



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:51 AM UTC

PDB ID : 3PPH / pdb_00003pph
Title : Crystal structure of the Candida albicans methionine synthase by surface entropy reduction, threonine variant
Authors : Ubhi, D.; Kavanagh, K.; Monzingo, A.F.; Robertus, J.D.
Deposited on : 2010-11-24
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 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

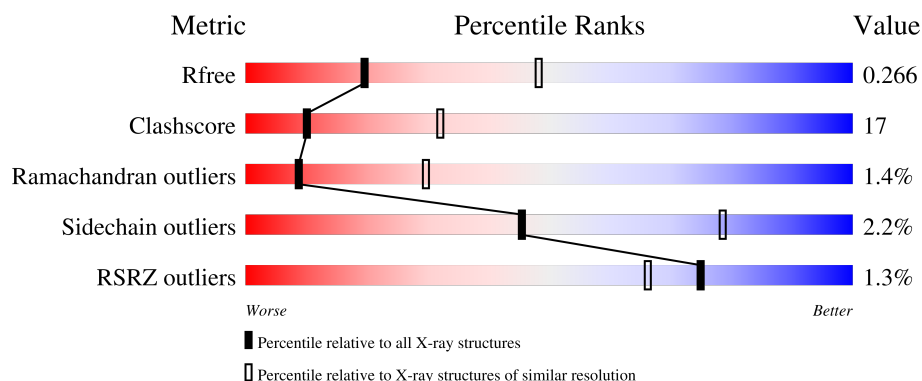
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	789	% 65% 29% • •
1	B	789	% 64% 29% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11040 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 5-methyltetrahydropteroyltriglutamate--homocysteine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	756	Total	C	N	O	S	0	0	0
			5510	3527	923	1050	10			
1	B	747	Total	C	N	O	S	0	0	0
			5479	3512	921	1036	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	THR	LYS	engineered mutation	UNP P82610
A	104	THR	LYS	engineered mutation	UNP P82610
A	107	THR	GLU	engineered mutation	UNP P82610
B	103	THR	LYS	engineered mutation	UNP P82610
B	104	THR	LYS	engineered mutation	UNP P82610
B	107	THR	GLU	engineered mutation	UNP P82610

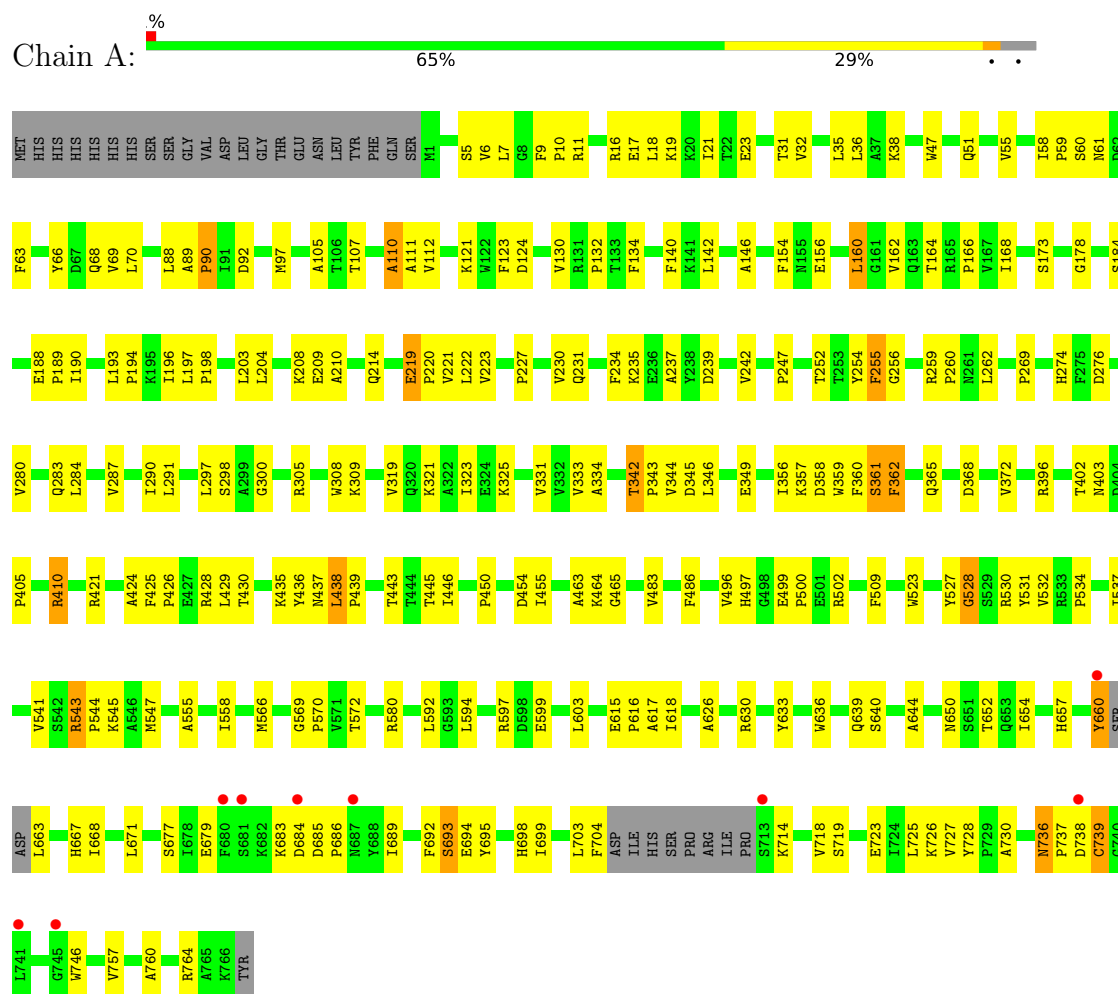
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	22	Total	O	0	0
			22	22		
2	B	29	Total	O	0	0
			29	29		

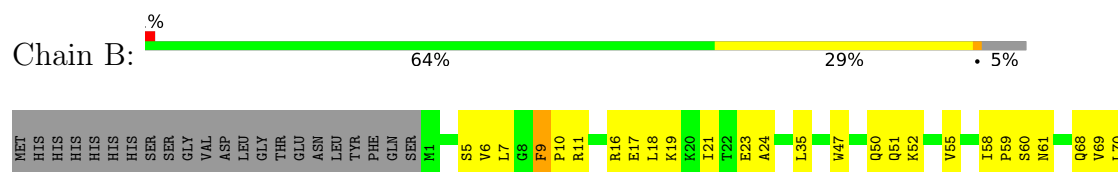
3 Residue-property plots

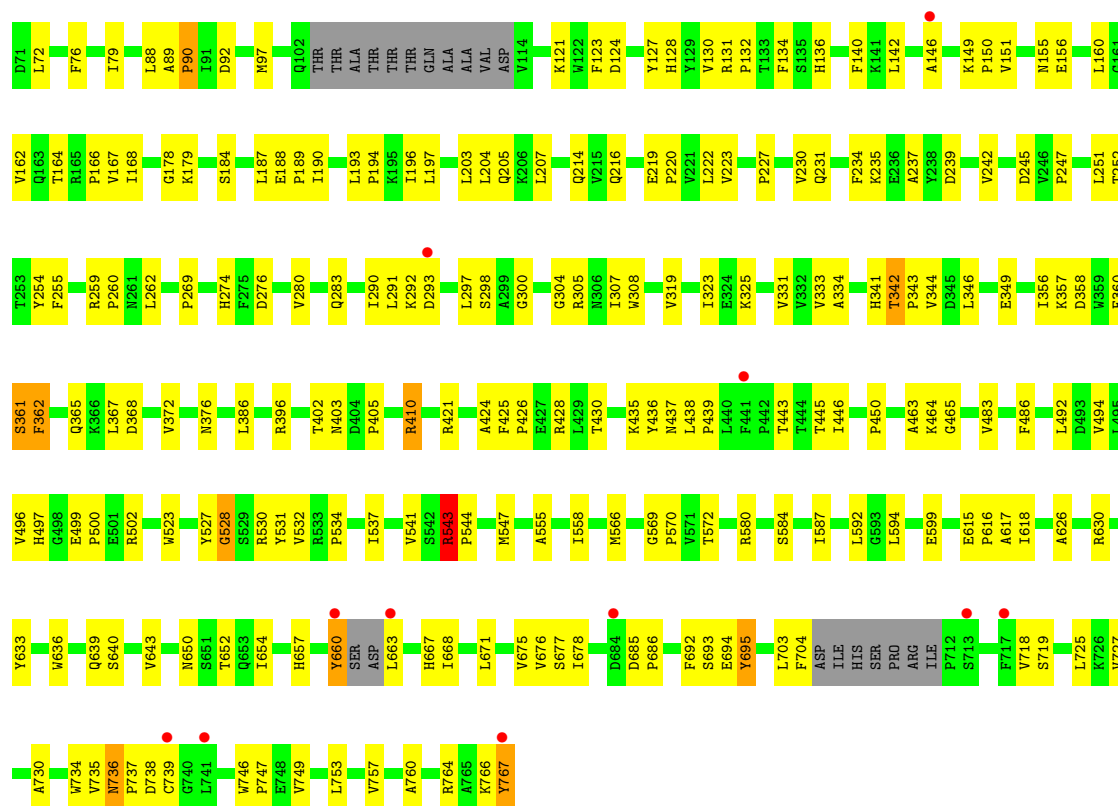
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 5-methyltetrahydropteroyltriglutamate--homocysteine methyltransferase



- Molecule 1: 5-methyltetrahydropteroyltriglutamate--homocysteine methyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.64Å 98.08Å 162.59Å 90.00° 131.10° 90.00°	Depositor
Resolution (Å)	47.66 – 2.80 47.66 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.66-2.80) 99.7 (47.66-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.210 , 0.276 0.203 , 0.266	Depositor DCC
R_{free} test set	2028 reflections (4.25%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.029 for 1/2*h-3/2*k,-1/2*h-1/2*k,-h+k-l 0.035 for 1/2*h+3/2*k,1/2*h-1/2*k,-h-k-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11040	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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	0.54	0/5626	0.94	18/7699 (0.2%)
1	B	0.56	0/5595	0.94	21/7644 (0.3%)
