



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:32 AM UTC

PDB ID : 5D1Y / pdb_00005d1y
Title : Low resolution crystal structure of human ribonucleotide reductase alpha6 hexamer in complex with dATP
Authors : Ando, N.; Li, H.; Brignole, E.J.; Thompson, S.; McLaughlin, M.I.; Page, J.; Asturias, F.; Stubbe, J.; Drennan, C.L.
Deposited on : 2015-08-04
Resolution : 9.01 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

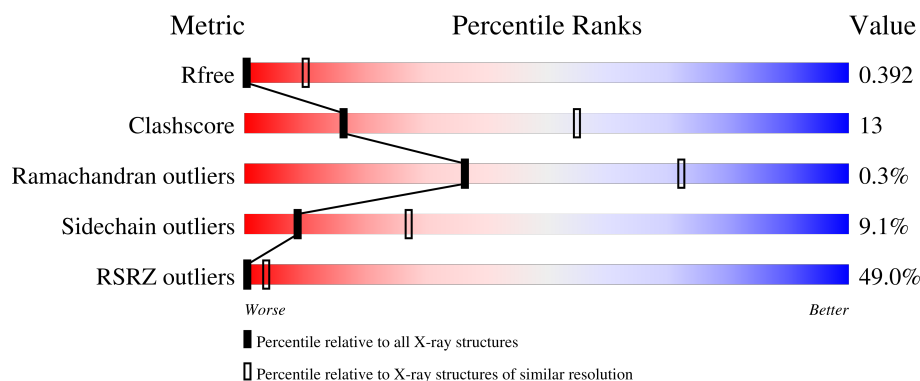
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 9.01 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}	180053	1168 (11.50-4.00)
Clashscore	190562	1001 (11.50-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

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 $\leq 5\%$. 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	812	43% 69% 16% • 12%
1	B	812	44% 73% 16% • 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11328 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 Ribonucleoside-diphosphate reductase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	714	Total	C	N	O	S	0	0	0
			5577	3567	926	1052	32			
1	B	738	Total	C	N	O	S	0	0	0
			5751	3669	968	1080	34			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P23921
A	-18	GLY	-	expression tag	UNP P23921
A	-17	SER	-	expression tag	UNP P23921
A	-16	SER	-	expression tag	UNP P23921
A	-15	HIS	-	expression tag	UNP P23921
A	-14	HIS	-	expression tag	UNP P23921
A	-13	HIS	-	expression tag	UNP P23921
A	-12	HIS	-	expression tag	UNP P23921
A	-11	HIS	-	expression tag	UNP P23921
A	-10	HIS	-	expression tag	UNP P23921
A	-9	SER	-	expression tag	UNP P23921
A	-8	SER	-	expression tag	UNP P23921
A	-7	GLY	-	expression tag	UNP P23921
A	-6	LEU	-	expression tag	UNP P23921
A	-5	VAL	-	expression tag	UNP P23921
A	-4	PRO	-	expression tag	UNP P23921
A	-3	ARG	-	expression tag	UNP P23921
A	-2	GLY	-	expression tag	UNP P23921
A	-1	SER	-	expression tag	UNP P23921
A	0	HIS	-	expression tag	UNP P23921
B	-19	MET	-	initiating methionine	UNP P23921
B	-18	GLY	-	expression tag	UNP P23921
B	-17	SER	-	expression tag	UNP P23921
B	-16	SER	-	expression tag	UNP P23921
B	-15	HIS	-	expression tag	UNP P23921

Continued on next page...

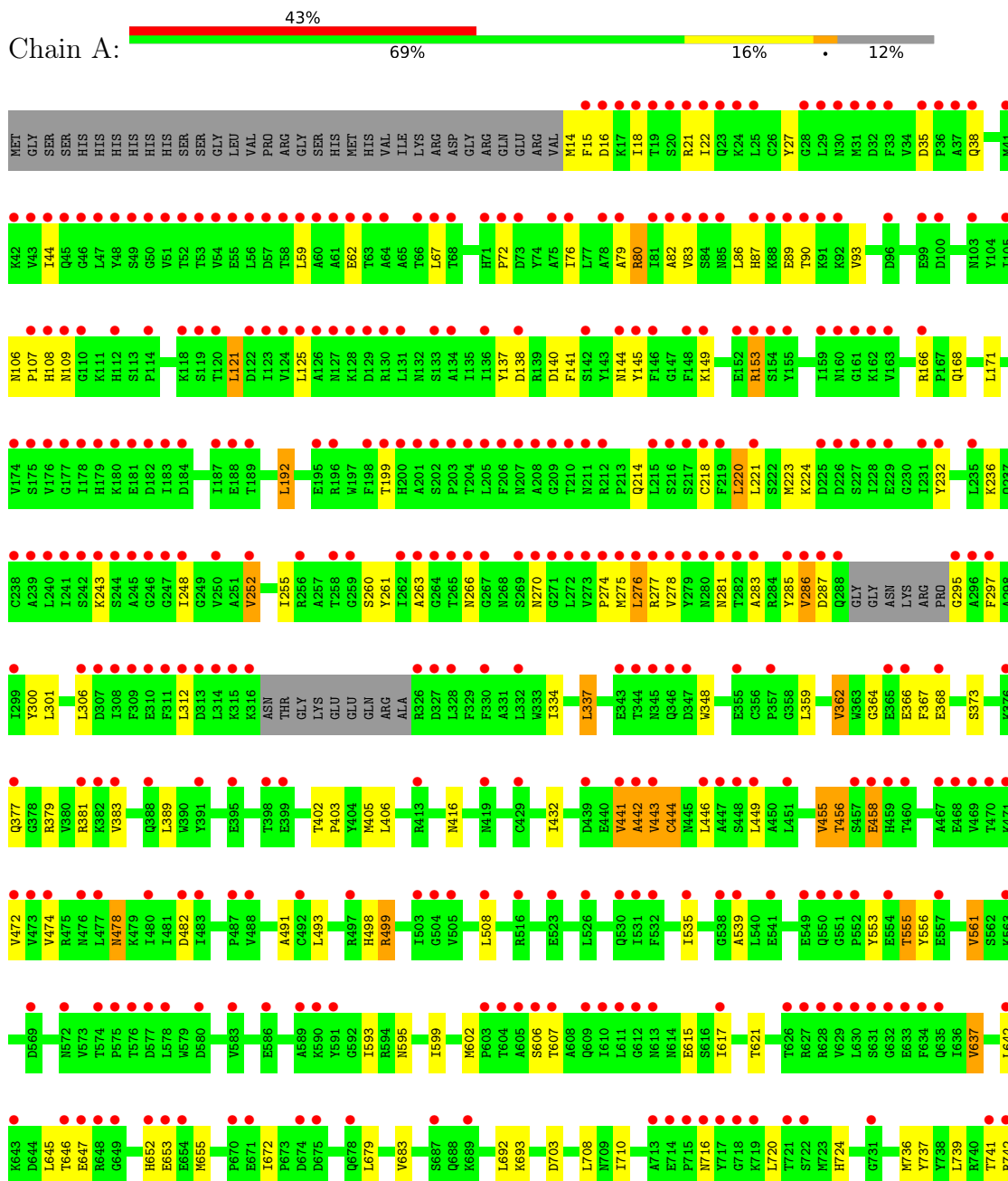
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P23921
B	-13	HIS	-	expression tag	UNP P23921
B	-12	HIS	-	expression tag	UNP P23921
B	-11	HIS	-	expression tag	UNP P23921
B	-10	HIS	-	expression tag	UNP P23921
B	-9	SER	-	expression tag	UNP P23921
B	-8	SER	-	expression tag	UNP P23921
B	-7	GLY	-	expression tag	UNP P23921
B	-6	LEU	-	expression tag	UNP P23921
B	-5	VAL	-	expression tag	UNP P23921
B	-4	PRO	-	expression tag	UNP P23921
B	-3	ARG	-	expression tag	UNP P23921
B	-2	GLY	-	expression tag	UNP P23921
B	-1	SER	-	expression tag	UNP P23921
B	0	HIS	-	expression tag	UNP P23921

