



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:12 PM UTC

PDB ID : 4KSD / pdb_00004ksd
Title : Structures of P-glycoprotein reveal its conformational flexibility and an epitope on the nucleotide-binding domain
Authors : Ward, A.; Szewczyk, P.; Grimard, V.; Lee, C.-W.; Martinez, L.; Doshi, R.; Caya, A.; Villaluz, M.; Pardon, E.; Cregger, C.; Swartz, D.J.; Falson, P.; Urbatsch, I.; Govaerts, C.; Steyaert, J.; Chang, G.
Deposited on : 2013-05-17
Resolution : 4.10 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

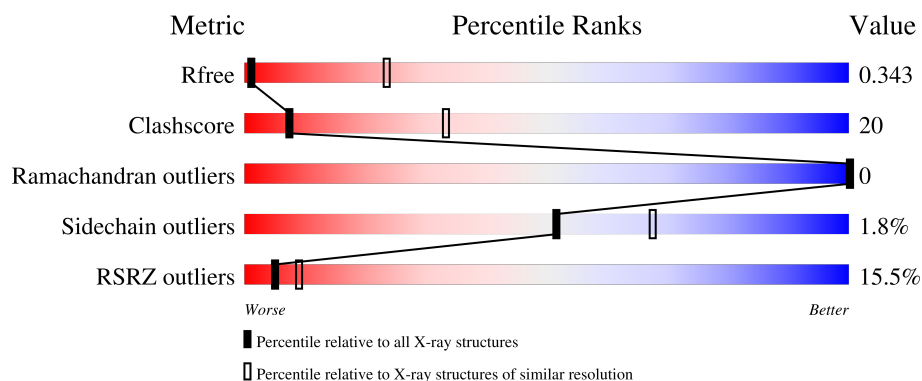
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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 $\leq 5\%$. 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	1284	13% 57% 33% 8%
2	B	124	29% 47% 48% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10084 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 Multidrug resistance protein 1A.

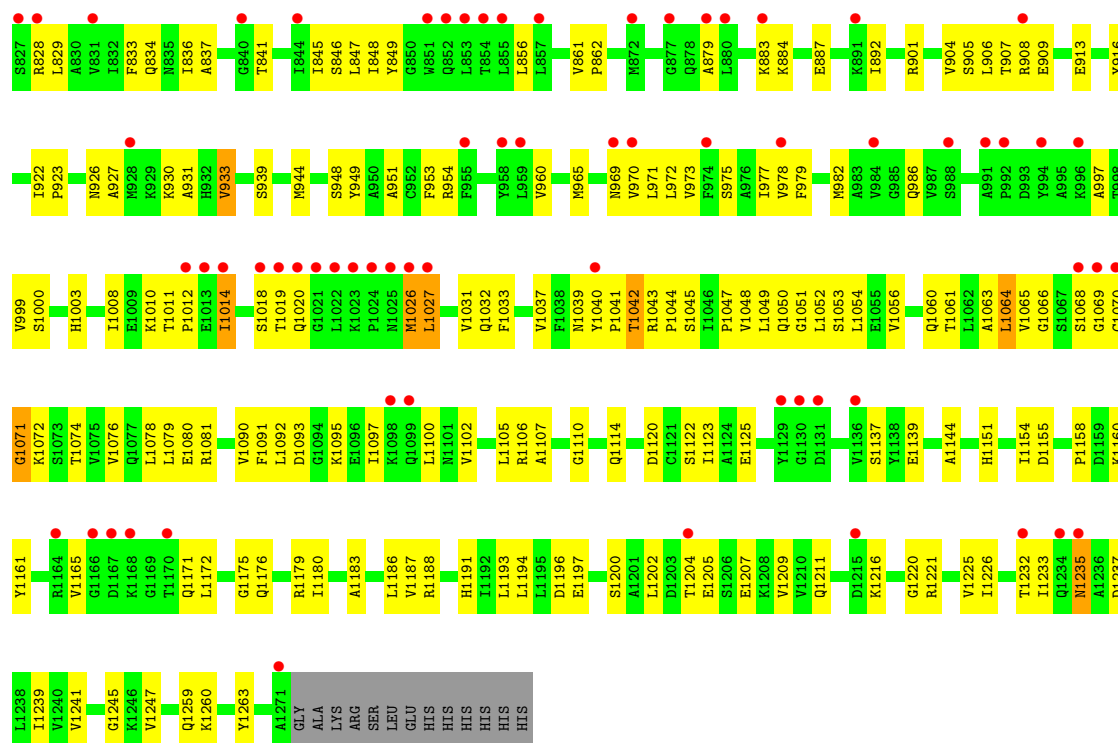
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1182	Total	C	N	O	S	0	0	0
			9171	5895	1552	1686	38			

There are 8 discrepancies between the modelled and reference sequences:

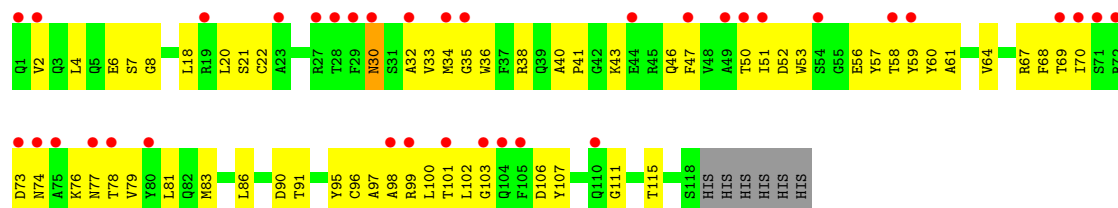
Chain	Residue	Modelled	Actual	Comment	Reference
A	1277	LEU	-	expression tag	UNP P21447
A	1278	GLU	-	expression tag	UNP P21447
A	1279	HIS	-	expression tag	UNP P21447
A	1280	HIS	-	expression tag	UNP P21447
A	1281	HIS	-	expression tag	UNP P21447
A	1282	HIS	-	expression tag	UNP P21447
A	1283	HIS	-	expression tag	UNP P21447
A	1284	HIS	-	expression tag	UNP P21447

- Molecule 2 is a protein called R2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	118	Total	C	N	O	S	8	0	0
			913	573	159	177	4			



• Molecule 2: R2 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.10Å 102.47Å 312.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.07 – 4.10 61.07 – 4.10	Depositor EDS
% Data completeness (in resolution range)	95.7 (61.07-4.10) 95.7 (61.07-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.43 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309), CNS	Depositor
R, R_{free}	0.323 , 0.344 0.322 , 0.343	Depositor DCC
R_{free} test set	1062 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	95.8	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 130.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.25$, $\langle L^2 \rangle = 0.09$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.66	EDS
Total number of atoms	10084	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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	0.40	0/9339	0.91	20/12626 (0.2%)
2	B	0.43	0/932	1.00	2/1261 (0.2%)
All	All	0.41	0/10271	0.92	22/13887 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	30	ASN	N-CA-C	10.75	122.75	111.14
1	A	1042	THR	N-CA-C	-8.61	92.90	107.80
1	A	1026	MET	N-CA-C	7.92	121.98	107.73
1	A	689	PRO	N-CA-C	6.92	119.14	110.70
1	A	623	MET	N-CA-C	6.81	118.79	111.36
1	A	515	GLN	CB-CA-C	-6.20	109.41	116.54
1	A	1071	GLY	N-CA-C	-6.10	106.07	114.67
1	A	317	VAL	CB-CA-C	-6.05	106.57	111.71
1	A	377	SER	CB-CA-C	-6.01	109.63	116.54
2	B	102	LEU	N-CA-C	-5.72	105.04	111.28
1	A	367	ASN	CB-CA-C	-5.53	109.21	115.79
1	A	1014	ILE	N-CA-C	5.48	116.66	108.54
1	A	162	HIS	N-CA-C	5.32	117.95	109.02
1	A	740	PRO	CA-C-N	-5.26	114.83	120.03