All	All	0.55	0/11221	0.94	39/15343 (0.3%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	695	TYR	CA-C-N	8.48	128.18	119.19
1	B	695	TYR	C-N-CA	8.48	128.18	119.19
1	A	410	ARG	NE-CZ-NH2	8.14	126.53	119.20
1	A	695	TYR	CA-C-N	8.07	127.74	119.19
1	A	695	TYR	C-N-CA	8.07	127.74	119.19
1	A	693	SER	N-CA-C	-7.28	104.14	112.87
1	A	410	ARG	NE-CZ-NH1	-7.24	114.27	121.50
1	B	693	SER	N-CA-C	-6.82	104.69	112.87
1	B	344	VAL	N-CA-C	6.72	116.84	110.53
1	B	736	ASN	N-CA-C	6.63	113.97	108.07
1	B	543	ARG	NE-CZ-NH2	6.63	125.17	119.20
1	A	438	LEU	CA-C-N	6.41	126.87	120.52
1	A	438	LEU	C-N-CA	6.41	126.87	120.52
1	B	543	ARG	NE-CZ-NH1	-6.35	115.15	121.50
1	B	438	LEU	CA-C-N	5.97	126.43	120.52
1	B	438	LEU	C-N-CA	5.97	126.43	120.52
1	A	736	ASN	N-CA-C	5.90	113.32	108.07
1	A	107	THR	N-CA-C	-5.82	106.80	114.31
1	A	219	GLU	CA-C-N	-5.73	114.34	120.47
1	A	219	GLU	C-N-CA	-5.73	114.34	120.47
1	A	410	ARG	CD-NE-CZ	5.67	132.34	124.40
1	B	410	ARG	NE-CZ-NH2	-5.53	114.22	119.20
1	B	654	ILE	CB-CA-C	-5.49	104.31	110.96
1	B	79	ILE	N-CA-C	5.46	113.56	108.15
1	A	739	CYS	N-CA-C	-5.39	106.83	113.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	GLU	CA-C-N	-5.38	114.72	120.47
1	B	219	GLU	C-N-CA	-5.38	114.72	120.47
1	A	345	ASP	N-CA-C	5.35	116.75	107.93
1	B	410	ARG	CD-NE-CZ	5.28	131.79	124.40
1	A	342	THR	CA-C-N	-5.27	115.30	120.52
1	A	342	THR	C-N-CA	-5.27	115.30	120.52
1	A	344	VAL	N-CA-C	5.23	115.90	110.82
1	B	342	THR	CA-C-N	-5.22	115.35	120.52
1	B	342	THR	C-N-CA	-5.22	115.35	120.52
1	B	9	PHE	CA-C-N	5.17	125.42	119.83
1	B	9	PHE	C-N-CA	5.17	125.42	119.83
1	B	739	CYS	N-CA-C	-5.09	107.20	113.41
1	B	543	ARG	CD-NE-CZ	5.08	131.51	124.40
1	A	654	ILE	CB-CA-C	-5.04	104.86	110.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5510	0	5051	182	0
1	B	5479	0	5062	183	0
2	A	22	0	0	0	0
2	B	29	0	0	0	0
All	All	11040	0	10113	365	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 17.

All (365) 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:B:252:THR:HG23	1:B:274:HIS:HB3	1.29	1.14
1:A:252:THR:HG23	1:A:274:HIS:HB3	1.37	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:VAL:HG11	1:B:269:PRO:O	1.71	0.90
1:A:255:PHE:CE1	1:A:305:ARG:HD2	2.07	0.89
1:B:190:ILE:HD13	1:B:230:VAL:HG22	1.54	0.86
1:B:252:THR:HG23	1:B:274:HIS:CB	2.05	0.86
1:B:255:PHE:CE1	1:B:305:ARG:HD2	2.11	0.86
1:A:242:VAL:HG11	1:A:269:PRO:O	1.76	0.85
1:B:446:ILE:HD13	1:B:657:HIS:CE1	2.12	0.85
