA	1:B:161:LYS:HE2	2.24	0.65
1:D:178:LEU:C	1:D:179:LEU:HD12	2.17	0.65
1:C:171:THR:CG2	1:C:172:ASP:H	2.00	0.64
1:A:34:ARG:CZ	1:A:34:ARG:HB2	2.21	0.64
1:B:8:ARG:HH11	1:B:12:GLN:HE21	1.44	0.64
1:C:125:ASN:OD1	2:C:401:HOH:O	2.15	0.64
1:C:43:ARG:O	1:C:43:ARG:CG	2.46	0.64
1:B:41:LYS:O	1:B:45:GLU:HG3	1.98	0.63
1:C:145:ARG:NH2	1:C:149:LEU:HG	2.12	0.63
1:A:53:GLY:HA2	1:A:88:TYR:CE1	2.34	0.63
1:C:79:LEU:CD2	1:C:119:ARG:HG2	2.28	0.63
1:C:199:ASP:HA	1:C:200:HIS:HB2	1.80	0.63
1:D:165:GLU:CD	1:D:179:LEU:HD11	2.19	0.62
1:A:40:THR:HG23	1:A:43:ARG:NH2	2.15	0.62
1:C:112:ASN:ND2	1:C:112:ASN:H	1.97	0.62
1:D:171:THR:CG2	1:D:208:SER:HB3	2.30	0.62
1:C:165:GLU:O	1:C:166:ASP:HB2	1.97	0.62
1:C:270:ARG:NH1	1:C:277:VAL:O	2.32	0.62
1:D:135:GLU:HG2	1:D:136:PHE:HD1	1.65	0.62
1:D:122:TRP:HA	1:D:187:ARG:NH1	2.15	0.62
1:D:148:PRO:HA	1:D:155:ILE:HD11	1.82	0.61
1:D:85:ASP:O	1:D:85:ASP:CG	2.39	0.61
1:D:274:HIS:CE1	1:D:275:SER:HG	2.19	0.61
1:C:122:TRP:HA	1:C:187:ARG:NH2	2.15	0.61
1:A:40:THR:HG23	1:A:43:ARG:NH1	2.15	0.61
1:C:79:LEU:O	1:C:79:LEU:HD23	2.01	0.61
1:C:162:ILE:HD11	1:C:178:LEU:HD13	1.82	0.61
1:A:205:SER:HB2	1:A:206:PHE:CE2	2.35	0.61
1:B:21:ASP:HB3	1:B:23:ASN:N	2.15	0.60
1:A:200:HIS:HE1	1:A:281:GLU:HA	1.66	0.60
1:B:255:LYS:HA	2:B:401:HOH:O	2.02	0.60
1:D:122:TRP:HA	1:D:187:ARG:HH12	1.67	0.60
1:C:122:TRP:O	1:C:187:ARG:NH2	2.35	0.60
1:A:201:ASP:HA	1:A:205:SER:HB3	1.83	0.59
1:D:295:GLU:OE1	1:D:298:LEU:HD12	2.02	0.59
1:A:183:GLN:NE2	1:C:101:LYS:HD2	2.17	0.59
1:B:170:ARG:HG3	1:B:173:TYR:CE2	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:GLU:HG2	1:C:288:ARG:HD2	1.84	0.59
1:A:40:THR:HG23	1:A:43:ARG:CZ	2.32	0.58
1:B:8:ARG:HH11	1:B:12:GLN:NE2	1.99	0.58
1:D:206:PHE:O	1:D:209:ILE:N	2.32	0.58
1:C:81:THR:C	1:C:83:SER:HA	2.23	0.58
1:C:122:TRP:HA	1:C:187:ARG:HH22	1.69	0.58
1:A:197:TRP:O	2:A:401:HOH:O	2.17	0.58
1:C:199:ASP:HA	2:C:405:HOH:O	2.04	0.58
1:D:55:LYS:HZ2	1:D:55:LYS:HB2	1.67	0.58
1:A:69:PRO:HA	2:A:462:HOH:O	2.03	0.58
1:D:171:THR:HG21	1:D:208:SER:HB3	1.86	0.58
1:D:43:ARG:HH11	1:D:43:ARG:HG3	1.69	0.57
1:C:229:ILE:HD12	1:C:242:CYS:SG	2.44	0.57
1:D:152:GLU:HG2	1:D:153:ASP:N	2.19	0.57
1:D:79:LEU:HD23	1:D:119:ARG:HG2	1.86	0.57
1:D:214:SER:HB3	1:D:248:TRP:CH2	2.39	0.57