1	A	740	PRO	C-N-CA	-5.26	114.83	120.03
1	A	162	HIS	CB-CA-C	-5.24	108.97	115.89
1	A	376	LYS	N-CA-C	5.22	116.92	109.14
1	A	166	GLU	N-CA-C	-5.21	105.66	112.23
1	A	1031	VAL	N-CA-C	5.20	116.18	108.23
1	A	163	ASP	N-CA-C	5.17	119.86	113.50
1	A	585	LEU	N-CA-C	5.09	119.55	113.23
1	A	933	VAL	N-CA-C	5.03	115.26	110.53

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	9171	0	9344	354	0
2	B	913	0	877	71	0
All	All	10084	0	10221	413	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 (413) 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:704:TRP:CZ2	1:A:707:PHE:HB2	1.43	1.51
1:A:310:PHE:CE1	1:A:332:PHE:CE2	2.20	1.29
1:A:310:PHE:CE1	1:A:332:PHE:CZ	2.25	1.24
1:A:1026:MET:C	1:A:1027:LEU:HD12	1.67	1.17
1:A:704:TRP:CZ2	1:A:707:PHE:CB	2.29	1.15
1:A:707:PHE:CE2	1:A:776:ALA:HB2	1.87	1.08
1:A:310:PHE:CZ	1:A:332:PHE:CE2	2.41	1.07
1:A:306:TYR:CD1	1:A:332:PHE:CE1	2.42	1.06
1:A:584:ARG:HD2	2:B:101:THR:HG23	1.05	1.04
1:A:704:TRP:HZ2	1:A:707:PHE:CB	1.66	1.04
1:A:584:ARG:HD2	2:B:101:THR:CG2	1.86	1.04
1:A:306:TYR:CE1	1:A:332:PHE:CE1	2.48	1.02
1:A:704:TRP:CE2	1:A:707:PHE:HB2	1.96	1.01
1:A:704:TRP:NE1	1:A:707:PHE:CD2	2.29	1.00
1:A:310:PHE:CE1	1:A:332:PHE:HE2	1.70	0.98
1:A:584:ARG:CD	2:B:101:THR:HG23	1.93	0.97
1:A:310:PHE:CZ	1:A:332:PHE:CZ	2.53	0.95
1:A:310:PHE:HE1	1:A:332:PHE:CE2	1.71	0.95
1:A:310:PHE:CE1	1:A:332:PHE:HZ	1.81	0.93
1:A:704:TRP:HE1	1:A:707:PHE:HD2	0.95	0.92
1:A:707:PHE:CD2	1:A:776:ALA:HB2	2.07	0.90
2:B:33:VAL:HG12	2:B:53:TRP:H	1.37	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:TRP:HZ2	1:A:707:PHE:HB2	1.12	0.89
2:B:33:VAL:HG22	2:B:99:ARG:HD3	1.55	0.86
2:B:91:THR:HG23	2:B:115:THR:HA	1.57	0.84
2:B:36:TRP:CD2	2:B:81:LEU:HD21	2.14	0.81
1:A:306:TYR:CE1	1:A:332:PHE:CD1	2.68	0.81
1:A:704:TRP:NE1	1:A:707:PHE:HD2	1.74	0.79
2:B:38:ARG:HG3	2:B:46:GLN:HG3	1.64	0.79
1:A:1110:GLY:HA3	1:A:1193:LEU:HA	1.66	0.78
1:A:707:PHE:CE2	1:A:776:ALA:CB	2.65	0.78
1:A:369:PRO:O	1:A:371:ILE:HG23	1.84	0.76
2:B:33:VAL:H	2:B:99:ARG:HB2	1.50	0.75
1:A:132:TRP:HD1	1:A:133:CYS:HG	1.34	0.75
1:A:370:SER:O	1:A:371:ILE:HG12	1.87	0.74
1:A:310:PHE:HE1	1:A:332:PHE:HE2	1.09	0.74
1:A:707:PHE:HE2	1:A:776:ALA:HB2	1.50	0.74
1:A:228:TRP:HZ2	1:A:295:MET:HB2	1.52	0.73
1:A:329:THR:HA	1:A:332:PHE:HD2	1.53	0.73
1:A:132:TRP:HB2	1:A:184:ASP:HB3	1.70	0.73
1:A:707:PHE:HE2	1:A:776:ALA:CB	2.00	0.73
2:B:33:VAL:CG2	2:B:99:ARG:HD3	2.20	0.72
1:A:707:PHE:HE2	1:A:776:ALA:CA	2.02	0.72
1:A:92:SER:OG	1:A:96:LYS:NZ	2.23	0.71
1:A:306:TYR:CD1	1:A:332:PHE:HE1	2.06	0.71
1:A:1090:VAL:HG13	1:A:1097:ILE:HB	1.72	0.71
1:A:370:SER:O	1:A:371:ILE:CG1	2.38	0.71
1:A:704:TRP:HZ2	1:A:707:PHE:HB3	1.55	0.70
1:A:1026:MET:O	1:A:1027:LEU:HD12	1.92	0.69
1:A:585:LEU:N	2:B:101:THR:O	2.21	0.69
1:A:328:LEU:O	1:A:332:PHE:CE2	2.45	0.69
1:A:901:ARG:O	1:A:904:VAL:HG12	1.93	0.69
1:A:132:TRP:HE3	1:A:184:ASP:H	1.40	0.69
2:B:70:ILE:HD11	2:B:79:VAL:HB	1.73	0.69
1:A:326:GLN:O	1:A:330:VAL:HG23	1.92	0.68
2:B:81:LEU:HD12	2:B:81:LEU:O	1.93	0.68
1:A:132:TRP:CD1	1:A:133:CYS:HG	2.12	0.67
1:A:625:GLN:HB3	2:B:103:GLY:O	1.94	0.67
1:A:328:LEU:O	1:A:332:PHE:CD2	2.48	0.67
1:A:1039:ASN:HD22	1:A:1047:PRO:HG3	1.59	0.67
1:A:239:GLU:OE1	1:A:287:LYS:NZ	2.28	0.67
1:A:1048:VAL:HG21	1:A:1074:THR:HG21	1.77	0.66
2:B:33:VAL:HG22	2:B:99:ARG:HB2	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1049:LEU:HD12	1:A:1052:LEU:HD22	1.77	0.66