3 Residue-property plots

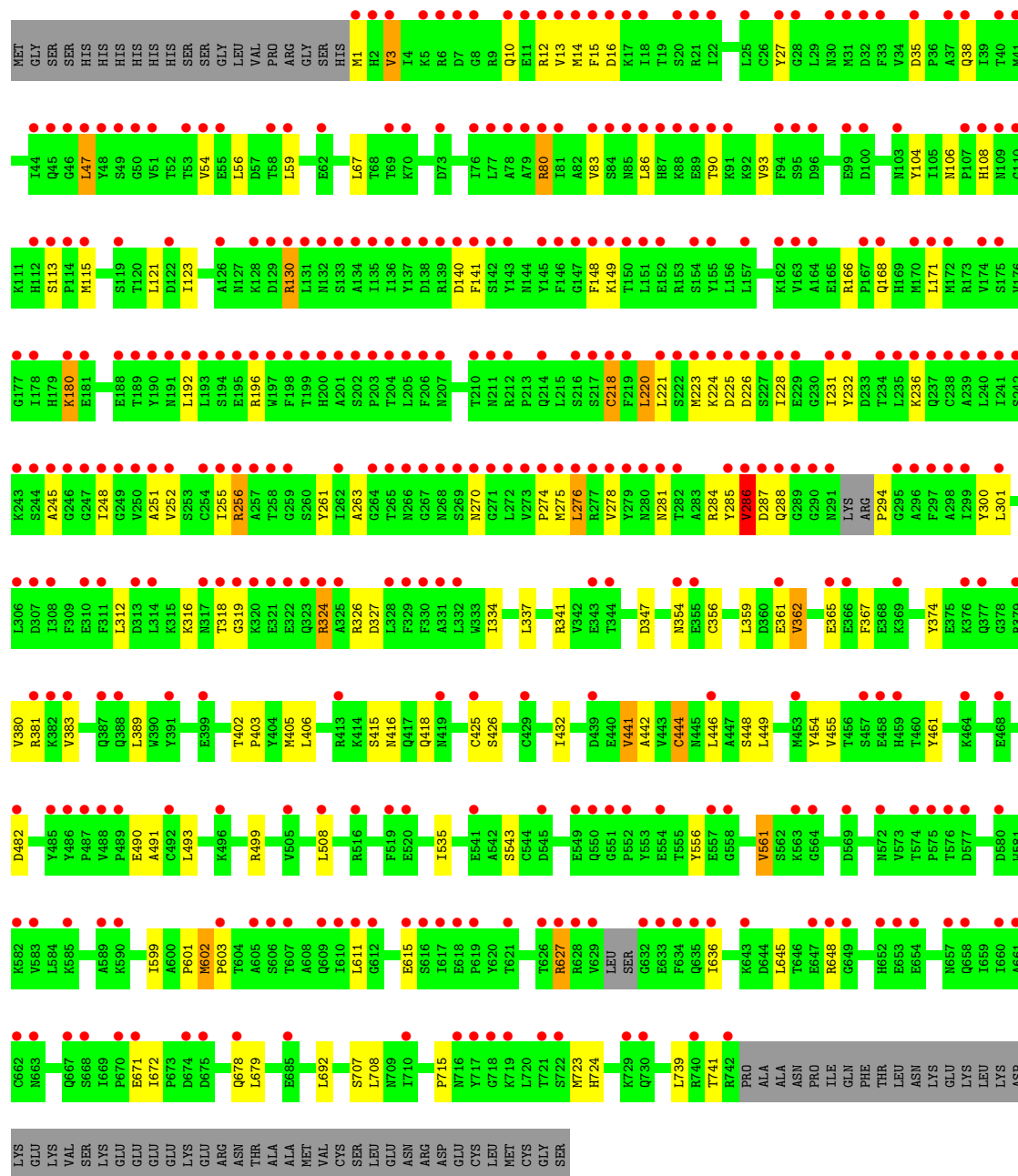
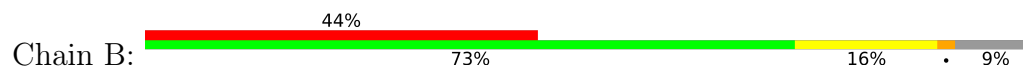
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ribonucleoside-diphosphate reductase large subunit



PRO	ALA	ALA	ASN	PRO	ILE	GLN	PHE	THR	ASN	LYS	GLY	LYS	LEU	LYS	ASP	GLY	LYS	GLY	LYS	VAL	SER	THR	ASN	THR	ALA	ALA	MET	VAL	CYS	SER	LEU	GLY	ASN	ARG	ASP	GLY	CYS	LEU	MET	CYS	GLY	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 1: Ribonucleoside-diphosphate reductase large subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	356.01Å 356.01Å 356.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.90 – 9.01 75.90 – 9.01	Depositor EDS
% Data completeness (in resolution range)	99.9 (75.90-9.01) 87.9 (75.90-9.01)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 8.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.405 , 0.426 0.388 , 0.392	Depositor DCC
R_{free} test set	707 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	407.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.03 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	11328	wwPDB-VP
Average B, all atoms (Å ²)	633.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.67	3/5699 (0.1%)	0.91	7/7751 (0.1%)
1	B	0.58	0/5876	0.88	3/7986 (0.0%)
All	All	0.63	3/11575 (0.0%)	0.89	10/15737 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	VAL	C-O	-6.39	1.17	1.24
1	A	286	VAL	CA-CB	5.33	1.60	1.53
1	A	442	ALA	CA-CB	-5.10	1.45	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	ILE	N-CA-C	6.52	115.07	107.77
1	A	334	ILE	N-CA-C	6.37	114.90	107.77
1	B	446	LEU	N-CA-C	6.08	119.11	109.50
1	A	443	VAL	CA-C-N	-5.95	112.81	122.81
1	A	443	VAL	C-N-CA	-5.95	112.81	122.81
1	A	444	CYS	N-CA-C	5.56	118.63	109.85
1	A	455	VAL	N-CA-CB	5.38	116.58	110.72
1	A	499	ARG	CA-C-N	-5.10	114.73	120.14
1	A	499	ARG	C-N-CA	-5.10	114.73	120.14
1	B	286	VAL	N-CA-C	5.02	111.58	106.21

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	5577	0	5412	201	28
1	B	5751	0	5584	184	14
All	All	11328	0	10996	290	28

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 13.