1:D:182:PHE:O	1:D:185:GLU:HG3	2.04	0.57
1:A:206:PHE:CE1	1:A:285:LEU:HD13	2.40	0.56
1:B:128:ILE:HB	1:B:227:ILE:HG12	1.86	0.56
1:C:54:GLU:HG2	1:C:68:LEU:HD13	1.88	0.56
1:D:206:PHE:HE2	1:D:288:ARG:HB3	1.70	0.56
1:B:199:ASP:OD2	1:B:199:ASP:C	2.43	0.56
1:A:285:LEU:O	1:A:285:LEU:HD12	2.05	0.56
1:D:154:PRO:HB2	1:D:161:LYS:HE3	1.87	0.56
1:B:198:PRO:O	1:B:199:ASP:C	2.44	0.56
1:D:95:LYS:HG3	1:D:272:GLN:OE1	2.05	0.56
1:A:222:HIS:HA	2:A:457:HOH:O	2.05	0.56
1:C:81:THR:HB	1:C:82:PRO:CD	2.35	0.56
1:B:259:GLU:CD	1:B:259:GLU:N	2.58	0.56
1:B:21:ASP:HB2	1:B:25:GLU:N	2.16	0.55
1:B:156:THR:HG22	1:B:156:THR:O	2.06	0.55
1:A:198:PRO:HB2	1:A:200:HIS:O	2.06	0.55
1:B:156:THR:N	1:B:161:LYS:NZ	2.53	0.55
1:C:197:TRP:HD1	1:C:199:ASP:HB3	1.71	0.55
1:D:148:PRO:CG	1:D:164:CYS:H	2.19	0.55
1:A:214:SER:HB3	1:A:248:TRP:CH2	2.42	0.55
1:C:7:LEU:HD21	1:C:251:LEU:HD21	1.89	0.55
1:D:218:LYS:NZ	2:D:406:HOH:O	2.38	0.54
1:A:204:SER:N	1:A:205:SER:HG	2.04	0.54
1:B:156:THR:OG1	1:B:161:LYS:NZ	2.28	0.54
1:B:112:ASN:H	1:B:112:ASN:HD22	1.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ILE:HB	1:A:227:ILE:HG12	1.90	0.54
1:A:30:ARG:HH11	1:A:30:ARG:HG2	1.73	0.54
1:D:45:GLU:CB	1:D:47:ILE:HD11	2.38	0.54
1:D:229:ILE:HD12	1:D:242:CYS:SG	2.48	0.53
1:A:172:ASP:HB3	1:A:196:ASN:HB3	1.90	0.53
1:D:299:GLN:OE1	1:D:299:GLN:HA	2.08	0.53
1:A:162:ILE:HD11	1:A:178:LEU:HB3	1.90	0.53
1:B:95:LYS:HG3	1:B:272:GLN:OE1	2.08	0.53
1:C:128:ILE:HG22	1:C:227:ILE:HG23	1.91	0.53
1:C:13:ARG:CZ	1:C:16:ALA:HB3	2.38	0.53
1:A:34:ARG:CZ	1:A:34:ARG:CB	2.83	0.53
1:C:175:ILE:HD11	1:C:215:LEU:HD23	1.90	0.53
1:D:165:GLU:O	1:D:166:ASP:HB2	2.08	0.53
1:D:16:ALA:O	1:D:17:MET:C	2.46	0.53
1:B:106:THR:O	1:B:230:HIS:HB2	2.09	0.53
1:A:200:HIS:CE1	1:A:281:GLU:HA	2.43	0.53
1:D:154:PRO:CB	1:D:161:LYS:HE3	2.39	0.53
1:A:204:SER:CA	1:A:205:SER:CB	2.86	0.52
1:C:44:THR:OG1	1:C:45:GLU:HB2	2.08	0.52
1:A:167:GLU:HG3	1:A:176:ARG:HG2	1.91	0.52
1:B:91:ALA:HB2	1:B:106:THR:OG1	2.10	0.52
1:C:197:TRP:CZ2	1:C:285:LEU:HD23	2.44	0.52
1:C:79:LEU:HD23	1:C:119:ARG:HG2	1.92	0.52
1:C:15:GLN:NE2	2:C:410:HOH:O	2.42	0.52
1:C:206:PHE:CE1	1:C:285:LEU:HD13	2.45	0.52
1:C:79:LEU:HD22	1:C:119:ARG:HG2	1.92	0.52
1:C:38:LEU:HG	1:C:42:TYR:CE2	2.45	0.52
1:A:57:GLU:OE1	2:A:402:HOH:O	2.18	0.52