1:A:190:ILE:HD13	1:A:230:VAL:HG22	1.55	0.85
1:A:403:ASN:O	1:A:405:PRO:HD3	1.79	0.83
1:A:446:ILE:HD13	1:A:657:HIS:CE1	2.17	0.80
1:B:121:LYS:HE3	1:B:124:ASP:HA	1.64	0.79
1:B:6:VAL:O	1:B:59:PRO:HG3	1.83	0.79
1:B:376:ASN:ND2	1:B:386:LEU:HD11	1.98	0.79
1:A:121:LYS:HE3	1:A:124:ASP:HA	1.65	0.78
1:A:252:THR:HG23	1:A:274:HIS:CB	2.13	0.78
1:B:403:ASN:O	1:B:405:PRO:HD3	1.84	0.78
1:A:242:VAL:HG21	1:A:269:PRO:HB2	1.63	0.77
1:B:376:ASN:HD21	1:B:386:LEU:HD11	1.50	0.76
1:B:242:VAL:HG21	1:B:269:PRO:HB2	1.67	0.75
1:B:254:TYR:HA	1:B:276:ASP:HB2	1.68	0.75
1:A:6:VAL:O	1:A:59:PRO:HG3	1.87	0.73
1:A:220:PRO:O	1:A:223:VAL:HG22	1.87	0.73
1:A:727:VAL:HG13	1:A:728:TYR:CD2	2.24	0.72
1:B:220:PRO:O	1:B:223:VAL:HG22	1.89	0.72
1:A:254:TYR:HA	1:A:276:ASP:HB2	1.71	0.71
1:A:5:SER:HB3	1:A:334:ALA:HB2	1.72	0.71
1:B:499:GLU:HG2	1:B:502:ARG:HD2	1.75	0.69
1:A:227:PRO:O	1:A:231:GLN:HG2	1.93	0.68
1:B:51:GLN:NE2	1:B:162:VAL:HG22	2.09	0.68
1:B:227:PRO:O	1:B:231:GLN:HG2	1.94	0.68
1:B:19:LYS:HE3	1:B:23:GLU:OE2	1.94	0.68
1:A:723:GLU:HA	1:A:726:LYS:HD3	1.74	0.67
1:B:259:ARG:HB2	1:B:260:PRO:HD3	1.77	0.67
1:B:497:HIS:CD2	1:B:499:GLU:H	2.13	0.67
1:B:291:LEU:HD11	1:B:297:LEU:HB2	1.78	0.66
1:A:51:GLN:NE2	1:A:162:VAL:HG22	2.11	0.65
1:A:497:HIS:CD2	1:A:499:GLU:H	2.14	0.65
1:B:131:ARG:HH11	1:B:179:LYS:HD3	1.61	0.65
1:B:572:THR:HA	1:B:617:ALA:HB3	1.80	0.64
1:B:584:SER:OG	1:B:587:ILE:HD12	1.99	0.63
1:B:5:SER:HB3	1:B:334:ALA:HB2	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ARG:HD3	1:B:523:TRP:CD1	2.33	0.63
1:B:323:ILE:HA	1:B:331:VAL:HG21	1.82	0.62
1:A:254:TYR:O	1:A:255:PHE:HB2	1.99	0.62
1:B:60:SER:HB3	1:B:164:THR:OG1	2.00	0.61
1:B:204:LEU:O	1:B:247:PRO:HD3	2.00	0.61
1:A:255:PHE:HE1	1:A:305:ARG:HD2	1.62	0.61
1:A:204:LEU:O	1:A:247:PRO:HD3	2.01	0.61
1:A:463:ALA:C	1:A:465:GLY:H	2.09	0.61
1:A:19:LYS:HE3	1:A:23:GLU:OE2	2.01	0.61
1:A:291:LEU:HD11	1:A:297:LEU:HB2	1.82	0.60
1:A:319:VAL:HG21	1:A:333:VAL:HG22	1.83	0.60
1:B:463:ALA:C	1:B:465:GLY:H	2.09	0.60
1:A:16:ARG:HD3	1:A:523:TRP:CD1	2.36	0.60
1:B:51:GLN:HE22	1:B:162:VAL:HG22	1.66	0.60
1:B:569:GLY:HA3	1:B:615:GLU:CD	2.26	0.60
1:A:421:ARG:NH2	1:A:428:ARG:HD2	2.16	0.60
1:B:421:ARG:NH2	1:B:428:ARG:HD2	2.17	0.60
1:A:51:GLN:HE22	1:A:162:VAL:HG22	1.65	0.60
1:B:319:VAL:HG21	1:B:333:VAL:HG22	1.82	0.60
1:A:70:LEU:HD11	1:A:97:MET:HE2	1.84	0.59
1:A:572:THR:HA	1:A:617:ALA:HB3	1.84	0.59
1:A:323:ILE:HA	1:A:331:VAL:HG21	1.84	0.59