1:A:306:TYR:HE1	1:A:332:PHE:CD1	2.14	0.66
1:A:416:GLY:H	1:A:577:THR:HG22	1.60	0.66
1:A:1026:MET:C	1:A:1027:LEU:CD1	2.60	0.66
1:A:263:PHE:HA	1:A:1188:ARG:HH12	1.62	0.65
1:A:706:TYR:O	1:A:707:PHE:CD1	2.49	0.65
1:A:270:LEU:HG	1:A:790:LYS:HD2	1.79	0.65
1:A:267:LYS:HA	1:A:270:LEU:HD22	1.79	0.65
2:B:36:TRP:CE2	2:B:81:LEU:HD21	2.31	0.65
2:B:76:LYS:HG3	2:B:77:ASN:H	1.61	0.65
1:A:306:TYR:CD1	1:A:332:PHE:CD1	2.85	0.64
1:A:1018:SER:C	1:A:1020:GLN:H	2.05	0.64
2:B:32:ALA:HA	2:B:99:ARG:HB3	1.79	0.64
1:A:272:ARG:O	1:A:276:ASN:ND2	2.28	0.62
1:A:684:LEU:HD13	1:A:806:THR:HG21	1.81	0.62
1:A:1123:ILE:HD11	1:A:1161:TYR:HA	1.82	0.62
1:A:385:GLN:HG2	1:A:386:GLY:H	1.65	0.62
1:A:552:GLU:HB3	1:A:555:SER:HB2	1.82	0.62
1:A:1027:LEU:HD12	1:A:1027:LEU:N	2.15	0.62
1:A:1048:VAL:HG23	1:A:1049:LEU:HD22	1.81	0.62
1:A:820:GLN:HB3	1:A:997:ALA:HA	1.81	0.62
1:A:484:ILE:HG21	1:A:496:ILE:HG13	1.80	0.61
1:A:1144:ALA:HA	1:A:1186:LEU:HD11	1.81	0.61
1:A:687:ASP:H	1:A:813:ARG:HH22	1.47	0.61
1:A:562:GLU:OE2	2:B:101:THR:HG21	2.01	0.60
1:A:1048:VAL:HG11	1:A:1070:CYS:HB2	1.81	0.60
1:A:796:ASP:OD1	1:A:796:ASP:N	2.34	0.60
1:A:219:PRO:O	1:A:223:LEU:N	2.35	0.60
1:A:362:PHE:HA	1:A:365:ILE:HB	1.82	0.60
2:B:47:PHE:HZ	2:B:50:THR:HB	1.66	0.60
1:A:707:PHE:HE2	1:A:776:ALA:HA	1.67	0.60
1:A:382:ASP:O	1:A:384:ILE:HG12	2.01	0.59
1:A:1176:GLN:OE1	1:A:1176:GLN:N	2.34	0.59
1:A:131:PHE:HE2	1:A:186:ILE:HB	1.67	0.59
2:B:40:ALA:HB3	2:B:43:LYS:HE2	1.84	0.59
1:A:715:ILE:HD12	1:A:836:ILE:HG13	1.84	0.59
1:A:1220:GLY:O	1:A:1221:ARG:NH1	2.35	0.59
1:A:396:SER:HB2	1:A:404:GLN:HG3	1.84	0.59
1:A:1014:ILE:HB	1:A:1102:VAL:HG11	1.85	0.59
1:A:463:ARG:HG3	1:A:906:LEU:HD13	1.85	0.59
1:A:1076:VAL:HG13	1:A:1194:LEU:HD13	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:TRP:O	1:A:212:LEU:HG	2.03	0.58
2:B:22:CYS:HB2	2:B:36:TRP:CZ2	2.39	0.58
1:A:923:PRO:HA	1:A:926:ASN:HB3	1.86	0.58
2:B:64:VAL:HB	2:B:68:PHE:CD2	2.39	0.58
1:A:1033:PHE:HB2	1:A:1054:LEU:H	1.68	0.57
2:B:2:VAL:HG11	2:B:107:TYR:CE2	2.40	0.57
1:A:1037:VAL:HG12	1:A:1051:GLY:H	1.69	0.57
2:B:33:VAL:HB	2:B:51:ILE:O	2.03	0.57
1:A:312:TYR:O	1:A:316:LEU:HG	2.04	0.57
1:A:1204:THR:OG1	1:A:1205:GLU:N	2.36	0.57
1:A:125:ALA:HA	1:A:128:GLN:HE21	1.70	0.57
1:A:1040:TYR:O	1:A:1042:THR:N	2.29	0.57
1:A:81:VAL:HG13	1:A:99:MET:HB3	1.85	0.57
1:A:429:LYS:HB3	1:A:581:ILE:HG12	1.87	0.57
1:A:243:TYR:O	1:A:247:GLY:N	2.30	0.57
1:A:686:GLU:HB3	1:A:813:ARG:HH22	1.70	0.57
1:A:44:TRP:HD1	1:A:45:LEU:HD12	1.69	0.56
1:A:1063:ALA:HB3	1:A:1239:ILE:HA	1.87	0.56
1:A:310:PHE:HZ	1:A:332:PHE:CE2	2.13	0.56
1:A:1122:SER:HB3	1:A:1125:GLU:HG2	1.89	0.55
1:A:586:SER:HB3	2:B:30:ASN:HB3	1.88	0.55
1:A:377:SER:O	1:A:458:ASN:ND2	2.39	0.55
1:A:156:ILE:HG12	1:A:439:LEU:O	2.06	0.55
1:A:1155:ASP:O	1:A:1160:LYS:NZ	2.39	0.55
2:B:2:VAL:HG11	2:B:107:TYR:HE2	1.71	0.55
2:B:36:TRP:CE2	2:B:81:LEU:CD2	2.90	0.55
1:A:768:LEU:O	1:A:772:THR:HG23	2.06	0.55
1:A:1037:VAL:HG12	1:A:1050:GLN:HA	1.89	0.55
2:B:95:TYR:HA	2:B:111:GLY:HA2	1.88	0.55
1:A:1039:ASN:ND2	1:A:1043:ARG:O	2.40	0.54
1:A:486:TYR:HB3	1:A:908:ARG:HH21	1.71	0.54
1:A:163:ASP:HB3	1:A:166:GLU:HB2	1.89	0.54
2:B:4:LEU:HD21	2:B:98:ALA:HB2	1.90	0.54
2:B:58:THR:HG21	2:B:70:ILE:HG21	1.89	0.54
1:A:214:ILE:O	1:A:217:ILE:HG12	2.08	0.54
1:A:534:ARG:HA	1:A:537:ILE:HD12	1.89	0.54