1:C:255:LYS:NZ	2:C:409:HOH:O	2.42	0.52
1:A:79:LEU:C	1:A:79:LEU:HD23	2.29	0.52
1:D:112:ASN:HD22	1:D:112:ASN:H	1.57	0.52
1:D:43:ARG:CG	1:D:43:ARG:NH1	2.71	0.52
1:D:135:GLU:OE2	1:D:145:ARG:HB2	2.09	0.51
1:C:199:ASP:CA	1:C:200:HIS:HB2	2.40	0.51
1:D:122:TRP:O	1:D:187:ARG:NH2	2.35	0.51
1:C:126:VAL:HG12	1:C:127:VAL:N	2.25	0.51
1:B:6:ILE:HD11	1:B:258:GLU:HG2	1.92	0.51
1:D:45:GLU:HB3	1:D:47:ILE:HD11	1.92	0.51
1:B:297:GLN:HG3	1:B:297:GLN:O	2.09	0.51
1:C:171:THR:HG21	1:C:208:SER:HB3	1.93	0.51
1:D:114:VAL:O	1:D:117:PHE:HB3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:PRO:CG	1:D:164:CYS:N	2.73	0.51
1:D:41:LYS:O	1:D:41:LYS:HG2	2.11	0.51
1:B:156:THR:CA	1:B:161:LYS:NZ	2.73	0.51
1:C:44:THR:HB	1:C:45:GLU:HB2	1.93	0.50
1:D:254:GLY:HA2	2:D:426:HOH:O	2.11	0.50
1:A:197:TRP:CE2	1:A:237:ARG:HG2	2.47	0.50
1:C:155:ILE:HG22	1:C:156:THR:H	1.76	0.50
1:A:15:GLN:NE2	2:A:411:HOH:O	2.45	0.50
1:D:53:GLY:HA2	1:D:88:TYR:CE1	2.46	0.50
1:A:40:THR:CG2	1:A:43:ARG:NH2	2.75	0.50
1:C:85:ASP:C	1:C:85:ASP:OD1	2.50	0.50
1:A:162:ILE:CD1	1:A:178:LEU:HB3	2.42	0.49
1:B:156:THR:CB	1:B:161:LYS:HZ1	2.23	0.49
1:C:216:MET:SD	1:C:227:ILE:HD13	2.52	0.49
1:D:171:THR:HG23	1:D:172:ASP:N	2.26	0.49
1:A:106:THR:O	1:A:230:HIS:HB2	2.12	0.49
1:B:284:GLU:HG2	1:B:288:ARG:HD2	1.94	0.49
1:C:136:PHE:CZ	1:C:141:LYS:HD3	2.48	0.49
1:D:157:PHE:O	1:D:158:ALA:C	2.51	0.49
1:D:55:LYS:HB2	1:D:55:LYS:NZ	2.28	0.49
1:D:77:LEU:O	1:D:87:ASP:HA	2.13	0.49
1:C:206:PHE:O	1:C:209:ILE:N	2.46	0.49
1:C:43:ARG:O	1:C:44:THR:HG23	2.13	0.49
1:C:77:LEU:O	1:C:87:ASP:HA	2.12	0.49
1:D:72:HIS:CE1	1:D:271:THR:O	2.66	0.49
1:D:37:ARG:NH2	2:D:407:HOH:O	2.41	0.49
1:A:183:GLN:O	1:A:184:ASN:CB	2.60	0.49
1:A:184:ASN:HB2	1:C:123:GLU:OE2	2.13	0.49
1:D:295:GLU:HA	1:D:295:GLU:OE1	2.12	0.49
1:C:148:PRO:HG2	1:C:164:CYS:HB2	1.96	0.48
1:C:148:PRO:HG3	1:C:163:SER:HA	1.94	0.48
1:D:97:VAL:HG23	1:D:98:TYR:HD2	1.78	0.48
1:D:164:CYS:SG	1:D:165:GLU:N	2.86	0.48
1:D:39:SER:O	1:D:42:TYR:HB2	2.13	0.48
1:C:110:LEU:O	1:C:114:VAL:HG23	2.13	0.48
1:C:82:PRO:N	1:C:83:SER:HA	2.27	0.48
1:D:43:ARG:HD3	1:D:43:ARG:O	2.14	0.48
1:A:285:LEU:C	1:A:285:LEU:HD12	2.32	0.48
1:A:288:ARG:HD2	2:A:441:HOH:O	2.13	0.48
1:D:125:ASN:HA	1:D:187:ARG:NH2	2.28	0.48