1:B:262:LEU:HD22	1:B:290:ILE:HG21	1.85	0.59
1:B:166:PRO:HD2	1:B:214:GLN:O	2.03	0.59
1:A:259:ARG:HB2	1:A:260:PRO:HD3	1.83	0.59
1:B:70:LEU:HD11	1:B:97:MET:HE2	1.85	0.58
1:A:454:ASP:O	1:A:455:ILE:C	2.45	0.58
1:A:55:VAL:HG12	1:A:58:ILE:HG12	1.84	0.58
1:A:527:TYR:O	1:A:528:GLY:C	2.45	0.57
1:B:16:ARG:HD3	1:B:523:TRP:CG	2.39	0.57
1:B:497:HIS:HD2	1:B:499:GLU:H	1.50	0.57
1:B:749:VAL:HG13	1:B:753:LEU:HD12	1.86	0.57
1:A:300:GLY:HA2	1:A:334:ALA:O	2.03	0.57
1:A:570:PRO:HG2	1:A:640:SER:HB3	1.87	0.57
1:B:492:LEU:HD21	1:B:753:LEU:HD22	1.86	0.57
1:A:166:PRO:HD2	1:A:214:GLN:O	2.04	0.57
1:B:677:SER:HB3	1:B:736:ASN:HD21	1.70	0.57
1:B:88:LEU:HD22	1:B:92:ASP:HB3	1.86	0.57
1:B:235:LYS:HE3	1:B:239:ASP:OD2	2.06	0.56
1:A:88:LEU:HD22	1:A:92:ASP:HB3	1.88	0.56
1:A:235:LYS:HE3	1:A:239:ASP:OD2	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:GLU:HG2	1:A:502:ARG:HD2	1.87	0.56
1:A:7:LEU:HD21	1:A:274:HIS:CD2	2.40	0.56
1:A:497:HIS:HD2	1:A:499:GLU:H	1.51	0.56
1:A:569:GLY:HA3	1:A:615:GLU:CD	2.31	0.56
1:A:683:LYS:C	1:A:685:ASP:H	2.13	0.55
1:A:692:PHE:C	1:A:694:GLU:N	2.61	0.55
1:A:446:ILE:HG21	1:A:657:HIS:CD2	2.41	0.55
1:A:677:SER:HB3	1:A:736:ASN:HD21	1.72	0.55
1:B:543:ARG:HD2	1:B:547:MET:HG3	1.88	0.55
1:B:570:PRO:HG2	1:B:640:SER:HB3	1.88	0.55
1:A:692:PHE:C	1:A:694:GLU:H	2.14	0.55
1:A:16:ARG:HD3	1:A:523:TRP:CG	2.41	0.55
1:B:616:PRO:HB2	1:B:660:TYR:HE2	1.72	0.55
1:B:60:SER:HB3	1:B:164:THR:CB	2.37	0.54
1:B:446:ILE:HG21	1:B:657:HIS:CD2	2.43	0.54
1:A:362:PHE:N	1:A:362:PHE:CD1	2.74	0.54
1:A:365:GLN:H	1:A:365:GLN:CD	2.16	0.54
1:B:255:PHE:HE1	1:B:305:ARG:HD2	1.69	0.54
1:A:9:PHE:CG	1:A:10:PRO:HD2	2.42	0.54
1:B:767:TYR:CD1	1:B:767:TYR:N	2.75	0.54
1:A:633:TYR:HA	1:A:636:TRP:NE1	2.23	0.53
1:A:190:ILE:CD1	1:A:230:VAL:HG22	2.35	0.53
1:B:362:PHE:N	1:B:362:PHE:CD1	2.74	0.53
1:B:11:ARG:O	1:B:18:LEU:HD22	2.08	0.53
1:B:193:LEU:HB3	1:B:194:PRO:HD3	1.90	0.53
1:A:555:ALA:O	1:A:558:ILE:HG12	2.08	0.53
1:A:667:HIS:NE2	1:A:671:LEU:HD21	2.24	0.53
1:B:300:GLY:HA2	1:B:334:ALA:O	2.09	0.53
1:B:618:ILE:HG13	1:B:667:HIS:CE1	2.43	0.53
1:B:17:GLU:O	1:B:21:ILE:HG22	2.09	0.53
1:A:70:LEU:HD22	1:A:130:VAL:HG21	1.90	0.53
1:A:105:ALA:HA	1:A:110:ALA:O	2.08	0.53
1:A:209:GLU:HG2	1:A:209:GLU:O	2.09	0.53
1:B:89:ALA:HB1	1:B:90:PRO:HD2	1.91	0.53
1:B:616:PRO:CB	1:B:660:TYR:HE2	2.22	0.52
1:A:450:PRO:HG2	1:A:746:TRP:CE2	2.44	0.52
1:A:531:TYR:CD1	1:A:531:TYR:N	2.75	0.52
1:B:439:PRO:HB2	1:B:764:ARG:HD3	1.91	0.52