All (290) 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:261:TYR:HB2	1:B:108:HIS:CE1	1.10	1.62
1:B:83:VAL:CG1	1:B:141:PHE:HD1	1.16	1.59
1:A:281:ASN:CG	1:B:281:ASN:HB3	1.23	1.58
1:B:86:LEU:HD13	1:B:148:PHE:CE1	1.39	1.54
1:B:90:THR:CG2	1:B:140:ASP:OD1	1.63	1.43
1:A:261:TYR:CB	1:B:108:HIS:HE1	1.30	1.42
1:A:285:TYR:CD1	1:B:278:VAL:CG1	1.85	1.41
1:A:261:TYR:CB	1:B:108:HIS:CE1	2.03	1.38
1:A:106:ASN:HD22	1:B:263:ALA:CB	1.35	1.37
1:A:285:TYR:CE1	1:B:278:VAL:HG11	1.58	1.36
1:B:83:VAL:CG1	1:B:141:PHE:CD1	2.07	1.35
1:A:285:TYR:CD1	1:B:278:VAL:HG11	1.08	1.35
1:A:281:ASN:ND2	1:B:281:ASN:HB3	1.44	1.32
1:A:285:TYR:CE1	1:B:232:TYR:CZ	2.20	1.28
1:A:86:LEU:CD1	1:A:140:ASP:HB2	1.64	1.27
1:A:86:LEU:HD11	1:A:140:ASP:CB	1.67	1.25
1:A:281:ASN:CG	1:B:281:ASN:CB	2.09	1.24
1:A:90:THR:CB	1:A:137:TYR:CB	2.03	1.23
1:B:90:THR:HG23	1:B:166:ARG:CB	1.68	1.23
1:A:90:THR:CA	1:A:137:TYR:HB2	1.70	1.21
1:A:72:PRO:HG3	1:A:646:THR:CG2	1.70	1.21
1:B:90:THR:CG2	1:B:166:ARG:HD3	1.60	1.19
1:A:90:THR:HA	1:A:137:TYR:CB	1.72	1.18
1:A:232:TYR:OH	1:B:286:VAL:HB	1.05	1.18
1:A:89:GLU:O	1:A:166:ARG:NH1	1.78	1.17
1:A:90:THR:CA	1:A:137:TYR:CB	2.20	1.17
1:B:90:THR:HG22	1:B:166:ARG:HD3	1.17	1.16
1:B:83:VAL:HG12	1:B:141:PHE:HD1	1.04	1.15
1:A:236:LYS:HD2	1:B:236:LYS:HD2	1.18	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:TYR:OH	1:B:286:VAL:CB	1.95	1.13
1:B:86:LEU:CD1	1:B:148:PHE:CE1	2.31	1.12
1:A:232:TYR:CZ	1:B:286:VAL:HB	1.85	1.10
1:B:83:VAL:HG13	1:B:141:PHE:CD1	1.86	1.10
1:A:106:ASN:ND2	1:B:263:ALA:HB2	1.63	1.09
1:A:106:ASN:ND2	1:B:263:ALA:CB	2.12	1.09
1:A:236:LYS:HZ2	1:B:236:LYS:NZ	1.52	1.07
1:A:261:TYR:OH	1:B:104:TYR:HE2	1.38	1.07
1:A:281:ASN:CB	1:B:281:ASN:HB3	1.84	1.06
1:A:86:LEU:CD1	1:A:140:ASP:CB	2.28	1.06
1:B:123:ILE:CD1	1:B:180:LYS:HG2	1.86	1.05
1:A:236:LYS:NZ	1:B:236:LYS:HZ3	1.52	1.04
1:A:263:ALA:HB1	1:B:113:SER:HB3	1.40	1.04
1:A:72:PRO:HG3	1:A:646:THR:HG21	1.35	1.04
1:A:90:THR:HB	1:A:137:TYR:CB	1.83	1.04
1:B:83:VAL:HG12	1:B:141:PHE:CD1	1.79	1.02
1:A:90:THR:CB	1:A:137:TYR:HB2	1.79	1.02
1:A:263:ALA:HB1	1:B:113:SER:CB	1.90	1.01
1:B:90:THR:CG2	1:B:166:ARG:CD	2.40	0.99
1:B:90:THR:CG2	1:B:166:ARG:HB3	1.91	0.99
1:A:275:MET:O	1:B:285:TYR:CE2	2.16	0.98
1:A:261:TYR:OH	1:B:104:TYR:CE2	2.11	0.98
1:A:106:ASN:HD22	1:B:263:ALA:HB2	1.16	0.98
1:A:106:ASN:HD22	1:B:263:ALA:CA	1.77	0.97
1:A:90:THR:HA	1:A:137:TYR:HB3	1.43	0.97
1:B:83:VAL:HG13	1:B:141:PHE:HD1	1.22	0.97
1:A:86:LEU:HD11	1:A:140:ASP:HB2	0.98	0.97
1:A:285:TYR:CD1	1:B:232:TYR:OH	2.14	0.97
1:A:281:ASN:ND2	1:B:281:ASN:CB	2.25	0.96
1:A:285:TYR:CE1	1:B:232:TYR:OH	2.17	0.96
1:B:90:THR:HG23	1:B:166:ARG:HB3	0.95	0.95
1:A:106:ASN:ND2	1:B:263:ALA:CA	2.30	0.95
1:B:90:THR:HG21	1:B:140:ASP:CG	1.91	0.94
1:A:72:PRO:HG2	1:A:646:THR:HB	1.47	0.94
1:A:90:THR:HB	1:A:137:TYR:HB2	1.46	0.93
1:A:87:HIS:CD2	1:A:138:ASP:OD1	2.22	0.92
1:A:106:ASN:ND2	1:B:263:ALA:HA	1.84	0.92
1:A:90:THR:CA	1:A:137:TYR:HB3	1.90	0.91
1:A:72:PRO:CG	1:A:646:THR:HB	1.99	0.91
1:A:108:HIS:CB	1:B:261:TYR:CB	2.49	0.90
1:A:108:HIS:CB	1:B:261:TYR:CD1	2.53	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LEU:HD13	1:B:148:PHE:CZ	2.07	0.89
1:A:275:MET:HA	1:B:285:TYR:HE2	1.37	0.87
1:A:285:TYR:CD1	1:B:278:VAL:HG13	2.10	0.87
1:A:108:HIS:CB	1:B:261:TYR:CG	2.57	0.87
1:A:236:LYS:HD2	1:B:236:LYS:CD	2.04	0.87
1:B:86:LEU:CD1	1:B:148:PHE:HE1	1.77	0.87
1:B:86:LEU:HD13	1:B:148:PHE:HE1	1.12	0.86
1:A:109:ASN:HD21	1:B:263:ALA:CB	1.88	0.86
1:A:277:ARG:HH12	1:B:284:ARG:CZ	1.88	0.86
1:A:86:LEU:HD21	1:A:138:ASP:O	1.77	0.85
1:A:285:TYR:CE1	1:B:232:TYR:CE2	2.66	0.84
1:A:236:LYS:NZ	1:B:236:LYS:NZ	2.15	0.83
1:A:275:MET:HA	1:B:285:TYR:CE2	2.14	0.82
1:A:72:PRO:HG3	1:A:646:THR:CB	2.09	0.82
1:B:90:THR:HG23	1:B:166:ARG:CG	2.08	0.82
1:A:285:TYR:HE1	1:B:232:TYR:CZ	1.97	0.81
1:A:275:MET:CA	1:B:285:TYR:HE2	1.93	0.81
1:B:90:THR:HG21	1:B:140:ASP:OD1	0.67	0.80
1:A:261:TYR:CD1	1:B:106:ASN:CB	2.67	0.77
1:A:86:LEU:HD11	1:A:140:ASP:CA	2.14	0.77
1:A:109:ASN:ND2	1:B:263:ALA:HB2	1.99	0.77
1:A:263:ALA:HB1	1:B:113:SER:OG	1.84	0.76
1:A:281:ASN:HB3	1:B:281:ASN:CB	2.16	0.75
1:B:223:MET:HG2	1:B:255:ILE:HD11	1.69	0.75
1:A:72:PRO:CG	1:A:646:THR:CB	2.63	0.75
1:A:62:GLU:CG	1:A:145:TYR:CE1	2.65	0.75
1:A:109:ASN:HD21	1:B:263:ALA:HB2	1.54	0.73
1:A:655:MET:HE1	1:A:672:ILE:HD11	1.69	0.73
1:B:448:SER:HB3	1:B:602:MET:CE	2.17	0.73
1:B:196:ARG:HG2	1:B:611:LEU:HD22	1.71	0.73
1:B:83:VAL:HG11	1:B:141:PHE:HD1	1.46	0.72
1:A:106:ASN:HD22	1:B:263:ALA:HB1	1.51	0.72
1:A:86:LEU:CD2	1:A:138:ASP:O	2.37	0.72
1:B:123:ILE:HD13	1:B:180:LYS:HG2	1.70	0.72
1:A:261:TYR:CE1	1:B:106:ASN:CB	2.73	0.71
1:A:281:ASN:CB	1:B:281:ASN:CB	2.57	0.71
1:B:90:THR:CG2	1:B:166:ARG:CG	2.67	0.71
1:B:275:MET:HE2	1:B:276:LEU:HD13	1.74	0.70
1:A:285:TYR:CD1	1:B:232:TYR:CZ	2.72	0.70
1:A:275:MET:HE2	1:A:276:LEU:HD13	1.75	0.69
1:B:402:THR:HB	1:B:403:PRO:HA	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:HIS:CB	1:B:261:TYR:HB3	2.22	0.68
1:A:261:TYR:CB	1:B:108:HIS:ND1	2.57	0.67
1:A:281:ASN:CG	1:B:281:ASN:CG	2.62	0.67
1:A:223:MET:HE2	1:A:252:VAL:HG22	1.76	0.66
1:A:416:ASN:OD1	1:A:561:VAL:HG13	1.95	0.66
1:A:285:TYR:HE1	1:B:232:TYR:CE2	2.09	0.66
1:B:123:ILE:HD13	1:B:180:LYS:CG	2.26	0.66
1:A:478:ASN:HD22	1:A:499:ARG:HH11	1.44	0.65
1:A:281:ASN:OD1	1:B:281:ASN:CG	2.39	0.65
1:A:285:TYR:CE1	1:B:278:VAL:CG1	2.50	0.65
1:A:281:ASN:HB3	1:B:281:ASN:HB2	1.77	0.64
1:B:123:ILE:HD11	1:B:180:LYS:HG2	1.80	0.64
1:A:90:THR:C	1:A:137:TYR:HB2	2.22	0.64
1:A:87:HIS:HD2	1:A:138:ASP:OD1	1.76	0.63
1:A:223:MET:HG2	1:A:255:ILE:HD11	1.79	0.63
1:A:498:HIS:ND1	1:A:555:THR:HG21	2.14	0.63
1:A:285:TYR:HE2	1:B:275:MET:HA	1.64	0.62
1:B:270:ASN:HB3	1:B:274:PRO:HG2	1.80	0.62
1:A:283:ALA:HB1	1:A:295:GLY:O	2.00	0.62
1:B:218:CYS:HB3	1:B:444:CYS:SG	2.40	0.62
1:A:482:ASP:OD2	1:A:499:ARG:NH2	2.32	0.62
1:A:275:MET:C	1:B:285:TYR:HE2	2.07	0.61
1:B:220:LEU:HG	1:B:442:ALA:HB3	1.82	0.61
1:A:285:TYR:OH	1:B:231:ILE:CG2	2.49	0.61
1:B:83:VAL:HG12	1:B:141:PHE:CE1	2.34	0.61
1:B:223:MET:HE3	1:B:231:ILE:HA	1.83	0.61
1:B:226:ASP:OD1	1:B:256:ARG:HD2	2.00	0.61
1:A:90:THR:HA	1:A:137:TYR:HB2	1.46	0.60
1:B:645:LEU:HD21	1:B:672:ILE:HD12	1.83	0.60
1:A:86:LEU:CD1	1:A:140:ASP:C	2.73	0.60
1:B:123:ILE:CD1	1:B:180:LYS:CG	2.70	0.60
1:B:221:LEU:HD13	1:B:248:ILE:HG21	1.84	0.59
1:A:62:GLU:HG2	1:A:145:TYR:CE1	2.36	0.59
1:A:87:HIS:NE2	1:A:138:ASP:OD1	2.34	0.59