1:C:97:VAL:HG21	2:C:449:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLU:CD	1:A:188:ARG:NH2	2.68	0.47
1:A:18:LYS:HE2	1:A:288:ARG:CZ	2.44	0.47
1:C:270:ARG:HG3	1:C:276:ALA:HB3	1.96	0.47
1:C:50:THR:O	1:C:54:GLU:HG3	2.14	0.47
1:D:121:ILE:O	1:D:187:ARG:NH1	2.44	0.47
1:B:152:GLU:HG2	1:B:153:ASP:O	2.15	0.47
1:B:97:VAL:HG13	2:B:417:HOH:O	2.14	0.47
1:D:292:GLN:O	1:D:296:LYS:HB2	2.14	0.47
1:A:298:LEU:O	1:A:299:GLN:HB2	2.13	0.47
1:A:181:GLU:HG3	2:A:423:HOH:O	2.14	0.47
1:C:9:LYS:O	1:C:12:GLN:CB	2.62	0.47
1:D:50:THR:O	1:D:54:GLU:HG2	2.14	0.47
1:C:32:PHE:CE2	1:C:36:ARG:HD3	2.50	0.47
1:D:171:THR:HG22	1:D:172:ASP:N	2.07	0.47
1:C:195:VAL:HG23	1:C:196:ASN:HD22	1.79	0.47
1:C:2:GLU:OE1	1:C:5:GLU:OE1	2.32	0.47
1:C:125:ASN:HA	1:C:187:ARG:NH2	2.29	0.47
1:D:156:THR:HG22	1:D:157:PHE:N	2.30	0.47
1:B:298:LEU:O	1:B:299:GLN:C	2.54	0.47
1:D:206:PHE:O	1:D:207:ASP:C	2.52	0.47
1:A:112:ASN:H	1:A:112:ASN:HD22	1.63	0.47
1:C:261:ASN:CG	1:C:264:ASN:HD22	2.18	0.47
1:B:148:PRO:HB3	1:B:155:ILE:HG13	1.96	0.46
1:B:194:TYR:CE1	1:B:196:ASN:O	2.68	0.46
1:C:262:VAL:O	1:C:266:ILE:HG12	2.15	0.46
1:C:43:ARG:HG2	1:C:43:ARG:O	2.15	0.46
1:D:154:PRO:HB3	1:D:161:LYS:CE	2.45	0.46
1:D:72:HIS:HE1	1:D:271:THR:O	1.98	0.46
1:D:115:ILE:HG23	1:D:116:ASP:N	2.29	0.46
1:C:152:GLU:HG2	1:C:153:ASP:O	2.15	0.46
1:A:205:SER:HB2	1:A:206:PHE:CD2	2.50	0.46
1:C:125:ASN:HA	1:C:187:ARG:CZ	2.46	0.46
1:C:130:VAL:HG21	1:C:216:MET:HE1	1.97	0.46
1:D:81:THR:HB	1:D:82:PRO:HD3	1.96	0.46
1:C:206:PHE:CE2	1:C:288:ARG:HB3	2.50	0.46
1:A:148:PRO:HG2	1:A:164:CYS:HB2	1.97	0.46
1:C:198:PRO:O	1:C:200:HIS:HB2	2.16	0.46
1:C:55:LYS:HB2	1:C:55:LYS:HE3	1.56	0.46
1:D:55:LYS:CB	1:D:55:LYS:NZ	2.79	0.46
1:C:8:ARG:O	1:C:9:LYS:C	2.54	0.46
1:A:34:ARG:HG2	1:A:263:PHE:HZ	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:PHE:HE2	1:C:288:ARG:HB3	1.81	0.46
1:D:2:GLU:O	1:D:3:GLN:C	2.54	0.46
1:A:204:SER:HB3	1:A:292:GLN:CD	2.36	0.46
1:D:57:GLU:CD	1:D:57:GLU:H	2.15	0.46
1:D:174:PHE:HE2	1:D:195:VAL:HG21	1.81	0.45
1:D:237:ARG:O	1:D:241:ILE:HG13	2.16	0.45
1:B:87:ASP:OD1	1:B:87:ASP:C	2.54	0.45
1:C:177:THR:HG23	1:C:190:TYR:CE1	2.51	0.45
1:C:84:GLN:HA	1:C:84:GLN:NE2	2.28	0.45
1:C:5:GLU:O	1:C:8:ARG:N	2.40	0.45
1:D:179:LEU:CD1	1:D:179:LEU:N	2.79	0.45