1:B:555:ALA:O	1:B:558:ILE:HG12	2.08	0.52
1:B:692:PHE:C	1:B:694:GLU:N	2.65	0.52
1:B:308:TRP:CE3	1:B:396:ARG:CZ	2.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:TYR:O	1:B:528:GLY:C	2.50	0.52
1:A:626:ALA:HA	1:A:630:ARG:HD2	1.92	0.52
1:B:532:VAL:HG23	1:B:534:PRO:HD3	1.92	0.52
1:B:121:LYS:HE3	1:B:123:PHE:O	2.09	0.51
1:B:252:THR:HG23	1:B:274:HIS:CG	2.45	0.51
1:A:193:LEU:HB3	1:A:194:PRO:HD3	1.93	0.51
1:B:499:GLU:N	1:B:500:PRO:HD3	2.25	0.51
1:A:616:PRO:CB	1:A:660:TYR:HE2	2.24	0.51
1:A:17:GLU:O	1:A:21:ILE:HG22	2.11	0.51
1:A:308:TRP:CE3	1:A:396:ARG:CZ	2.94	0.51
1:A:424:ALA:O	1:A:428:ARG:HG3	2.11	0.51
1:A:252:THR:HG23	1:A:274:HIS:CG	2.45	0.51
1:A:262:LEU:HD22	1:A:290:ILE:HG21	1.91	0.51
1:A:142:LEU:HD21	1:A:203:LEU:HB2	1.93	0.51
1:B:11:ARG:H	1:B:11:ARG:HD3	1.76	0.51
1:B:7:LEU:HD21	1:B:274:HIS:CD2	2.46	0.50
1:B:70:LEU:CD1	1:B:97:MET:HE2	2.42	0.50
1:A:60:SER:HB3	1:A:164:THR:OG1	2.11	0.50
1:A:11:ARG:HD3	1:A:11:ARG:H	1.76	0.50
1:A:435:LYS:HG2	1:A:436:TYR:CE2	2.46	0.50
1:B:254:TYR:O	1:B:255:PHE:HB2	2.11	0.50
1:B:633:TYR:HA	1:B:636:TRP:NE1	2.27	0.50
1:A:60:SER:HB3	1:A:164:THR:CB	2.42	0.50
1:A:309:LYS:HB2	1:A:359:TRP:O	2.12	0.50
1:A:343:PRO:HB2	1:A:362:PHE:CD2	2.47	0.50
1:A:616:PRO:HB2	1:A:660:TYR:HE2	1.76	0.50
1:A:677:SER:CB	1:A:736:ASN:HD21	2.25	0.50
1:B:685:ASP:N	1:B:686:PRO:CD	2.74	0.50
1:A:499:GLU:N	1:A:500:PRO:HD3	2.26	0.50
1:B:9:PHE:CG	1:B:10:PRO:HD2	2.47	0.50
1:A:21:ILE:HG13	1:A:35:LEU:HD13	1.95	0.49
1:B:531:TYR:CD1	1:B:531:TYR:N	2.79	0.49
1:A:47:TRP:HZ3	1:A:156:GLU:HG2	1.77	0.49
1:A:197:LEU:HD21	1:A:237:ALA:HB1	1.93	0.49
1:B:677:SER:CB	1:B:736:ASN:HD21	2.25	0.49
1:A:197:LEU:HD11	1:A:237:ALA:HA	1.93	0.49
1:B:70:LEU:HD22	1:B:130:VAL:HG21	1.94	0.49
1:B:692:PHE:C	1:B:694:GLU:H	2.18	0.49
1:A:636:TRP:HA	1:A:639:GLN:HB3	1.95	0.49
1:B:142:LEU:HD21	1:B:203:LEU:HB2	1.94	0.49
1:B:450:PRO:HG2	1:B:746:TRP:CE2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:PHE:CD1	1:A:305:ARG:HD2	2.47	0.49
1:A:121:LYS:HE3	1:A:123:PHE:O	2.13	0.49
1:A:439:PRO:HB2	1:A:764:ARG:NE	2.28	0.49
1:B:307:ILE:C	1:B:307:ILE:HD12	2.38	0.49
1:B:131:ARG:HG2	1:B:179:LYS:HD3	1.95	0.49
1:B:190:ILE:CD1	1:B:230:VAL:HG22	2.36	0.49
1:A:105:ALA:HB2	1:A:111:ALA:HB2	1.94	0.49
1:A:668:ILE:HD12	1:A:692:PHE:HZ	1.77	0.48
1:B:51:GLN:O	1:B:52:LYS:C	2.56	0.48
1:A:70:LEU:CD1	1:A:97:MET:HE2	2.43	0.48
1:A:463:ALA:C	1:A:465:GLY:N	2.72	0.48
1:A:725:LEU:HD21	1:A:730:ALA:HA	1.96	0.48