1:A:923:PRO:O	1:A:927:ALA:N	2.39	0.54
2:B:61:ALA:HB3	2:B:64:VAL:HG22	1.90	0.54
1:A:35:VAL:HB	1:A:355:ARG:HE	1.73	0.54
1:A:370:SER:C	1:A:371:ILE:HG12	2.33	0.54
1:A:1197:GLU:HB3	1:A:1200:SER:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:PHE:HD1	1:A:376:LYS:H	1.56	0.54
1:A:1235:ASN:OD1	1:A:1235:ASN:N	2.40	0.54
1:A:258:ARG:NH2	1:A:801:ASP:O	2.36	0.53
2:B:57:TYR:CG	2:B:58:THR:N	2.76	0.53
1:A:384:ILE:HG22	1:A:384:ILE:O	2.08	0.53
1:A:538:ALA:O	1:A:542:VAL:HG23	2.08	0.53
2:B:36:TRP:CD2	2:B:81:LEU:CD2	2.90	0.53
1:A:1039:ASN:OD1	1:A:1045:SER:OG	2.27	0.53
1:A:722:PRO:HG2	1:A:841:THR:HB	1.90	0.53
1:A:281:LYS:HD3	1:A:782:LYS:HE2	1.91	0.53
1:A:385:GLN:NE2	1:A:415:SER:HB2	2.23	0.53
1:A:713:CYS:HG	1:A:765:THR:HG1	1.55	0.53
1:A:529:GLY:HA2	1:A:532:LYS:HD3	1.91	0.53
1:A:845:ILE:HG23	1:A:972:LEU:HD23	1.90	0.53
1:A:892:ILE:O	1:A:916:TYR:OH	2.26	0.52
1:A:756:LEU:HA	1:A:760:ILE:HD13	1.92	0.52
1:A:808:GLY:O	1:A:812:THR:OG1	2.25	0.52
1:A:1010:LYS:HG2	1:A:1011:THR:H	1.73	0.52
1:A:1179:ARG:HH21	1:A:1209:VAL:HG11	1.74	0.52
1:A:437:GLN:HB2	1:A:439:LEU:HD23	1.91	0.52
1:A:1043:ARG:HB3	1:A:1044:PRO:HD3	1.91	0.52
1:A:1071:GLY:HA2	1:A:1074:THR:OG1	2.09	0.52
1:A:1092:LEU:HB3	1:A:1097:ILE:HD11	1.92	0.52
2:B:35:GLY:O	2:B:97:ALA:N	2.26	0.52
1:A:603:VAL:HG23	1:A:604:GLU:H	1.75	0.52
1:A:970:VAL:HG23	1:A:971:LEU:HD22	1.90	0.52
1:A:94:ALA:HA	1:A:97:ARG:HE	1.74	0.52
1:A:906:LEU:HG	1:A:909:GLU:HG3	1.92	0.52
1:A:421:LEU:HB2	1:A:581:ILE:HG13	1.91	0.51
1:A:471:GLN:OE1	1:A:471:GLN:N	2.43	0.51
1:A:313:GLY:O	1:A:317:VAL:HG23	2.11	0.51
1:A:1060:GLN:HB2	1:A:1237:ASP:CG	2.35	0.51
1:A:703:GLU:O	1:A:705:PRO:HD3	2.10	0.51
2:B:22:CYS:HB3	2:B:79:VAL:HG23	1.91	0.51
1:A:1000:SER:HA	1:A:1003:HIS:CD2	2.46	0.51
1:A:527:LEU:H	1:A:527:LEU:HD23	1.76	0.51
2:B:68:PHE:CD1	2:B:83:MET:HG2	2.46	0.51
1:A:419:VAL:HG13	1:A:579:ILE:HG13	1.93	0.50
1:A:509:ILE:HD13	1:A:516:PHE:CE1	2.46	0.50
1:A:786:TYR:O	1:A:790:LYS:HG2	2.12	0.50
1:A:173:ASP:O	1:A:177:LYS:HG3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1137:SER:OG	1:A:1139:GLU:OE2	2.29	0.50
1:A:327:VAL:HA	1:A:330:VAL:HB	1.94	0.50
1:A:466:ILE:HG23	1:A:549:LEU:HD13	1.94	0.50
1:A:550:LEU:HD23	1:A:569:LEU:HD13	1.93	0.50
1:A:696:ILE:HG13	1:A:697:LEU:H	1.77	0.50
1:A:327:VAL:O	1:A:331:PHE:HD1	1.95	0.49
1:A:506:TYR:CD1	1:A:509:ILE:HD11	2.47	0.49
1:A:1027:LEU:CD1	1:A:1027:LEU:N	2.75	0.49
2:B:38:ARG:NH2	2:B:90:ASP:HA	2.27	0.49
1:A:922:ILE:HB	1:A:923:PRO:HD3	1.94	0.49
2:B:76:LYS:HG3	2:B:77:ASN:N	2.27	0.49
1:A:217:ILE:HG21	1:A:305:SER:HB2	1.93	0.49
1:A:700:ASN:O	1:A:704:TRP:N	2.45	0.49
2:B:51:ILE:HG22	2:B:58:THR:OG1	2.12	0.49
2:B:7:SER:HB2	2:B:21:SER:OG	2.12	0.49
1:A:213:VAL:O	1:A:217:ILE:HG23	2.12	0.49
1:A:488:ARG:HE	1:A:542:VAL:HG12	1.77	0.49
1:A:533:GLN:O	1:A:537:ILE:HG13	2.13	0.49
1:A:707:PHE:CD2	1:A:776:ALA:CB	2.90	0.49
1:A:879:ALA:O	1:A:883:LYS:HG2	2.12	0.49
1:A:1158:PRO:C	1:A:1160:LYS:H	2.20	0.49
2:B:6:GLU:OE1	2:B:111:GLY:N	2.46	0.49
1:A:469:VAL:HG13	1:A:533:GLN:NE2	2.27	0.49
1:A:724:PHE:HB2	1:A:758:LEU:HD11	1.94	0.49
1:A:861:VAL:HB	1:A:862:PRO:HD3	1.94	0.49
1:A:944:MET:O	1:A:948:SER:OG	2.20	0.49
2:B:18:LEU:HG	2:B:20:LEU:HD21	1.94	0.49
1:A:496:ILE:O	1:A:500:VAL:HG22	2.13	0.49
1:A:753:LEU:HD12	1:A:756:LEU:HD11	1.94	0.49
1:A:155:GLU:OE1	1:A:373:SER:OG	2.31	0.49
1:A:611:LEU:HD23	1:A:618:TYR:CG	2.48	0.49