1:C:206:PHE:CE1	1:C:285:LEU:CD1	3.00	0.45
1:B:34:ARG:HD2	2:B:449:HOH:O	2.16	0.45
1:D:63:ARG:HG2	1:D:64:TYR:CE2	2.51	0.45
1:D:210:LEU:HD22	1:D:293:LEU:HD21	1.98	0.45
1:D:9:LYS:O	1:D:12:GLN:HB2	2.17	0.45
1:B:299:GLN:OE1	1:B:299:GLN:CA	2.45	0.44
1:D:26:ASP:O	1:D:30:ARG:HG3	2.17	0.44
1:D:162:ILE:HD12	1:D:163:SER:N	2.32	0.44
1:C:9:LYS:HB2	1:C:9:LYS:HE2	1.69	0.44
1:D:156:THR:CG2	1:D:157:PHE:N	2.80	0.44
1:B:69:PRO:HA	2:B:468:HOH:O	2.18	0.44
1:C:170:ARG:O	1:C:171:THR:O	2.36	0.44
1:D:10:PHE:CE1	1:D:14:VAL:HG21	2.53	0.44
1:A:6:ILE:HD11	1:A:258:GLU:HG2	2.00	0.44
1:B:252:LYS:C	1:B:254:GLY:H	2.19	0.44
1:C:13:ARG:NE	1:C:13:ARG:HA	2.31	0.44
1:D:134:ARG:NH2	2:D:404:HOH:O	2.30	0.44
1:D:218:LYS:HE2	1:D:218:LYS:HB3	1.66	0.44
1:D:87:ASP:C	1:D:87:ASP:OD1	2.56	0.44
1:A:215:LEU:HA	1:A:218:LYS:HG3	2.00	0.44
1:D:274:HIS:CE1	1:D:275:SER:OG	2.70	0.44
1:C:206:PHE:O	1:C:207:ASP:C	2.56	0.44
1:D:28:PHE:CD2	1:D:284:GLU:HG3	2.52	0.44
1:D:154:PRO:CB	1:D:161:LYS:CE	2.96	0.43
1:D:275:SER:O	1:D:276:ALA:C	2.56	0.43
1:A:200:HIS:HB3	2:A:441:HOH:O	2.17	0.43
1:B:275:SER:O	1:B:276:ALA:C	2.56	0.43
1:C:82:PRO:HG3	1:C:159:PRO:HB3	2.00	0.43
1:C:121:ILE:HG23	1:C:126:VAL:HB	1.99	0.43
1:C:127:VAL:HG12	1:C:128:ILE:HD13	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ARG:HH22	1:D:149:LEU:HG	1.80	0.43
1:C:206:PHE:N	1:C:206:PHE:CD1	2.84	0.43
1:D:9:LYS:O	1:D:12:GLN:CB	2.66	0.43
1:A:165:GLU:OE1	1:A:188:ARG:NH2	2.52	0.43
1:B:8:ARG:HG3	2:B:531:HOH:O	2.19	0.43
1:A:40:THR:HG23	1:A:43:ARG:HH22	1.81	0.43
1:D:270:ARG:HG3	1:D:276:ALA:HB3	2.00	0.43
1:D:30:ARG:O	1:D:34:ARG:HG3	2.19	0.43
1:A:8:ARG:HH11	1:A:12:GLN:HE21	1.67	0.43
1:C:127:VAL:HG12	1:C:128:ILE:CD1	2.49	0.43
1:C:218:LYS:HE2	1:C:218:LYS:HB3	1.59	0.43
1:D:12:GLN:O	1:D:15:GLN:HB3	2.19	0.43
1:D:269:MET:HG2	1:D:276:ALA:CB	2.49	0.43
1:B:168:GLN:HB2	1:B:168:GLN:HE21	1.49	0.43
1:A:40:THR:HG23	1:A:43:ARG:HH12	1.82	0.42
1:A:79:LEU:HD23	1:A:80:LYS:N	2.35	0.42
1:D:232:SER:HB3	2:D:436:HOH:O	2.19	0.42
1:D:45:GLU:HB2	1:D:47:ILE:HD11	2.01	0.42
1:A:162:ILE:HD11	1:A:178:LEU:HD13	2.01	0.42
1:C:148:PRO:HA	1:C:155:ILE:HD11	2.01	0.42
1:D:63:ARG:NH2	1:D:110:LEU:HD23	2.33	0.42
1:C:183:GLN:HE21	1:C:183:GLN:HB2	1.67	0.42
1:A:204:SER:CA	1:A:205:SER:OG	2.67	0.42