1:B:415:SER:O	1:B:418:GLN:HB2	2.02	0.59
1:A:86:LEU:CD1	1:A:140:ASP:HB3	2.28	0.59
1:A:153:ARG:HB2	1:A:153:ARG:HH11	1.66	0.59
1:B:448:SER:HB3	1:B:602:MET:HE1	1.83	0.59
1:A:277:ARG:HH12	1:B:284:ARG:NH2	2.00	0.59
1:A:277:ARG:NH1	1:B:284:ARG:CZ	2.61	0.59
1:A:86:LEU:HD13	1:A:140:ASP:CB	2.29	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ALA:HB2	1:B:288:GLN:OE1	2.03	0.58
1:A:275:MET:C	1:B:285:TYR:CE2	2.81	0.58
1:A:72:PRO:CG	1:A:646:THR:CG2	2.62	0.57
1:A:236:LYS:HZ2	1:B:236:LYS:HZ3	0.70	0.57
1:A:446:LEU:HB3	1:A:602:MET:HE2	1.86	0.57
1:A:456:THR:HG23	1:A:458:GLU:H	1.68	0.57
1:A:248:ILE:HD12	1:A:297:PHE:CE2	2.40	0.57
1:A:285:TYR:CB	1:B:278:VAL:HG13	2.34	0.57
1:A:72:PRO:CG	1:A:646:THR:HG21	2.22	0.57
1:A:456:THR:CG2	1:A:458:GLU:H	2.17	0.57
1:B:3:VAL:HG22	1:B:13:VAL:HG22	1.87	0.57
1:B:535:ILE:HG22	1:B:599:ILE:HD12	1.86	0.57
1:A:86:LEU:HD13	1:A:140:ASP:C	2.29	0.56
1:B:448:SER:HB3	1:B:602:MET:HE3	1.85	0.56
1:A:82:ALA:O	1:A:141:PHE:CD1	2.59	0.56
1:B:324:ARG:HG3	1:B:326:ARG:NH2	2.20	0.56
1:A:478:ASN:ND2	1:A:499:ARG:HH11	2.04	0.56
1:A:637:VAL:HG22	1:A:642:LEU:HB2	1.88	0.56
1:A:108:HIS:CB	1:B:261:TYR:HB2	2.35	0.55
1:A:362:VAL:HG22	1:A:366:GLU:HB3	1.87	0.55
1:A:72:PRO:HG3	1:A:646:THR:HG22	1.78	0.55
1:A:263:ALA:CB	1:B:113:SER:OG	2.54	0.54
1:B:1:MET:HE3	1:B:47:LEU:HD12	1.88	0.54
1:A:109:ASN:ND2	1:B:263:ALA:CB	2.59	0.53
1:A:637:VAL:HG13	1:A:642:LEU:HD22	1.90	0.53
1:A:261:TYR:CZ	1:B:104:TYR:HE2	2.24	0.53
1:A:285:TYR:CD1	1:B:232:TYR:CE2	2.97	0.53
1:B:221:LEU:HD13	1:B:248:ILE:CG2	2.38	0.53
1:A:402:THR:HB	1:A:403:PRO:HA	1.90	0.53
1:A:275:MET:CA	1:B:285:TYR:CE2	2.82	0.53
1:A:478:ASN:HD22	1:A:499:ARG:NH1	2.07	0.53
1:B:130:ARG:CG	1:B:130:ARG:HH11	2.22	0.53
1:A:275:MET:CE	1:A:276:LEU:HD13	2.38	0.52
1:A:416:ASN:CG	1:A:561:VAL:HG13	2.35	0.52
1:A:153:ARG:HB2	1:A:153:ARG:NH1	2.23	0.52
1:A:27:TYR:O	1:A:80:ARG:NH2	2.39	0.52
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.10	0.51
1:B:362:VAL:CG1	1:B:367:PHE:HA	2.40	0.51
1:B:482:ASP:OD2	1:B:499:ARG:NH2	2.44	0.51
1:A:281:ASN:ND2	1:B:281:ASN:CA	2.73	0.50
1:B:287:ASP:HB3	1:B:294:PRO:HA	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:ASN:CG	1:B:561:VAL:HG13	2.36	0.50
1:B:441:VAL:O	1:B:491:ALA:HA	2.11	0.50
1:A:645:LEU:HD13	1:A:655:MET:HE3	1.93	0.50
1:A:221:LEU:CD1	1:A:248:ILE:HG23	2.42	0.50
1:A:260:SER:OG	1:A:381:ARG:NH2	2.44	0.50
1:B:90:THR:HG22	1:B:166:ARG:CD	2.11	0.50
1:A:109:ASN:HD21	1:B:263:ALA:HB3	1.72	0.49
1:A:232:TYR:CZ	1:B:286:VAL:CB	2.78	0.49
1:B:86:LEU:HD23	1:B:140:ASP:O	2.12	0.49
1:A:121:LEU:HD22	1:A:125:LEU:HG	1.93	0.49
1:A:261:TYR:HD1	1:B:106:ASN:CB	2.23	0.49
1:A:261:TYR:CG	1:B:108:HIS:CE1	2.95	0.49
1:A:553:TYR:CE1	1:A:555:THR:HG22	2.47	0.49
1:A:285:TYR:CE1	1:B:232:TYR:CE1	2.92	0.49
1:A:535:ILE:HG22	1:A:599:ILE:HD12	1.95	0.49
1:B:83:VAL:HG11	1:B:141:PHE:CD1	2.31	0.49
1:B:482:ASP:CG	1:B:499:ARG:HH22	2.20	0.49
1:B:627:ARG:HB2	1:B:636:ILE:HD12	1.95	0.49
1:A:652:HIS:O	1:A:655:MET:HB3	2.12	0.49
1:A:86:LEU:HD13	1:A:140:ASP:HB3	1.94	0.48
1:A:621:THR:HA	1:A:683:VAL:HG12	1.95	0.48
1:B:27:TYR:O	1:B:80:ARG:NH2	2.46	0.48
1:B:356:CYS:HB3	1:B:374:TYR:CD1	2.49	0.47
1:A:364:GLY:O	1:A:368:GLU:HG3	2.14	0.47
1:A:18:ILE:O	1:A:22:ILE:HG12	2.14	0.47
1:A:277:ARG:NH1	1:B:284:ARG:NH2	2.62	0.47
1:A:35:ASP:HB3	1:A:38:GLN:HG3	1.96	0.47
1:A:655:MET:CE	1:A:672:ILE:HD11	2.41	0.46
1:A:285:TYR:CZ	1:B:232:TYR:CZ	2.96	0.46
1:A:232:TYR:OH	1:B:286:VAL:CA	2.61	0.46
1:A:86:LEU:HD12	1:A:140:ASP:HB2	1.83	0.46
1:B:627:ARG:HB2	1:B:636:ILE:CD1	2.46	0.46
1:A:86:LEU:CD1	1:A:140:ASP:CA	2.86	0.46
1:A:266:ASN:HB2	1:B:115:MET:HE3	1.98	0.46
1:B:341:ARG:HD2	1:B:347:ASP:O	2.16	0.46
1:B:90:THR:HA	1:B:166:ARG:HG2	0.81	0.46
1:A:278:VAL:N	1:B:285:TYR:CD2	2.82	0.46
1:A:362:VAL:HG13	1:A:367:PHE:HA	1.98	0.46
1:B:556:TYR:HE2	1:B:561:VAL:CG2	2.29	0.45
1:A:300:TYR:HE2	1:A:406:LEU:HD13	1.81	0.45
1:B:86:LEU:CD2	1:B:140:ASP:O	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:PRO:HD3	1:B:707:SER:OG	2.16	0.45
1:A:90:THR:HA	1:A:137:TYR:CG	2.47	0.45
1:B:319:GLY:HA3	1:B:324:ARG:NH1	2.32	0.45
1:B:406:LEU:HD22	1:B:426:SER:HB2	1.99	0.45
1:B:256:ARG:HG3	1:B:354:ASN:HB2	1.99	0.45
1:A:106:ASN:HA	1:A:107:PRO:HD3	1.83	0.45
1:A:474:VAL:HG21	1:A:539:ALA:HA	1.99	0.45
1:A:76:ILE:O	1:A:80:ARG:HG3	2.18	0.44
1:A:218:CYS:SG	1:A:432:ILE:HG13	2.58	0.44
1:A:285:TYR:OH	1:B:231:ILE:HG22	2.18	0.44
1:B:284:ARG:HD2	1:B:327:ASP:OD2	2.17	0.44
1:B:715:PRO:HG3	1:B:741:THR:HG21	1.98	0.44
1:A:285:TYR:OH	1:B:231:ILE:HG21	2.16	0.44
1:B:140:ASP:OD2	1:B:168:GLN:HG2	2.18	0.44
1:B:454:TYR:HB2	1:B:461:TYR:CZ	2.52	0.44
1:B:251:ALA:HB2	1:B:425:CYS:HB3	1.99	0.44
1:B:432:ILE:HG13	1:B:444:CYS:SG	2.58	0.44
1:B:90:THR:CB	1:B:166:ARG:CG	2.80	0.44
1:A:199:THR:HG21	1:A:607:THR:HB	2.00	0.43
1:B:221:LEU:CD1	1:B:248:ILE:CG2	2.95	0.43
1:A:278:VAL:HA	1:B:285:TYR:HB2	1.54	0.43
1:A:90:THR:OG1	1:A:138:ASP:N	2.47	0.43
1:B:405:MET:HG3	1:B:724:HIS:CE1	2.53	0.43
1:A:270:ASN:HB3	1:A:274:PRO:HG3	2.01	0.42
1:A:62:GLU:HG3	1:A:145:TYR:CE1	2.50	0.42
1:A:261:TYR:CZ	1:B:104:TYR:CE2	3.02	0.42
1:A:362:VAL:CG1	1:A:367:PHE:HA	2.49	0.42
1:B:223:MET:HE2	1:B:231:ILE:HG12	2.02	0.42
1:A:243:LYS:HD2	1:B:228:ILE:HG22	2.01	0.42
1:A:261:TYR:HB3	1:B:108:HIS:ND1	2.33	0.42
1:A:82:ALA:O	1:A:141:PHE:CE1	2.73	0.42
1:A:236:LYS:HZ3	1:B:236:LYS:NZ	2.11	0.42
1:B:300:TYR:HE2	1:B:406:LEU:HD13	1.84	0.42
1:A:220:LEU:HG	1:A:442:ALA:HB3	2.02	0.41
1:A:306:LEU:HD22	1:A:381:ARG:HG2	2.02	0.41
1:A:593:ILE:HD12	1:A:595:ASN:O	2.20	0.41
1:A:441:VAL:HG22	1:A:491:ALA:HB2	2.01	0.41
1:A:405:MET:HG3	1:A:724:HIS:CE1	2.56	0.41
1:B:123:ILE:HD12	1:B:180:LYS:HG2	1.86	0.41
1:B:441:VAL:HG13	1:B:490:GLU:HB2	2.01	0.41
1:A:192:LEU:HD23	1:A:472:VAL:HG11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ASP:O	1:B:38:GLN:HB2	2.21	0.41
1:A:79:ALA:O	1:A:83:VAL:HG23	2.21	0.41
1:B:130:ARG:CG	1:B:130:ARG:NH1	2.82	0.41
1:A:337:LEU:HD13	1:A:348:TRP:HZ3	1.86	0.41
1:A:362:VAL:HG13	1:A:367:PHE:CA	2.50	0.41
1:A:553:TYR:HE1	1:A:555:THR:HG22	1.85	0.41
1:A:261:TYR:HH	1:B:104:TYR:HE2	0.56	0.41
1:A:710:ILE:HG12	1:A:736:MET:HG3	2.03	0.41
1:B:221:LEU:CD1	1:B:248:ILE:HG23	2.51	0.41
1:A:144:ASN:OD1	1:A:144:ASN:C	2.65	0.40
1:A:285:TYR:CE2	1:B:275:MET:HA	2.50	0.40
1:A:90:THR:HG22	1:A:137:TYR:HB3	1.08	0.40
1:B:196:ARG:HG2	1:B:611:LEU:CD2	2.46	0.40
1:A:373:SER:O	1:A:377:GLN:HG3	2.21	0.40
1:A:556:TYR:HE2	1:A:561:VAL:HG22	1.87	0.40