1:B:47:TRP:HZ3	1:B:156:GLU:HG2	1.78	0.48
1:B:362:PHE:N	1:B:362:PHE:HD1	2.11	0.48
1:B:365:GLN:CD	1:B:365:GLN:H	2.21	0.48
1:B:436:TYR:O	1:B:437:ASN:C	2.55	0.48
1:A:362:PHE:N	1:A:362:PHE:HD1	2.12	0.48
1:A:436:TYR:O	1:A:437:ASN:C	2.56	0.48
1:B:410:ARG:HG2	1:B:594:LEU:HD13	1.96	0.48
1:A:256:GLY:C	1:A:280:VAL:HG21	2.39	0.48
1:A:618:ILE:HG13	1:A:667:HIS:CE1	2.48	0.48
1:B:749:VAL:CG1	1:B:753:LEU:HD12	2.44	0.48
1:B:541:VAL:HG11	1:B:592:LEU:HD23	1.96	0.48
1:B:636:TRP:HA	1:B:639:GLN:HB3	1.95	0.48
1:A:89:ALA:HB1	1:A:90:PRO:HD2	1.96	0.48
1:A:660:TYR:C	1:A:663:LEU:HA	2.39	0.47
1:A:736:ASN:HB2	1:A:737:PRO:CD	2.44	0.47
1:B:255:PHE:CD1	1:B:305:ARG:HD2	2.49	0.47
1:B:660:TYR:C	1:B:663:LEU:HA	2.38	0.47
1:B:435:LYS:HG2	1:B:436:TYR:CE2	2.49	0.47
1:B:439:PRO:HB2	1:B:764:ARG:NE	2.29	0.47
1:B:736:ASN:HB2	1:B:737:PRO:CD	2.43	0.47
1:A:259:ARG:HA	1:A:262:LEU:HG	1.96	0.47
1:B:668:ILE:HD12	1:B:692:PHE:HZ	1.79	0.47
1:B:308:TRP:CE3	1:B:396:ARG:NH1	2.82	0.47
1:A:537:ILE:O	1:A:580:ARG:HG3	2.14	0.47
1:A:703:LEU:O	1:A:704:PHE:CB	2.63	0.47
1:B:132:PRO:HD2	1:B:178:GLY:HA2	1.96	0.47
1:B:360:PHE:O	1:B:361:SER:HB2	2.15	0.47
1:A:70:LEU:HD13	1:A:130:VAL:HG11	1.96	0.47
1:A:160:LEU:N	1:A:160:LEU:HD23	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLN:O	1:A:287:VAL:HG22	2.15	0.47
1:B:570:PRO:CG	1:B:640:SER:HB3	2.45	0.47
1:B:572:THR:OG1	1:B:615:GLU:HA	2.15	0.47
1:B:678:ILE:HD13	1:B:692:PHE:CE2	2.49	0.47
1:B:50:GLN:HG2	1:B:367:LEU:CD2	2.44	0.47
1:A:368:ASP:O	1:A:372:VAL:HG23	2.15	0.47
1:B:131:ARG:NH1	1:B:179:LYS:HD3	2.28	0.47
1:B:140:PHE:CD1	1:B:196:ILE:HG13	2.51	0.46
1:B:222:LEU:HD21	1:B:234:PHE:CE1	2.50	0.46
1:B:343:PRO:HB2	1:B:362:PHE:CD2	2.50	0.46
1:A:725:LEU:HA	1:A:725:LEU:HD23	1.78	0.46
1:A:356:ILE:C	1:A:358:ASP:N	2.70	0.46
1:A:445:THR:OG1	1:A:496:VAL:HG13	2.16	0.46
1:B:463:ALA:C	1:B:465:GLY:N	2.71	0.46
1:B:530:ARG:C	1:B:531:TYR:HD1	2.24	0.46
1:A:439:PRO:HB2	1:A:764:ARG:HD3	1.96	0.46
1:A:760:ALA:O	1:A:764:ARG:HG3	2.16	0.46
1:B:136:HIS:CE1	1:B:187:LEU:HD13	2.50	0.46
1:A:429:LEU:HD12	1:A:429:LEU:O	2.15	0.46
1:A:63:PHE:CD1	1:A:63:PHE:C	2.94	0.46
1:B:197:LEU:HD21	1:B:237:ALA:HB1	1.97	0.46
1:B:356:ILE:C	1:B:358:ASP:N	2.69	0.46
1:A:55:VAL:CG1	1:A:58:ILE:HG12	2.46	0.46
1:B:149:LYS:HB3	1:B:150:PRO:HD3	1.98	0.46
1:B:445:THR:OG1	1:B:496:VAL:HG13	2.15	0.46
1:A:35:LEU:O	1:A:36:LEU:C	2.59	0.46
1:A:679:GLU:OE2	1:A:739:CYS:N	2.49	0.46
1:B:424:ALA:O	1:B:428:ARG:HG3	2.15	0.46