1:A:53:GLY:HA2	1:A:88:TYR:CZ	2.54	0.42
1:C:140:ARG:HB2	1:C:140:ARG:HE	1.40	0.42
1:C:99:GLY:HA2	1:C:100:PRO:HD3	1.91	0.42
1:C:7:LEU:O	1:C:11:ILE:HG13	2.19	0.42
1:A:172:ASP:HB3	1:A:196:ASN:CB	2.49	0.42
1:B:235:CYS:HB2	1:B:275:SER:O	2.20	0.42
1:A:148:PRO:HB3	1:A:155:ILE:HG13	2.01	0.42
1:C:167:GLU:CG	1:C:176:ARG:HG2	2.50	0.42
1:D:125:ASN:HA	1:D:187:ARG:CZ	2.50	0.42
1:A:2:GLU:N	2:A:418:HOH:O	2.53	0.41
1:A:40:THR:CG2	1:A:43:ARG:HH22	2.32	0.41
1:C:167:GLU:HG2	1:C:176:ARG:HG2	2.02	0.41
1:C:74:ARG:NH2	1:C:76:LYS:HG3	2.35	0.41
1:D:148:PRO:O	1:D:164:CYS:HB2	2.20	0.41
1:A:134:ARG:NH2	2:A:405:HOH:O	2.34	0.41
1:D:110:LEU:O	1:D:114:VAL:HG23	2.19	0.41
1:D:285:LEU:HD12	1:D:285:LEU:O	2.20	0.41
1:D:36:ARG:CG	1:D:36:ARG:HH11	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:ARG:HB3	1:D:140:ARG:HE	1.49	0.41
1:A:157:PHE:O	1:A:158:ALA:C	2.59	0.41
1:C:165:GLU:O	1:C:165:GLU:HG2	2.20	0.41
1:C:97:VAL:HG22	1:C:223:GLU:OE2	2.20	0.41
1:D:299:GLN:OE1	1:D:299:GLN:CA	2.68	0.41
1:A:253:ALA:O	1:A:255:LYS:HG3	2.21	0.41
1:D:27:ASN:N	2:D:412:HOH:O	2.52	0.41
1:D:97:VAL:CG2	1:D:98:TYR:CD2	3.03	0.41
1:B:181:GLU:HG2	1:B:186:SER:HB3	2.03	0.41
1:B:60:LYS:HB3	1:B:60:LYS:HE3	1.79	0.41
1:C:266:ILE:HD12	1:C:277:VAL:HG21	2.02	0.41
1:C:9:LYS:NZ	1:C:258:GLU:O	2.54	0.41
1:D:152:GLU:OE2	1:D:155:ILE:HG12	2.20	0.41
1:C:206:PHE:HD2	1:C:292:GLN:OE1	2.04	0.41
1:D:197:TRP:HA	1:D:198:PRO:HD3	1.87	0.41
1:D:32:PHE:CE2	1:D:36:ARG:HD2	2.56	0.41
1:C:144:GLU:OE2	1:C:144:GLU:HA	2.20	0.41
1:D:167:GLU:HA	1:D:175:ILE:O	2.21	0.41
1:D:112:ASN:H	1:D:112:ASN:ND2	2.18	0.41
1:A:200:HIS:CE1	1:A:281:GLU:CA	3.03	0.41
1:A:23:ASN:N	1:A:23:ASN:HD22	2.19	0.41
1:B:194:TYR:HE1	1:B:196:ASN:O	2.04	0.41
1:B:2:GLU:N	2:B:414:HOH:O	2.54	0.41
1:C:55:LYS:NZ	1:C:57:GLU:OE1	2.43	0.41
1:D:154:PRO:HB3	1:D:161:LYS:HE2	2.03	0.41
1:A:150:TYR:HB2	1:A:167:GLU:HB2	2.04	0.40
1:A:217:ARG:HD3	1:A:217:ARG:HA	1.93	0.40
1:D:148:PRO:HG3	1:D:163:SER:CA	2.44	0.40
1:D:179:LEU:HA	1:D:187:ARG:O	2.22	0.40
1:A:192:PHE:CZ	1:A:216:MET:HA	2.56	0.40
1:A:262:VAL:HG12	1:A:266:ILE:HD12	2.02	0.40
1:B:218:LYS:NZ	2:B:415:HOH:O	2.55	0.40
1:B:298:LEU:HD23	1:B:298:LEU:HA	1.97	0.40
1:C:197:TRP:HA	1:C:198:PRO:HD3	1.82	0.40
1:C:269:MET:HG2	1:C:276:ALA:CB	2.50	0.40