1:A:698:LYS:O	1:A:702:THR:OG1	2.25	0.49
1:A:714:ALA:HB1	1:A:833:PHE:HB2	1.94	0.48
1:A:787:MET:HE2	1:A:1008:ILE:HD11	1.95	0.48
1:A:1019:THR:O	1:A:1020:GLN:HG2	2.13	0.48
1:A:573:ARG:C	1:A:575:GLY:H	2.21	0.48
1:A:1202:LEU:HB3	1:A:1207:GLU:HG2	1.94	0.48
1:A:65:PRO:O	1:A:69:LEU:N	2.45	0.48
1:A:105:GLU:O	1:A:109:THR:HG23	2.14	0.48
1:A:296:GLY:O	1:A:300:LEU:HG	2.14	0.48
1:A:711:ILE:O	1:A:715:ILE:HG12	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:LEU:HB3	1:A:1226:ILE:HG22	1.96	0.48
2:B:22:CYS:HB3	2:B:79:VAL:CG2	2.44	0.48
1:A:38:MET:HA	1:A:41:TYR:HB3	1.96	0.48
1:A:111:ALA:HA	1:A:114:TYR:CE1	2.49	0.48
1:A:1010:LYS:HD2	1:A:1012:PRO:HA	1.95	0.48
1:A:1241:VAL:HG21	1:A:1263:TYR:HB2	1.95	0.48
1:A:132:TRP:HD1	1:A:133:CYS:SG	2.36	0.47
1:A:1068:SER:OG	1:A:1069:GLY:N	2.46	0.47
1:A:824:ALA:O	1:A:828:ARG:HG2	2.14	0.47
1:A:846:SER:HA	1:A:849:TYR:CE2	2.49	0.47
1:A:257:ILE:HG12	1:A:800:PHE:CD1	2.50	0.47
1:A:906:LEU:HA	1:A:909:GLU:HG2	1.96	0.47
1:A:109:THR:HB	1:A:113:TYR:CZ	2.48	0.47
1:A:569:LEU:O	1:A:573:ARG:N	2.47	0.47
1:A:626:THR:C	2:B:99:ARG:HD2	2.39	0.47
1:A:156:ILE:HG22	1:A:160:ASP:OD1	2.14	0.47
1:A:453:ASP:OD1	1:A:454:ILE:N	2.48	0.47
1:A:969:ASN:H	1:A:972:LEU:HD13	1.79	0.47
2:B:38:ARG:CG	2:B:46:GLN:HG3	2.41	0.47
1:A:603:VAL:HG23	1:A:604:GLU:N	2.29	0.47
1:A:1120:ASP:HA	1:A:1165:VAL:HG21	1.97	0.47
2:B:100:LEU:HD22	2:B:106:ASP:HB2	1.97	0.47
1:A:528:SER:HB3	1:A:531:GLN:CD	2.40	0.47
1:A:1011:THR:HG23	1:A:1011:THR:O	2.15	0.47
1:A:1120:ASP:OD1	1:A:1120:ASP:N	2.48	0.47
2:B:64:VAL:O	2:B:68:PHE:HD2	1.97	0.47
1:A:1000:SER:HA	1:A:1003:HIS:HD2	1.80	0.47
2:B:67:ARG:HG3	2:B:67:ARG:HH11	1.79	0.47
1:A:390:PHE:CD1	1:A:447:VAL:HG23	2.50	0.46
1:A:510:MET:HA	1:A:515:GLN:OE1	2.14	0.46
2:B:52:ASP:OD2	2:B:56:GLU:HB3	2.15	0.46
1:A:215:LEU:O	1:A:219:PRO:HD3	2.14	0.46
1:A:247:GLY:O	1:A:251:GLU:N	2.47	0.46
1:A:1076:VAL:O	1:A:1080:GLU:HG2	2.15	0.46
1:A:590:ASN:OD1	1:A:590:ASN:N	2.38	0.46
2:B:33:VAL:CG1	2:B:52:ASP:HA	2.45	0.46
1:A:884:LYS:O	1:A:887:GLU:HB3	2.16	0.46
1:A:186:ILE:HD11	1:A:351:PHE:CD1	2.50	0.46
1:A:390:PHE:HB3	1:A:409:LEU:HD12	1.97	0.46
1:A:530:GLY:HA3	1:A:561:SER:OG	2.15	0.46
1:A:1081:ARG:O	1:A:1106:ARG:NH2	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:ASP:O	2:B:74:ASN:HB2	2.16	0.46
1:A:300:LEU:HD22	1:A:759:GLY:HA2	1.98	0.46
1:A:459:VAL:O	1:A:463:ARG:HG2	2.16	0.46
1:A:311:TRP:HZ3	1:A:748:SER:HA	1.81	0.46
1:A:773:PHE:HB3	1:A:829:LEU:HD22	1.98	0.46
1:A:107:MET:HE1	1:A:954:ARG:HG2	1.98	0.46
1:A:784:LEU:O	1:A:788:VAL:HG23	2.16	0.46
1:A:93:GLU:O	1:A:97:ARG:HG3	2.16	0.45
1:A:132:TRP:CE3	1:A:183:GLY:HA3	2.51	0.45
1:A:208:TRP:O	1:A:211:THR:OG1	2.35	0.45
2:B:34:MET:HE1	2:B:78:THR:N	2.30	0.45
1:A:461:TYR:O	1:A:465:ILE:HG12	2.16	0.45
1:A:385:GLN:HG2	1:A:386:GLY:N	2.31	0.45
1:A:133:CYS:SG	1:A:931:ALA:HA	2.56	0.45
1:A:777:GLY:O	1:A:781:THR:OG1	2.31	0.45
1:A:834:GLN:HA	1:A:837:ALA:HB3	1.98	0.45
1:A:1061:THR:N	1:A:1237:ASP:OD1	2.38	0.45
1:A:1114:GLN:HG2	1:A:1197:GLU:HB2	1.98	0.45
1:A:1175:GLY:O	1:A:1179:ARG:HG3	2.16	0.45
1:A:1211:GLN:NE2	1:A:1232:THR:HB	2.31	0.45
1:A:1176:GLN:O	1:A:1180:ILE:HG13	2.16	0.45
1:A:1202:LEU:HD23	1:A:1207:GLU:HA	1.97	0.45
1:A:74:MET:HB2	1:A:110:TYR:OH	2.17	0.45
1:A:43:GLY:CA	1:A:46:ASP:HB2	2.46	0.45
1:A:370:SER:C	1:A:371:ILE:CG1	2.90	0.45
1:A:626:THR:HG22	2:B:99:ARG:HD2	1.98	0.45