All (28) 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:27:TYR:CD1	1:A:27:TYR:CD1[22_554]	0.73	1.47
1:A:27:TYR:CG	1:A:27:TYR:CE1[22_554]	0.90	1.30
1:A:27:TYR:CE2	1:A:27:TYR:CZ[22_554]	1.07	1.13
1:A:27:TYR:CD2	1:A:27:TYR:CZ[22_554]	1.15	1.05
1:A:27:TYR:CD2	1:A:27:TYR:CE1[22_554]	1.27	0.93
1:A:27:TYR:CE2	1:A:27:TYR:CE2[22_554]	1.27	0.93
1:A:27:TYR:CG	1:A:27:TYR:CD1[22_554]	1.45	0.75
1:A:14:MET:CE	1:B:15:PHE:O[9_555]	1.67	0.53
1:A:27:TYR:CD2	1:A:27:TYR:OH[22_554]	1.67	0.53
1:A:14:MET:CE	1:B:15:PHE:C[9_555]	1.69	0.51
1:A:27:TYR:CD1	1:A:27:TYR:CE1[22_554]	1.69	0.51
1:A:27:TYR:CE2	1:A:27:TYR:OH[22_554]	1.78	0.42
1:A:16:ASP:CB	1:B:14:MET:CG[9_555]	1.79	0.41
1:A:14:MET:CG	1:B:15:PHE:CA[9_555]	1.82	0.38
1:A:14:MET:N	1:B:16:ASP:OD2[9_555]	1.84	0.36
1:A:14:MET:CG	1:B:15:PHE:CD2[9_555]	1.86	0.34
1:A:27:TYR:CZ	1:A:27:TYR:CZ[22_554]	1.93	0.27
1:A:14:MET:CB	1:B:15:PHE:C[9_555]	1.95	0.25
1:A:15:PHE:CD2	1:B:13:VAL:O[9_555]	1.96	0.24
1:A:14:MET:SD	1:B:15:PHE:CG[9_555]	2.03	0.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:MET:CG	1:B:15:PHE:C[9_555]	2.04	0.16
1:A:27:TYR:CG	1:A:27:TYR:CZ[22_554]	2.04	0.16
1:A:14:MET:SD	1:B:15:PHE:CA[9_555]	2.05	0.15
1:A:27:TYR:CB	1:A:27:TYR:CE1[22_554]	2.06	0.14
1:A:14:MET:N	1:B:16:ASP:CG[9_555]	2.08	0.12
1:A:14:MET:CB	1:B:15:PHE:CB[9_555]	2.09	0.11
1:A:14:MET:SD	1:B:15:PHE:CD2[9_555]	2.10	0.10
1:A:27:TYR:CE1	1:A:27:TYR:CE2[22_554]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	706/812 (87%)	683 (97%)	21 (3%)	2 (0%)	36	72
1	B	730/812 (90%)	700 (96%)	28 (4%)	2 (0%)	36	72
All	All	1436/1624 (88%)	1383 (96%)	49 (3%)	4 (0%)	36	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	LYS
1	B	224	LYS
1	A	737	TYR
1	B	601	PRO