1:C:57:GLU:CD	2:C:406:HOH:O	2.58	0.40
1:A:30:ARG:NH1	1:A:30:ARG:HG2	2.37	0.40
1:C:155:ILE:HG22	1:C:156:THR:N	2.37	0.40
1:D:26:ASP:OD1	1:D:28:PHE:HB2	2.20	0.40
1:A:259:GLU:HG2	1:A:259:GLU:O	2.22	0.40
1:D:207:ASP:O	1:D:211:ASP:N	2.44	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	293/311 (94%)	278 (95%)	12 (4%)	3 (1%)	19 8
1	B	290/311 (93%)	279 (96%)	8 (3%)	3 (1%)	19 8
1	C	280/311 (90%)	245 (88%)	27 (10%)	8 (3%)	6 1
1	D	274/311 (88%)	232 (85%)	36 (13%)	6 (2%)	8 1
All	All	1137/1244 (91%)	1034 (91%)	83 (7%)	20 (2%)	11 2

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	ASP
1	C	82	PRO
1	C	171	THR
1	D	171	THR
1	A	171	THR
1	C	46	LYS
1	C	184	ASN
1	D	15	GLN
1	D	165	GLU
1	A	198	PRO
1	B	21	ASP
1	C	165	GLU
1	D	182	PHE
1	D	187	ARG
1	C	166	ASP
1	B	171	THR
1	C	12	GLN
1	D	207	ASP
1	B	198	PRO
1	C	127	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	268/282 (95%)	249 (93%)	19 (7%)	18 10
1	B	265/282 (94%)	244 (92%)	21 (8%)	15 7
1	C	258/282 (92%)	231 (90%)	27 (10%)	8 2
1	D	255/282 (90%)	224 (88%)	31 (12%)	6 2
All	All	1046/1128 (93%)	948 (91%)	98 (9%)	11 4

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	13	ARG
1	A	15	GLN
1	A	34	ARG
1	A	38	LEU
1	A	55	LYS
1	A	60	LYS
1	A	83	SER
1	A	112	ASN
1	A	138	MET
1	A	162	ILE
1	A	170	ARG
1	A	183	GLN
1	A	184	ASN
1	A	188	ARG
1	A	235	CYS
1	A	285	LEU
1	A	297	GLN
1	A	299	GLN
1	B	13	ARG
1	B	21	ASP
1	B	38	LEU
1	B	46	LYS
1	B	55	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	112	ASN
1	B	138	MET
1	B	161	LYS
1	B	184	ASN
1	B	196	ASN
1	B	199	ASP
1	B	205	SER
1	B	207	ASP
1	B	235	CYS
1	B	250	LEU
1	B	251	LEU
1	B	259	GLU
1	B	266	ILE
1	B	285	LEU
1	B	297	GLN
1	B	299	GLN
1	C	1	MET
1	C	11	ILE
1	C	12	GLN
1	C	13	ARG
1	C	15	GLN
1	C	39	SER
1	C	44	THR
1	C	45	GLU
1	C	60	LYS
1	C	76	LYS
1	C	81	THR
1	C	84	GLN
1	C	85	ASP
1	C	112	ASN
1	C	128	ILE
1	C	140	ARG
1	C	150	TYR
1	C	162	ILE
1	C	167	GLU
1	C	171	THR
1	C	178	LEU
1	C	180	LEU
1	C	218	LYS
1	C	231	CYS
1	C	235	CYS
1	C	251	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	259	GLU
1	D	7	LEU
1	D	8	ARG
1	D	12	GLN
1	D	26	ASP
1	D	39	SER
1	D	43	ARG
1	D	44	THR
1	D	46	LYS
1	D	74	ARG
1	D	76	LYS
1	D	79	LEU
1	D	81	THR
1	D	83	SER
1	D	95	LYS
1	D	112	ASN
1	D	149	LEU
1	D	161	LYS
1	D	162	ILE