1:A:66:TYR:CE2	1:A:528:GLY:HA3	2.51	0.45
1:A:438:LEU:HB3	1:A:439:PRO:HD2	1.98	0.45
1:A:111:ALA:O	1:A:112:VAL:C	2.58	0.45
1:A:308:TRP:CE3	1:A:396:ARG:NH1	2.84	0.45
1:A:566:MET:HE3	1:A:566:MET:HB3	1.71	0.45
1:A:222:LEU:HD21	1:A:234:PHE:CE1	2.51	0.45
1:B:537:ILE:O	1:B:580:ARG:HG3	2.16	0.45
1:A:90:PRO:HB3	1:A:146:ALA:HB2	1.99	0.45
1:A:693:SER:N	1:A:728:TYR:OH	2.50	0.45
1:B:55:VAL:HG12	1:B:58:ILE:HG12	1.98	0.45
1:B:70:LEU:HD13	1:B:130:VAL:HG11	1.97	0.45
1:B:443:THR:HG21	1:B:757:VAL:HA	1.98	0.45
1:A:219:GLU:OE1	1:A:219:GLU:HA	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:THR:CG2	1:B:274:HIS:HB3	2.22	0.45
1:B:274:HIS:HA	1:B:298:SER:HB3	1.98	0.45
1:A:425:PHE:HB3	1:A:426:PRO:HD3	1.99	0.45
1:B:486:PHE:C	1:B:486:PHE:CD2	2.95	0.45
1:B:667:HIS:NE2	1:B:671:LEU:HD21	2.32	0.45
1:B:259:ARG:CB	1:B:260:PRO:HD3	2.46	0.45
1:B:342:THR:HG22	1:B:343:PRO:HD2	1.99	0.45
1:B:446:ILE:CD1	1:B:657:HIS:CE1	2.93	0.45
1:A:239:ASP:HA	1:A:269:PRO:HG3	2.00	0.44
1:B:167:VAL:HG13	1:B:216:GLN:HG2	1.99	0.44
1:B:274:HIS:CB	1:B:298:SER:HB3	2.48	0.44
1:A:254:TYR:O	1:A:255:PHE:CB	2.65	0.44
1:B:280:VAL:HG12	1:B:283:GLN:HB3	1.98	0.44
1:B:639:GLN:O	1:B:643:VAL:HG23	2.17	0.44
1:A:274:HIS:HA	1:A:298:SER:HB3	1.99	0.44
1:B:439:PRO:HB2	1:B:764:ARG:CD	2.48	0.44
1:A:532:VAL:HG23	1:A:534:PRO:HD3	2.00	0.44
1:B:703:LEU:O	1:B:704:PHE:CB	2.65	0.44
1:A:346:LEU:O	1:A:346:LEU:HG	2.17	0.44
1:A:486:PHE:CD2	1:A:486:PHE:C	2.96	0.44
1:A:154:PHE:HE2	1:A:210:ALA:O	2.00	0.44
1:B:425:PHE:HB3	1:B:426:PRO:HD3	1.99	0.44
1:B:725:LEU:HD21	1:B:730:ALA:HA	1.99	0.44
1:A:360:PHE:O	1:A:361:SER:HB2	2.17	0.44
1:A:570:PRO:CG	1:A:640:SER:HB3	2.47	0.44
1:A:736:ASN:HB2	1:A:737:PRO:HD2	1.99	0.44
1:B:692:PHE:HD1	1:B:695:TYR:CB	2.31	0.44
1:A:280:VAL:HG12	1:A:283:GLN:HB3	1.99	0.44
1:A:428:ARG:HA	1:A:650:ASN:HB3	2.00	0.44
1:B:72:LEU:HD22	1:B:76:PHE:CE2	2.53	0.44
1:B:68:GLN:HG2	1:B:69:VAL:N	2.33	0.43
1:A:274:HIS:CB	1:A:298:SER:HB3	2.47	0.43
1:B:205:GLN:NE2	1:B:245:ASP:OD2	2.51	0.43
1:B:292:LYS:O	1:B:293:ASP:C	2.62	0.43
1:A:718:VAL:O	1:A:719:SER:C	2.61	0.43
1:B:727:VAL:O	1:B:727:VAL:HG22	2.18	0.43
1:A:365:GLN:CD	1:A:365:GLN:N	2.76	0.43
1:A:197:LEU:N	1:A:198:PRO:CD	2.82	0.43
1:A:297:LEU:HD23	1:A:297:LEU:C	2.44	0.43
1:A:572:THR:HG23	1:A:617:ALA:HB2	2.00	0.43
1:A:173:SER:OG	1:A:221:VAL:HG13	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:GLU:H	1:B:17:GLU:CD	2.25	0.43
1:A:11:ARG:O	1:A:18:LEU:HD22	2.18	0.43