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	592/710 (83%)	539 (91%)	53 (9%)	9	27
1	B	607/710 (86%)	551 (91%)	56 (9%)	8	27
All	All	1199/1420 (84%)	1090 (91%)	109 (9%)	9	27

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	44	ILE
1	A	59	LEU
1	A	67	LEU
1	A	80	ARG
1	A	93	VAL
1	A	121	LEU
1	A	149	LYS
1	A	153	ARG
1	A	171	LEU
1	A	192	LEU
1	A	214	GLN
1	A	220	LEU
1	A	252	VAL
1	A	276	LEU
1	A	286	VAL
1	A	287	ASP
1	A	301	LEU
1	A	312	LEU
1	A	337	LEU
1	A	359	LEU
1	A	362	VAL
1	A	379	ARG
1	A	383	VAL
1	A	389	LEU
1	A	441	VAL
1	A	443	VAL
1	A	444	CYS
1	A	449	LEU
1	A	455	VAL
1	A	456	THR
1	A	458	GLU
1	A	478	ASN
1	A	493	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	508	LEU
1	A	555	THR
1	A	561	VAL
1	A	606	SER
1	A	615	GLU
1	A	617	ILE
1	A	637	VAL
1	A	647	GLU
1	A	653	GLU
1	A	679	LEU
1	A	692	LEU
1	A	693	LYS
1	A	703	ASP
1	A	708	LEU
1	A	716	ASN
1	A	720	LEU
1	A	739	LEU
1	A	741	THR
1	A	742	ARG
1	B	3	VAL
1	B	10	GLN
1	B	12	ARG
1	B	47	LEU
1	B	54	VAL
1	B	56	LEU
1	B	59	LEU
1	B	67	LEU
1	B	80	ARG
1	B	93	VAL
1	B	121	LEU
1	B	130	ARG
1	B	149	LYS
1	B	171	LEU
1	B	180	LYS
1	B	192	LEU
1	B	218	CYS
1	B	220	LEU
1	B	225	ASP
1	B	252	VAL
1	B	256	ARG
1	B	276	LEU
1	B	286	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	301	LEU
1	B	312	LEU
1	B	316	LYS
1	B	318	THR
1	B	324	ARG
1	B	337	LEU
1	B	359	LEU
1	B	361	GLU
1	B	362	VAL
1	B	365	GLU
1	B	380	VAL
1	B	381	ARG
1	B	383	VAL
1	B	389	LEU
1	B	441	VAL
1	B	444	CYS
1	B	449	LEU
1	B	455	VAL
1	B	493	LEU
1	B	508	LEU
1	B	543	SER
1	B	561	VAL
1	B	602	MET
1	B	615	GLU
1	B	627	ARG
1	B	648	ARG
1	B	671	GLU
1	B	678	GLN
1	B	679	LEU
1	B	692	LEU
1	B	708	LEU
1	B	723	MET
1	B	739	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	87	HIS
1	A	106	ASN
1	A	127	ASN
1	A	160	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	266	ASN
1	A	418	GLN
1	A	550	GLN
1	A	667	GLN
1	B	108	HIS
1	B	160	ASN
1	B	207	ASN
1	B	268	ASN
1	B	270	ASN
1	B	346	GLN
1	B	525	GLN
1	B	711	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 oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	90:THR	C	91:LYS	N	11.08
1	B	90:THR	C	91:LYS	N	5.88

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	714/812 (87%)	2.65	352 (49%) 0 3	631, 631, 660, 660	0
1	B	738/812 (90%)	2.64	360 (48%) 0 3	631, 631, 642, 642	0
All	All	1452/1624 (89%)	2.64	712 (49%) 0 3	631, 631, 660, 660	0