1	D	163	SER
1	D	171	THR
1	D	185	GLU
1	D	187	ARG
1	D	188	ARG
1	D	199	ASP
1	D	208	SER
1	D	231	CYS
1	D	251	LEU
1	D	255	LYS
1	D	261	ASN
1	D	285	LEU
1	D	296	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	23	ASN
1	A	112	ASN
1	A	183	GLN
1	A	200	HIS
1	A	264	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	12	GLN
1	B	15	GLN
1	B	23	ASN
1	B	27	ASN
1	B	112	ASN
1	B	168	GLN
1	B	264	ASN
1	C	84	GLN
1	C	112	ASN
1	C	168	GLN
1	C	183	GLN
1	C	191	GLN
1	C	196	ASN
1	C	264	ASN
1	C	299	GLN
1	D	72	HIS
1	D	112	ASN
1	D	183	GLN
1	D	196	ASN
1	D	264	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

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	296/311 (95%)	0.48	6 (2%)	68	73	21, 33, 53, 69	0
1	B	293/311 (94%)	0.45	6 (2%)	68	73	24, 33, 52, 63	0
1	C	286/311 (91%)	0.93	26 (9%)	11	12	30, 54, 74, 86	0
1	D	284/311 (91%)	0.95	27 (9%)	10	11	30, 54, 74, 84	0
All	All	1159/1244 (93%)	0.70	65 (5%)	28	32	21, 42, 71, 86	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	179	LEU	4.8
1	B	255	LYS	4.7
1	D	77	LEU	4.5
1	C	14	VAL	4.4
1	D	200	HIS	4.4
1	D	186	SER	4.1
1	D	150	TYR	3.7
1	C	154	PRO	3.7
1	D	67	ILE	3.6
1	C	174	PHE	3.6
1	D	206	PHE	3.5
1	D	42	TYR	3.5
1	C	47	ILE	3.2
1	C	42	TYR	3.2
1	D	14	VAL	3.2
1	D	59	VAL	3.2
1	C	44	THR	3.2
1	C	155	ILE	3.1
1	C	149	LEU	3.0
1	D	161	LYS	2.8
1	C	189	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	158	ALA	2.8
1	B	198	PRO	2.7
1	D	136	PHE	2.7
1	C	79	LEU	2.7
1	C	180	LEU	2.6
1	A	34	ARG	2.5
1	D	115	ILE	2.5
1	C	77	LEU	2.4
1	D	11	ILE	2.4
1	D	169	ALA	2.4
1	C	200	HIS	2.4
1	C	16	ALA	2.4
1	C	17	MET	2.4
1	D	43	ARG	2.4
1	D	79	LEU	2.3
1	D	157	PHE	2.3
1	C	84	GLN	2.3
1	C	168	GLN	2.3
1	D	17	MET	2.3
1	B	276	ALA	2.2
1	B	248	TRP	2.2
1	D	160	PHE	2.2
1	C	196	ASN	2.2
1	B	189	LEU	2.2
1	A	255	LYS	2.2
1	A	204	SER	2.2
1	D	140	ARG	2.2
1	C	185	GLU	2.2
1	D	180	LEU	2.2
1	C	136	PHE	2.1
1	C	188	ARG	2.1
1	D	148	PRO	2.1
1	B	42	TYR	2.1
1	C	156	THR	2.1
1	A	179	LEU	2.1
1	C	276	ALA	2.1
1	D	32	PHE	2.1
1	D	8	ARG	2.0
1	D	70	PHE	2.0
1	C	146	TYR	2.0
1	A	229	ILE	2.0
1	C	160	PHE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	86	SER	2.0
1	A	200	HIS	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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.