1:A:686:GLU:HB3	1:A:813:ARG:NH2	2.32	0.45
1:A:1151:HIS:HA	1:A:1154:ILE:HB	1.98	0.45
2:B:33:VAL:HG21	2:B:99:ARG:HH11	1.81	0.45
1:A:438:ARG:CZ	1:A:455:ARG:HA	2.47	0.45
1:A:1093:ASP:HB3	1:A:1095:LYS:HD3	1.99	0.45
1:A:484:ILE:HG23	1:A:542:VAL:HG21	1.99	0.45
1:A:802:ASP:CB	1:A:1041:PRO:HD2	2.47	0.45
1:A:999:VAL:HG12	1:A:1003:HIS:NE2	2.32	0.45
2:B:8:GLY:O	2:B:18:LEU:HD11	2.16	0.45
1:A:96:LYS:HA	1:A:100:PHE:CE1	2.52	0.45
1:A:132:TRP:HE3	1:A:184:ASP:N	2.11	0.45
1:A:619:PHE:CE1	1:A:623:MET:HG3	2.52	0.44
1:A:235:PHE:HB3	1:A:287:LYS:HE2	1.99	0.44
1:A:1107:ALA:O	1:A:1188:ARG:HD3	2.17	0.44
1:A:1196:ASP:CG	1:A:1226:ILE:HD11	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:ARG:HG3	2:B:67:ARG:NH1	2.32	0.44
2:B:70:ILE:HA	2:B:81:LEU:HA	1.99	0.44
1:A:111:ALA:HA	1:A:114:TYR:HE1	1.82	0.44
1:A:72:GLY:O	1:A:326:GLN:HG2	2.17	0.44
1:A:172:THR:HA	1:A:175:VAL:HG22	2.00	0.44
1:A:727:ILE:O	1:A:731:VAL:HG23	2.17	0.44
2:B:22:CYS:HB2	2:B:36:TRP:CE2	2.52	0.44
1:A:83:ASN:HA	1:A:738:GLY:O	2.18	0.44
1:A:569:LEU:O	1:A:573:ARG:HG3	2.17	0.44
1:A:1032:GLN:HB2	1:A:1091:PHE:HB2	2.00	0.44
1:A:44:TRP:CD1	1:A:45:LEU:HD12	2.49	0.44
1:A:513:PRO:C	1:A:515:GLN:H	2.25	0.44
1:A:43:GLY:HA3	1:A:46:ASP:HB2	1.99	0.44
1:A:905:SER:C	1:A:907:THR:H	2.25	0.44
2:B:36:TRP:CD1	2:B:81:LEU:HD23	2.53	0.44
1:A:359:TYR:HA	1:A:362:PHE:HB2	2.00	0.44
1:A:845:ILE:O	1:A:848:ILE:HG12	2.18	0.44
1:A:949:TYR:HD1	1:A:953:PHE:HE2	1.65	0.44
1:A:71:PHE:HA	1:A:74:MET:HE3	2.00	0.43
1:A:306:TYR:CE1	1:A:332:PHE:CZ	3.02	0.43
1:A:329:THR:HA	1:A:332:PHE:CD2	2.43	0.43
1:A:358:ALA:O	1:A:362:PHE:N	2.51	0.43
1:A:366:ASP:CG	1:A:367:ASN:H	2.26	0.43
1:A:797:VAL:O	1:A:797:VAL:HG13	2.17	0.43
1:A:33:VAL:HG23	1:A:34:SER:H	1.82	0.43
1:A:204:PHE:HA	1:A:211:THR:HG21	1.99	0.43
2:B:18:LEU:O	2:B:83:MET:HB2	2.19	0.43
1:A:121:VAL:HA	1:A:124:VAL:HG22	2.00	0.43
1:A:1191:HIS:HA	1:A:1221:ARG:HD2	1.99	0.43
1:A:1079:LEU:HD23	1:A:1194:LEU:HD11	2.00	0.43
1:A:463:ARG:O	1:A:543:ARG:NH2	2.52	0.43
1:A:973:VAL:O	1:A:977:ILE:HG13	2.18	0.43
1:A:1260:LYS:HD3	2:B:41:PRO:HB2	2.01	0.43
1:A:171:LEU:O	1:A:175:VAL:HG13	2.19	0.43
1:A:208:TRP:C	1:A:211:THR:HG1	2.27	0.43
1:A:746:GLN:O	1:A:750:LEU:HG	2.19	0.43
1:A:790:LYS:N	1:A:790:LYS:HD3	2.34	0.43
1:A:33:VAL:HG23	1:A:34:SER:N	2.34	0.42
1:A:370:SER:OG	1:A:371:ILE:N	2.52	0.42
1:A:1049:LEU:HD21	1:A:1074:THR:OG1	2.19	0.42
1:A:1074:THR:O	1:A:1078:LEU:HG	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1171:GLN:HG3	1:A:1172:LEU:HG	2.01	0.42
1:A:355:ARG:HG2	1:A:359:TYR:HD2	1.85	0.42
1:A:122:LEU:HD12	1:A:939:SER:HB2	2.01	0.42
1:A:315:SER:O	1:A:320:LYS:HG3	2.20	0.42
1:A:724:PHE:HB2	1:A:758:LEU:HD21	2.02	0.42
1:A:780:LEU:O	1:A:784:LEU:HB2	2.19	0.42
1:A:385:GLN:CG	1:A:386:GLY:H	2.31	0.42
1:A:528:SER:O	1:A:532:LYS:HG3	2.18	0.42
1:A:960:VAL:HG12	1:A:965:MET:SD	2.59	0.42
1:A:257:ILE:HA	1:A:260:VAL:HG12	2.00	0.42
1:A:800:PHE:O	1:A:803:PRO:HD3	2.20	0.42
1:A:1018:SER:C	1:A:1020:GLN:N	2.72	0.42
1:A:107:MET:HA	1:A:110:TYR:HD2	1.85	0.42
1:A:1066:GLY:H	1:A:1072:LYS:HE2	1.84	0.42
1:A:1259:GLN:HG3	1:A:1260:LYS:H	1.85	0.42
2:B:58:THR:HG22	2:B:59:TYR:N	2.34	0.42
1:A:156:ILE:H	1:A:156:ILE:HD12	1.84	0.42
1:A:471:GLN:HB3	1:A:552:GLU:HB2	2.01	0.42
1:A:721:GLN:HB3	1:A:722:PRO:HD3	2.01	0.42
1:A:979:PHE:HA	1:A:982:MET:HG2	2.02	0.42
1:A:856:LEU:HD21	1:A:951:ALA:HB1	2.02	0.42