All (712) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	THR	21.7
1	A	288	GLN	21.4
1	A	264	GLY	20.6
1	B	265	THR	20.2
1	A	47	LEU	17.1
1	B	275	MET	16.7
1	B	276	LEU	15.1
1	A	49	SER	15.0
1	B	288	GLN	14.5
1	B	273	VAL	13.2
1	A	46	GLY	13.1
1	B	617	ILE	13.1
1	A	200	HIS	13.1
1	B	228	ILE	13.0
1	B	264	GLY	12.8
1	A	629	VAL	12.7
1	B	279	TYR	12.4
1	B	487	PRO	12.3
1	B	297	PHE	12.2
1	B	47	LEU	12.2
1	B	318	THR	12.0
1	B	272	LEU	11.5
1	B	238	CYS	11.2
1	B	319	GLY	11.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	142	SER	10.8
1	B	299	ILE	10.8
1	A	53	THR	10.5
1	B	35	ASP	10.4
1	A	177	GLY	10.1
1	B	245	ALA	10.0
1	B	146	PHE	10.0
1	A	243	LYS	10.0
1	A	28	GLY	9.9
1	A	88	LYS	9.9
1	A	470	THR	9.7
1	A	45	GLN	9.6
1	A	84	SER	9.6
1	A	227	SER	9.6
1	B	11	GLU	9.5
1	A	211	ASN	9.4
1	A	473	VAL	9.4
1	B	48	TYR	9.2
1	A	54	VAL	9.1
1	A	176	VAL	9.1
1	A	263	ALA	9.1
1	B	232	TYR	9.1
1	A	316	LYS	9.0
1	A	20	SER	8.9
1	B	626	THR	8.9
1	B	241	ILE	8.9
1	A	295	GLY	8.8
1	A	285	TYR	8.8
1	A	279	TYR	8.7
1	A	202	SER	8.7
1	B	633	GLU	8.7
1	B	13	VAL	8.6
1	B	635	GLN	8.6
1	A	50	GLY	8.6
1	B	46	GLY	8.6
1	B	32	ASP	8.5
1	A	631	SER	8.5
1	B	219	PHE	8.4
1	A	44	ILE	8.4
1	A	160	ASN	8.3
1	B	274	PRO	8.3
1	A	90	THR	8.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	627	ARG	8.2
1	A	276	LEU	8.2
1	A	52	THR	8.2
1	B	628	ARG	8.2
1	B	195	GLU	8.1
1	B	258	THR	8.1
1	A	178	ILE	8.0
1	B	311	PHE	8.0
1	B	1	MET	7.9
1	A	476	ASN	7.9
1	A	238	CYS	7.9
1	B	248	ILE	7.8
1	A	311	PHE	7.8
1	A	129	ASP	7.8
1	A	633	GLU	7.7
1	A	245	ALA	7.7
1	B	330	PHE	7.7
1	B	140	ASP	7.7
1	A	133	SER	7.6
1	A	89	GLU	7.5
1	A	287	ASP	7.5
1	B	218	CYS	7.4
1	A	212	ARG	7.4
1	B	193	LEU	7.4
1	A	722	SER	7.4
1	B	49	SER	7.4
1	A	15	PHE	7.4
1	B	174	VAL	7.3
1	B	307	ASP	7.3
1	B	246	GLY	7.3
1	A	91	LYS	7.2
1	A	632	GLY	7.2
1	A	87	HIS	7.2
1	A	228	ILE	7.1
1	B	252	VAL	7.1
1	A	630	LEU	7.0
1	B	554	GLU	7.0
1	B	634	PHE	6.9
1	B	223	MET	6.9
1	B	227	SER	6.9
1	B	247	GLY	6.9
1	A	85	ASN	6.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	192	LEU	6.8
1	B	44	ILE	6.7
1	B	323	GLN	6.7
1	B	151	LEU	6.7
1	B	145	TYR	6.7
1	A	716	ASN	6.7
1	A	472	VAL	6.7
1	A	282	THR	6.6
1	A	17	LYS	6.6
1	B	718	GLY	6.6
1	B	134	ALA	6.6
1	A	239	ALA	6.6
1	B	141	PHE	6.6
1	A	103	ASN	6.5
1	A	503	ILE	6.5
1	B	328	LEU	6.5
1	B	632	GLY	6.5
1	A	161	GLY	6.5
1	A	262	ILE	6.5
1	A	226	ASP	6.5
1	B	629	VAL	6.5
1	B	618	GLU	6.5
1	B	89	GLU	6.4
1	B	150	THR	6.4
1	A	365	GLU	6.4
1	A	43	VAL	6.4
1	A	48	TYR	6.4
1	B	244	SER	6.4
1	A	199	THR	6.4
1	B	278	VAL	6.4
1	B	139	ARG	6.3
1	B	167	PRO	6.3
1	A	718	GLY	6.3
1	B	143	TYR	6.3
1	B	16	ASP	6.2
1	A	60	ALA	6.2
1	B	133	SER	6.2
1	B	369	LYS	6.2
1	B	6	ARG	6.2
1	B	250	VAL	6.2
1	A	286	VAL	6.1
1	B	45	GLN	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	202	SER	6.1
1	B	270	ASN	6.1
1	A	180	LYS	6.1
1	A	21	ARG	6.0
1	B	87	HIS	6.0
1	A	550	GLN	6.0
1	A	23	GLN	5.9
1	A	717	TYR	5.9
1	A	272	LEU	5.9
1	A	689	LYS	5.9
1	B	262	ILE	5.9
1	B	231	ILE	5.9
1	A	162	LYS	5.9
1	B	200	HIS	5.9
1	B	191	ASN	5.9
1	A	647	GLU	5.8
1	B	557	GLU	5.8
1	A	256	ARG	5.8
1	A	328	LEU	5.7
1	B	320	LYS	5.7
1	A	557	GLU	5.7
1	B	271	GLY	5.7
1	B	343	GLU	5.7
1	B	290	GLY	5.7
1	B	221	LEU	5.7
1	B	12	ARG	5.7
1	A	58	THR	5.7
1	B	110	GLY	5.7
1	B	365	GLU	5.6
1	B	136	ILE	5.6
1	A	201	ALA	5.6
1	A	574	THR	5.6
1	A	626	THR	5.6
1	B	492	CYS	5.6
1	A	309	PHE	5.5
1	A	366	GLU	5.5
1	B	577	ASP	5.5
1	B	196	ARG	5.5
1	A	314	LEU	5.5
1	A	326	ARG	5.5
1	A	152	GLU	5.5
1	B	197	TRP	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2	HIS	5.5
1	B	610	ILE	5.5
1	A	57	ASP	5.4
1	B	674	ASP	5.4
1	A	109	ASN	5.4
1	B	55	GLU	5.4
1	B	574	THR	5.4
1	B	663	ASN	5.4
1	A	35	ASP	5.4
1	B	668	SER	5.4
1	B	178	ILE	5.4
1	B	189	THR	5.4
1	A	217	SER	5.4
1	B	722	SER	5.3
1	A	219	PHE	5.3
1	B	198	PHE	5.3
1	B	322	GLU	5.3
1	A	92	LYS	5.3
1	B	308	ILE	5.3
1	B	282	THR	5.2
1	B	296	ALA	5.2
1	B	175	SER	5.2
1	A	38	GLN	5.2
1	B	131	LEU	5.2
1	B	661	ALA	5.2
1	B	217	SER	5.2
1	A	576	THR	5.2
1	A	474	VAL	5.2
1	A	577	ASP	5.1
1	B	317	ASN	5.1
1	B	508	LEU	5.1
1	A	535	ILE	5.1
1	A	270	ASN	5.1
1	A	297	PHE	5.1
1	B	86	LEU	5.1
1	A	606	SER	5.1
1	A	306	LEU	5.1
1	B	148	PHE	5.0
1	A	652	HIS	5.0
1	A	183	ILE	5.0
1	A	299	ILE	5.0
1	A	382	LYS	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	171	LEU	5.0
1	A	471	LYS	5.0
1	B	660	ILE	5.0
1	A	232	TYR	5.0
1	B	51	VAL	4.9
1	B	289	GLY	4.9
1	A	181	GLU	4.9
1	A	449	LEU	4.9
1	A	134	ALA	4.9
1	B	112	HIS	4.8
1	B	226	ASP	4.8
1	A	539	ALA	4.8
1	A	643	LYS	4.8
1	A	714	GLU	4.8
1	A	687	SER	4.8
1	A	628	ARG	4.8
1	B	721	THR	4.7
1	A	123	ILE	4.7
1	A	310	GLU	4.7
1	B	267	GLY	4.7
1	A	41	MET	4.7
1	A	204	THR	4.7
1	B	485	TYR	4.7
1	B	277	ARG	4.7
1	A	469	VAL	4.7
1	A	307	ASP	4.7
1	B	606	SER	4.7
1	A	76	ILE	4.7
1	B	729	LYS	4.7
1	A	447	ALA	4.7
1	A	56	LEU	4.6
1	A	235	LEU	4.6
1	B	103	ASN	4.6
1	B	580	ASP	4.6
1	B	15	PHE	4.6
1	B	242	SER	4.6
1	B	306	LEU	4.6
1	B	41	MET	4.6
1	B	135	ILE	4.6
1	A	18	ILE	4.6
1	A	55	GLU	4.6
1	B	83	VAL	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	177	GLY	4.5
1	B	605	ALA	4.5
1	A	51	VAL	4.5
1	A	313	ASP	4.5
1	A	482	ASP	4.5
1	B	564	GLY	4.5
1	A	99	GLU	4.5
1	B	130	ARG	4.5
1	A	634	PHE	4.5
1	B	332	LEU	4.5
1	B	109	ASN	4.5
1	B	331	ALA	4.5
1	B	199	THR	4.5
1	A	266	ASN	4.5
1	B	291	ASN	4.5
1	A	541	GLU	4.5
1	B	329	PHE	4.4
1	A	122	ASP	4.4
1	B	77	LEU	4.4
1	B	298	ALA	4.4
1	A	399	GLU	4.4
1	B	188	GLU	4.4
1	B	147	GLY	4.4
1	A	153	ARG	4.4
1	B	38	GLN	4.4
1	A	205	LEU	4.4
1	B	138	ASP	4.4
1	A	504	GLY	4.4
1	B	21	ARG	4.4
1	B	488	VAL	4.4
1	B	243	LYS	4.4
1	B	439	ASP	4.4
1	A	343	GLU	4.4
1	B	129	ASP	4.3
1	A	174	VAL	4.3
1	A	108	HIS	4.3
1	A	459	HIS	4.3
1	B	33	PHE	4.3
1	A	166	ARG	4.3
1	A	586	GLU	4.3
1	B	239	ALA	4.3
1	B	88	LYS	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	269	SER	4.3
1	A	275	MET	4.3
1	A	607	THR	4.2
1	B	391	TYR	4.2
1	A	32	ASP	4.2
1	A	649	GLY	4.2
1	B	457	SER	4.2
1	A	107	PRO	4.2
1	B	429	CYS	4.2
1	B	162	LYS	4.2
1	B	675	ASP	4.2
1	B	285	TYR	4.1
1	A	391	TYR	4.1
1	A	612	GLY	4.1
1	B	172	MET	4.1
1	A	480	ILE	4.1
1	A	33	PHE	4.1
1	B	211	ASN	4.1
1	B	603	PRO	4.1
1	B	91	LYS	4.1
1	A	155	TYR	4.1
1	A	487	PRO	4.1
1	B	194	SER	4.1
1	A	19	THR	4.0
1	B	657	ASN	4.0
1	A	154	SER	4.0
1	B	119	SER	4.0
1	B	671	GLU	4.0
1	A	124	VAL	4.0
1	A	258	THR	4.0
1	A	315	LYS	4.0
1	A	590	LYS	4.0
1	B	94	PHE	4.0
1	B	235	LEU	4.0
1	B	149	LYS	4.0
1	B	670	PRO	4.0
1	B	662	CYS	4.0
1	A	578	LEU	3.9
1	A	75	ALA	3.9
1	A	66	THR	3.9
1	B	58	THR	3.9
1	A	110	GLY	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	572	ASN	3.9
1	B	155	TYR	3.9
1	A	37	ALA	3.9
1	B	205	LEU	3.8
1	A	146	PHE	3.8
1	A	654	GLU	3.8
1	B	168	GLN	3.8
1	A	100	ASP	3.8
1	A	549	GLU	3.8
1	A	247	GLY	3.8
1	B	259	GLY	3.8
1	A	719	LYS	3.8
1	A	741	THR	3.8
1	A	145	TYR	3.8
1	A	225	ASP	3.8
1	B	81	ILE	3.8
1	B	251	ALA	3.8
1	B	170	MET	3.8
1	A	439	ASP	3.8
1	A	554	GLU	3.8
1	B	268	ASN	3.7
1	B	387	GLN	3.7
1	A	267	GLY	3.7
1	A	330	PHE	3.7
1	A	119	SER	3.7
1	A	278	VAL	3.7
1	B	84	SER	3.7
1	A	477	LEU	3.7
1	B	100	ASP	3.7
1	B	459	HIS	3.7
1	A	118	LYS	3.7
1	A	179	HIS	3.7
1	B	653	GLU	3.7
1	B	286	VAL	3.6
1	B	496	LYS	3.6
1	A	120	THR	3.6
1	B	654	GLU	3.6
1	B	376	LYS	3.6
1	B	222	SER	3.6
1	B	229	GLU	3.6
1	A	742	ARG	3.6
1	B	207	ASN	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	81	ILE	3.6
1	B	295	GLY	3.6
1	A	492	CYS	3.5
1	B	22	ILE	3.5
1	A	675	ASP	3.5
1	B	355	GLU	3.5
1	A	296	ALA	3.5
1	B	287	ASP	3.5
1	A	72	PRO	3.5
1	B	582	LYS	3.5
1	B	545	ASP	3.5
1	B	206	PHE	3.5
1	A	381	ARG	3.4
1	A	269	SER	3.4
1	B	611	LEU	3.4
1	B	5	LYS	3.4
1	B	114	PRO	3.4
1	B	53	THR	3.4
1	A	148	PHE	3.4
1	B	249	GLY	3.4
1	B	619	PRO	3.4
1	B	667	GLN	3.4
1	A	617	ILE	3.4
1	A	127	ASN	3.4
1	B	379	ARG	3.4
1	A	61	ALA	3.4
1	A	383	VAL	3.4
1	B	20	SER	3.4
1	A	105	ILE	3.4
1	B	399	GLU	3.4
1	A	589	ALA	3.3
1	B	324	ARG	3.3
1	A	59	LEU	3.3
1	A	175	SER	3.3
1	B	607	THR	3.3
1	B	382	LYS	3.3
1	A	273	VAL	3.3
1	B	28	GLY	3.3
1	B	157	LEU	3.3
1	A	82	ALA	3.3
1	A	671	GLU	3.3
1	A	142	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	152	GLU	3.3
1	A	246	GLY	3.3
1	B	122	ASP	3.3
1	A	198	PHE	3.3
1	A	163	VAL	3.3
1	A	419	ASN	3.3
1	A	131	LEU	3.3
1	B	234	THR	3.3
1	B	18	ILE	3.3
1	B	50	GLY	3.3
1	A	605	ALA	3.3
1	B	541	GLU	3.2
1	A	713	ALA	3.2
1	B	212	ARG	3.2
1	A	395	GLU	3.2
1	A	346	GLN	3.2
1	B	31	MET	3.2
1	B	552	PRO	3.2
1	B	163	VAL	3.2
1	B	14	MET	3.2
1	B	321	GLU	3.2
1	A	73	ASP	3.2
1	B	225	ASP	3.2
1	B	383	VAL	3.2
1	B	128	LYS	3.2
1	B	575	PRO	3.2
1	A	24	LYS	3.1
1	B	569	ASP	3.2
1	A	603	PRO	3.1
1	A	532	PHE	3.1
1	B	583	VAL	3.1
1	B	255	ILE	3.1
1	A	523	GLU	3.1
1	A	526	LEU	3.1
1	B	301	LEU	3.1
1	B	69	THR	3.1
1	B	62	GLU	3.1
1	A	68	THR	3.1
1	B	551	GLY	3.1
1	B	237	GLN	3.0
1	B	550	GLN	3.0
1	B	354	ASN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	30	ASN	3.0
1	B	616	SER	3.0
1	B	115	MET	3.0
1	B	254	CYS	3.0
1	B	17	LYS	3.0
1	A	613	ASN	3.0
1	A	203	PRO	3.0
1	B	482	ASP	3.0
1	B	201	ALA	3.0
1	B	256	ARG	3.0
1	A	347	ASP	3.0
1	B	257	ALA	3.0
1	B	615	GLU	3.0
1	A	277	ARG	3.0
1	A	388	GLN	3.0
1	B	652	HIS	2.9
1	B	325	ALA	2.9
1	B	572	ASN	2.9
1	B	458	GLU	2.9
1	A	221	LEU	2.9
1	A	377	GLN	2.9
1	A	580	ASP	2.9
1	A	721	THR	2.9
1	B	90	THR	2.9
1	A	31	MET	2.9
1	A	241	ILE	2.9
1	A	196	ARG	2.9
1	B	719	LYS	2.9
1	B	486	TYR	2.9
1	B	717	TYR	2.9
1	A	126	ALA	2.9
1	B	366	GLU	2.9
1	B	464	LYS	2.9
1	B	710	ILE	2.9
1	A	242	SER	2.9
1	B	132	ASN	2.9
1	B	576	THR	2.8
1	A	62	GLU	2.8
1	A	63	THR	2.8
1	B	95	SER	2.8
1	A	674	ASP	2.8
1	B	190	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	159	ILE	2.8
1	A	182	ASP	2.8
1	A	207	ASN	2.8
1	B	266	ASN	2.8
1	A	83	VAL	2.8
1	A	208	ALA	2.8
1	B	164	ALA	2.8
1	A	429	CYS	2.8
1	B	742	ARG	2.8
1	A	530	GLN	2.8
1	B	126	ALA	2.8
1	A	25	LEU	2.8
1	A	206	PHE	2.8
1	B	361	GLU	2.7
1	A	231	ILE	2.7
1	A	538	GLY	2.7
1	A	446	LEU	2.7
1	A	610	ILE	2.7
1	A	516	ARG	2.7
1	B	96	ASP	2.7
1	B	37	ALA	2.7
1	A	670	PRO	2.7
1	B	310	GLU	2.7
1	B	381	ARG	2.7
1	A	678	GLN	2.7
1	B	388	GLN	2.7
1	B	425	CYS	2.7
1	B	516	ARG	2.7
1	A	244	SER	2.7
1	B	7	ASP	2.7
1	A	248	ILE	2.7
1	B	80	ARG	2.7
1	B	647	GLU	2.7
1	B	649	GLY	2.7
1	A	458	GLU	2.7
1	B	70	LYS	2.6
1	B	648	ARG	2.6
1	A	138	ASP	2.6
1	A	483	ILE	2.6
1	B	281	ASN	2.6
1	A	653	GLU	2.6
1	A	448	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	648	ARG	2.6
1	B	240	LEU	2.6
1	A	531	ILE	2.6
1	B	59	LEU	2.6
1	A	355	GLU	2.6
1	B	489	PRO	2.6
1	A	497	ARG	2.6
1	A	552	PRO	2.6
1	B	236	LYS	2.6
1	B	313	ASP	2.6
1	A	136	ILE	2.6
1	A	218	CYS	2.6
1	A	468	GLU	2.6
1	B	730	GLN	2.6
1	A	413	ARG	2.6
1	B	280	ASN	2.6
1	B	505	VAL	2.6
1	B	609	GLN	2.5
1	A	646	THR	2.5
1	B	25	LEU	2.5
1	A	30	ASN	2.5
1	A	210	THR	2.5
1	A	604	THR	2.5
1	A	271	GLY	2.5
1	A	505	VAL	2.5
1	B	154	SER	2.5
1	A	209	GLY	2.5
1	A	250	VAL	2.5
1	A	627	ARG	2.5
1	B	612	GLY	2.5
1	B	10	GLN	2.5
1	A	563	LYS	2.5
1	B	590	LYS	2.5
1	A	345	ASN	2.5
1	B	419	ASN	2.5
1	A	259	GLY	2.5
1	B	678	GLN	2.5
1	A	16	ASP	2.5
1	B	79	ALA	2.5
1	A	308	ILE	2.5
1	B	76	ILE	2.5
1	A	575	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	130	ARG	2.5
1	A	467	ALA	2.5
1	B	643	LYS	2.5
1	A	29	LEU	2.4
1	A	398	THR	2.4
1	B	210	THR	2.4
1	A	195	GLU	2.4
1	A	457	SER	2.4
1	B	137	TYR	2.4
1	B	3	VAL	2.4
1	B	446	LEU	2.4
1	A	344	THR	2.4
1	A	79	ALA	2.4
1	A	281	ASN	2.4
1	A	327	ASP	2.4
1	A	551	GLY	2.4
1	B	377	GLN	2.4
1	A	642	LEU	2.4
1	B	520	GLU	2.4
1	A	216	SER	2.4
1	A	731	GLY	2.4
1	B	8	GLY	2.4
1	A	569	ASP	2.4
1	A	67	LEU	2.4
1	A	125	LEU	2.4
1	B	563	LYS	2.4
1	A	357	PRO	2.3
1	A	187	ILE	2.3
1	A	128	LYS	2.3
1	B	558	GLY	2.3
1	B	636	ILE	2.3
1	A	280	ASN	2.3
1	A	252	VAL	2.3
1	B	224	LYS	2.3
1	B	585	LYS	2.3
1	A	22	ILE	2.3
1	A	488	VAL	2.3
1	A	591	TYR	2.3
1	B	108	HIS	2.3
1	A	229	GLU	2.3
1	B	453	MET	2.3
1	B	40	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	508	LEU	2.3
1	B	589	ALA	2.3
1	A	215	LEU	2.2
1	A	441	VAL	2.2
1	A	609	GLN	2.2
1	B	344	THR	2.2
1	B	621	THR	2.2
1	A	114	PRO	2.2
1	B	413	ARG	2.2
1	A	368	GLU	2.2
1	B	181	GLU	2.2
1	B	658	GLN	2.2
1	B	107	PRO	2.2
1	B	716	ASN	2.2
1	B	740	ARG	2.2
1	A	71	HIS	2.2
1	B	113	SER	2.2
1	A	78	ALA	2.2
1	B	180	LYS	2.2
1	B	99	GLU	2.2
1	B	549	GLU	2.2
1	A	64	ALA	2.2
1	A	442	ALA	2.1
1	B	519	PHE	2.1
1	B	85	ASN	2.1
1	B	314	LEU	2.1
1	B	27	TYR	2.1
1	B	78	ALA	2.1
1	A	274	PRO	2.1
1	A	42	LYS	2.1
1	A	611	LEU	2.1
1	A	189	THR	2.1
1	A	283	ALA	2.1
1	B	685	GLU	2.1
1	A	144	ASN	2.1
1	A	149	LYS	2.1
1	A	312	LEU	2.1
1	A	332	LEU	2.1
1	A	376	LYS	2.1
1	A	451	LEU	2.1
1	B	214	GLN	2.1
1	A	715	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	203	PRO	2.1
1	B	54	VAL	2.1
1	A	583	VAL	2.1
1	A	96	ASP	2.0
1	A	443	VAL	2.0
1	A	240	LEU	2.0
1	A	184	ASP	2.0
1	B	73	ASP	2.0
1	A	112	HIS	2.0
1	A	188	GLU	2.0
1	A	460	THR	2.0
1	B	204	THR	2.0
1	B	216	SER	2.0
1	A	36	PRO	2.0
1	A	635	GLN	2.0
1	B	468	GLU	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 oligosaccharides 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.