1:A:930:LYS:HA	1:A:933:VAL:HB	2.02	0.42
1:A:1233:ILE:HD12	1:A:1233:ILE:HA	1.91	0.42
1:A:278:GLU:OE1	1:A:281:LYS:NZ	2.53	0.41
1:A:999:VAL:HG12	1:A:1003:HIS:HE2	1.85	0.41
2:B:36:TRP:CG	2:B:81:LEU:CD2	3.02	0.41
2:B:60:TYR:OH	2:B:70:ILE:HG22	2.20	0.41
1:A:180:GLU:O	1:A:185:LYS:HG3	2.20	0.41
2:B:68:PHE:CE1	2:B:83:MET:HG2	2.55	0.41
1:A:370:SER:O	1:A:371:ILE:HG13	2.17	0.41
1:A:405:ILE:H	1:A:405:ILE:HD12	1.85	0.41
1:A:214:ILE:HD11	1:A:331:PHE:HB3	2.01	0.41
1:A:1050:GLN:H	1:A:1245:GLY:HA3	1.86	0.41
1:A:1183:ALA:O	1:A:1187:VAL:HG23	2.21	0.41
1:A:74:MET:HE2	1:A:110:TYR:HE1	1.85	0.41
1:A:153:ASN:ND2	1:A:368:LYS:HB3	2.35	0.41
1:A:278:GLU:O	1:A:281:LYS:HG2	2.20	0.41
2:B:36:TRP:HA	2:B:96:CYS:HA	2.01	0.41
1:A:625:GLN:CB	2:B:103:GLY:O	2.66	0.41
1:A:846:SER:HA	1:A:849:TYR:CZ	2.55	0.41
1:A:1260:LYS:HD3	2:B:41:PRO:CB	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ILE:HG23	1:A:767:PHE:HE1	1.85	0.41
1:A:834:GLN:OE1	1:A:986:GLN:HB2	2.21	0.41
1:A:88:SER:OG	1:A:89:THR:N	2.53	0.41
1:A:148:PHE:HB3	1:A:913:GLU:OE2	2.20	0.41
1:A:197:PHE:O	1:A:201:ILE:HG13	2.21	0.41
1:A:244:ALA:O	1:A:248:ALA:N	2.43	0.41
1:A:260:VAL:O	1:A:264:GLY:N	2.53	0.41
1:A:1079:LEU:HD23	1:A:1194:LEU:HD21	2.02	0.41
1:A:1216:LYS:HD3	1:A:1216:LYS:HA	1.89	0.41
2:B:36:TRP:NE1	2:B:81:LEU:HD23	2.35	0.41
2:B:69:THR:HG22	2:B:70:ILE:N	2.36	0.41
1:A:361:VAL:O	1:A:365:ILE:HG13	2.21	0.41
1:A:392:ASN:OD1	1:A:394:HIS:NE2	2.54	0.40
1:A:461:TYR:CZ	1:A:465:ILE:HD11	2.56	0.40
1:A:292:ASN:CG	1:A:770:GLY:HA3	2.45	0.40
1:A:125:ALA:HA	1:A:128:GLN:NE2	2.35	0.40
1:A:1100:LEU:HD23	1:A:1105:LEU:HB2	2.02	0.40
1:A:35:VAL:HG12	1:A:359:TYR:CZ	2.56	0.40
1:A:975:SER:O	1:A:978:VAL:HG12	2.20	0.40
1:A:1053:SER:O	1:A:1054:LEU:HD13	2.21	0.40
1:A:1139:GLU:H	1:A:1139:GLU:CD	2.30	0.40
1:A:793:LEU:HD12	1:A:793:LEU:HA	1.94	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	1178/1284 (92%)	1071 (91%)	107 (9%)	0	100	100
2	B	116/124 (94%)	95 (82%)	21 (18%)	0	100	100
All	All	1294/1408 (92%)	1166 (90%)	128 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	976/1065 (92%)	958 (98%)	18 (2%)	51	67
2	B	94/100 (94%)	93 (99%)	1 (1%)	65	74
All	All	1070/1165 (92%)	1051 (98%)	19 (2%)	51	67

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	58	ILE
1	A	64	LEU
1	A	409	LEU
1	A	509	ILE
1	A	590	ASN
1	A	593	VAL
1	A	601	VAL
1	A	696	ILE
1	A	796	ASP
1	A	847	LEU
1	A	1027	LEU
1	A	1056	VAL
1	A	1064	LEU
1	A	1065	VAL
1	A	1225	VAL
1	A	1235	ASN
1	A	1247	VAL
2	B	86	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	179	ASN
1	A	385	GLN
1	A	533	GLN
1	A	544	ASN
1	A	746	GLN
1	A	749	ASN
1	A	820	GLN
1	A	932	HIS
1	A	942	GLN
1	A	969	ASN
1	A	1003	HIS
1	A	1108	GLN
1	A	1114	GLN
1	A	1211	GLN
1	A	1270	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 oligosaccharides 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, 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	1182/1284 (92%)	0.98	165 (13%) 6 10	46, 123, 185, 232	0
2	B	117/124 (94%)	1.63	36 (30%) 1 3	123, 157, 179, 198	0
All	All	1299/1408 (92%)	1.04	201 (15%) 5 9	46, 130, 185, 232	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	GLY	9.0
1	A	319	SER	6.2
2	B	34	MET	6.2
1	A	1025	ASN	6.1
1	A	828	ARG	6.1
1	A	1024	PRO	5.7
1	A	1167	ASP	5.6
2	B	51	ILE	5.5
2	B	73	ASP	4.8
1	A	225	ALA	4.8
1	A	229	ALA	4.8
1	A	827	SER	4.7
2	B	99	ARG	4.5
1	A	318	ILE	4.4
1	A	1168	LYS	4.4
1	A	626	THR	4.2
1	A	234	SER	4.1
1	A	1013	GLU	4.1
1	A	320	LYS	4.1
1	A	1018	SER	4.0
1	A	236	THR	4.0
1	A	599	GLY	3.9
1	A	227	ILE	3.9
1	A	230	LYS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	908	ARG	3.8
1	A	339	PHE	3.8
1	A	598	ASP	3.7
2	B	35	GLY	3.7
1	A	1131	ASP	3.7
1	A	1020	GLN	3.7
1	A	40	ARG	3.7
1	A	221	LEU	3.7
1	A	958	TYR	3.6
2	B	1	GLN	3.6
1	A	1022	LEU	3.5
2	B	75	ALA	3.5
1	A	730	LYS	3.5
2	B	32	ALA	3.4
1	A	559	THR	3.4
1	A	329	THR	3.4
2	B	49	ALA	3.3
1	A	798	SER	3.3
1	A	1271	ALA	3.3
1	A	984	VAL	3.3
1	A	959	LEU	3.3
1	A	299	PHE	3.2
1	A	1215	ASP	3.2
2	B	58	THR	3.2
1	A	104	GLU	3.2
1	A	102	LYS	3.2
1	A	826	GLY	3.1
1	A	238	LYS	3.1
1	A	1021	GLY	3.1
1	A	723	ALA	3.1
1	A	224	SER	3.1
2	B	44	GLU	3.1
2	B	110	GLN	3.1
1	A	241	HIS	3.1
1	A	314	THR	3.0
2	B	28	THR	3.0
1	A	969	ASN	3.0
1	A	426	GLY	3.0
1	A	360	GLU	3.0
1	A	1019	THR	3.0
2	B	71	SER	3.0
1	A	988	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	315	SER	2.9
1	A	694	TRP	2.9
1	A	851	TRP	2.9
1	A	1136	VAL	2.9
1	A	749	ASN	2.9
1	A	68	MET	2.8
1	A	521	GLY	2.8
1	A	794	ARG	2.8
1	A	872	MET	2.8
1	A	1234	GLN	2.8
1	A	240	LEU	2.8
2	B	27	ARG	2.8
2	B	69	THR	2.8
1	A	182	ILE	2.7
1	A	376	LYS	2.7
1	A	423	GLY	2.7
1	A	706	TYR	2.7
1	A	78	PHE	2.7
1	A	844	ILE	2.7
2	B	103	GLY	2.7
1	A	584	ARG	2.7
1	A	697	LEU	2.7
1	A	1232	THR	2.7
1	A	1069	GLY	2.7
2	B	59	TYR	2.7
2	B	70	ILE	2.7
1	A	497	GLU	2.7
1	A	525	ALA	2.6
1	A	158	TRP	2.6
1	A	689	PRO	2.6
1	A	1070	CYS	2.6
1	A	316	LEU	2.6
1	A	992	PRO	2.6
2	B	78	THR	2.6
1	A	978	VAL	2.6
1	A	100	PHE	2.6
1	A	891	LYS	2.6
2	B	2	VAL	2.6
1	A	312	TYR	2.6
1	A	1129	TYR	2.6
1	A	1235	ASN	2.5
1	A	333	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	322	TYR	2.5
1	A	427	CYS	2.5
1	A	71	PHE	2.5
1	A	1012	PRO	2.5
1	A	879	ALA	2.5
1	A	991	ALA	2.5
1	A	1026	MET	2.5
1	A	385	GLN	2.5
1	A	386	GLY	2.5
1	A	693	PHE	2.5
2	B	98	ALA	2.5
1	A	1023	LYS	2.5
1	A	1040	TYR	2.5
1	A	184	ASP	2.5
1	A	90	ASN	2.5
1	A	425	SER	2.4
2	B	30	ASN	2.4
2	B	47	PHE	2.4
1	A	366	ASP	2.4
1	A	302	ILE	2.4
1	A	107	MET	2.4
2	B	72	ARG	2.4
1	A	877	GLY	2.4
1	A	700	ASN	2.4
1	A	363	LYS	2.4
1	A	853	LEU	2.4
1	A	802	ASP	2.4
1	A	994	TYR	2.4
1	A	171	LEU	2.4
1	A	816	ASN	2.4
2	B	101	THR	2.3
1	A	235	PHE	2.3
1	A	1068	SER	2.3
1	A	1098	LYS	2.3
1	A	731	VAL	2.3
2	B	104	GLN	2.3
2	B	74	ASN	2.3
1	A	743	THR	2.3
1	A	162	HIS	2.3
1	A	99	MET	2.3
1	A	778	GLU	2.3
1	A	336	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	883	LYS	2.3
1	A	734	VAL	2.3
1	A	970	VAL	2.3
2	B	23	ALA	2.3
1	A	698	LYS	2.2
1	A	688	VAL	2.2
1	A	955	PHE	2.2
1	A	209	LYS	2.2
1	A	624	THR	2.2
1	A	1204	THR	2.2
1	A	1130	GLY	2.2
1	A	852	GLN	2.2
1	A	1014	ILE	2.2
1	A	1164	ARG	2.2
2	B	105	PHE	2.2
1	A	239	GLU	2.2
1	A	554	THR	2.2
2	B	54	SER	2.2
1	A	1099	GLN	2.1
1	A	974	PHE	2.1
1	A	424	ASN	2.1
1	A	233	SER	2.1
2	B	80	TYR	2.1
1	A	119	ALA	2.1
1	A	1166	GLY	2.1
1	A	687	ASP	2.1
1	A	726	VAL	2.1
1	A	1170	THR	2.1
2	B	50	THR	2.1
1	A	707	PHE	2.1
1	A	996	LYS	2.1
1	A	854	THR	2.1
1	A	840	GLY	2.1
1	A	831	VAL	2.1
1	A	695	ARG	2.1
1	A	855	LEU	2.1
1	A	857	LEU	2.1
2	B	29	PHE	2.1
2	B	19	ARG	2.1
1	A	557	LEU	2.0
1	A	685	ASP	2.0
1	A	1027	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	157	GLY	2.0
1	A	818	ALA	2.0
1	A	766	PHE	2.0
1	A	365	ILE	2.0
1	A	928	MET	2.0
2	B	77	ASN	2.0
1	A	223	LEU	2.0
1	A	301	LEU	2.0
1	A	880	LEU	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.