1:A:38:LYS:HA	1:A:38:LYS:HD3	1.84	0.43
1:A:541:VAL:HG11	1:A:592:LEU:HD23	2.01	0.43
1:B:155:ASN:O	1:B:156:GLU:C	2.62	0.43
1:B:718:VAL:O	1:B:719:SER:C	2.61	0.43
1:A:61:ASN:ND2	1:A:168:ILE:HG22	2.34	0.43
1:A:532:VAL:C	1:A:534:PRO:HD3	2.44	0.43
1:B:151:VAL:HG22	1:B:207:LEU:HD23	2.01	0.42
1:A:530:ARG:C	1:A:531:TYR:HD1	2.27	0.42
1:B:304:GLY:O	1:B:341:HIS:HB2	2.20	0.42
1:A:140:PHE:CD1	1:A:196:ILE:HG13	2.54	0.42
1:B:21:ILE:HG13	1:B:35:LEU:HD13	2.01	0.42
1:A:208:LYS:C	1:A:210:ALA:H	2.27	0.42
1:A:509:PHE:HD1	1:A:547:MET:CE	2.33	0.42
1:B:127:TYR:CG	1:B:128:HIS:N	2.86	0.42
1:B:307:ILE:C	1:B:307:ILE:CD1	2.93	0.42
1:B:346:LEU:HG	1:B:346:LEU:O	2.20	0.42
1:A:68:GLN:HG2	1:A:69:VAL:N	2.35	0.42
1:B:356:ILE:O	1:B:357:LYS:C	2.62	0.42
1:A:17:GLU:H	1:A:17:GLU:CD	2.26	0.42
1:A:349:GLU:HB2	1:A:357:LYS:HE2	2.00	0.42
1:B:90:PRO:HB3	1:B:146:ALA:HB2	2.02	0.42
1:B:368:ASP:O	1:B:372:VAL:HG23	2.18	0.42
1:B:626:ALA:HA	1:B:630:ARG:HD2	2.01	0.42
1:B:259:ARG:HA	1:B:262:LEU:HG	2.01	0.42
1:A:132:PRO:HD2	1:A:178:GLY:HA2	2.02	0.42
1:B:88:LEU:HA	1:B:88:LEU:HD23	1.77	0.42
1:B:428:ARG:HA	1:B:650:ASN:HB3	2.02	0.42
1:A:683:LYS:O	1:A:686:PRO:HD2	2.19	0.42
1:B:61:ASN:ND2	1:B:168:ILE:HG22	2.35	0.42
1:A:274:HIS:HB2	1:A:298:SER:HB3	2.02	0.42
1:A:439:PRO:HB2	1:A:764:ARG:CD	2.50	0.41
1:B:274:HIS:HB2	1:B:298:SER:HB3	2.02	0.41
1:B:566:MET:HE3	1:B:566:MET:HB3	1.67	0.41
1:B:60:SER:HB3	1:B:164:THR:HB	2.02	0.41
1:B:365:GLN:CD	1:B:365:GLN:N	2.78	0.41
1:B:543:ARG:HH21	1:B:599:GLU:HA	1.85	0.41
1:A:31:THR:O	1:A:32:VAL:C	2.64	0.41
1:A:342:THR:HG22	1:A:343:PRO:HD2	2.01	0.41
1:A:343:PRO:O	1:A:362:PHE:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ARG:HD3	1:A:594:LEU:HD13	2.03	0.41
1:B:494:VAL:HG21	1:B:734:TRP:HZ3	1.85	0.41
1:B:760:ALA:O	1:B:764:ARG:HG3	2.20	0.41
1:A:68:GLN:H	1:A:68:GLN:CD	2.29	0.41
1:A:543:ARG:CD	1:A:545:LYS:O	2.69	0.41
1:B:676:VAL:O	1:B:676:VAL:HG23	2.20	0.41
1:A:188:GLU:HA	1:A:189:PRO:HD3	1.87	0.41
1:A:425:PHE:HZ	1:A:698:HIS:ND1	2.19	0.41
1:A:509:PHE:HD1	1:A:547:MET:HE3	1.85	0.41
1:A:543:ARG:HH21	1:A:599:GLU:HA	1.85	0.41
1:B:58:ILE:HA	1:B:59:PRO:HD3	1.87	0.41
1:B:89:ALA:O	1:B:92:ASP:HB2	2.20	0.41
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.82	0.41
1:B:297:LEU:HD23	1:B:297:LEU:C	2.45	0.41
1:A:714:LYS:O	1:A:718:VAL:HG23	2.21	0.41
1:B:188:GLU:HA	1:B:189:PRO:HD3	1.87	0.41
1:B:736:ASN:HB2	1:B:737:PRO:HD2	2.02	0.41
1:A:11:ARG:HB2	1:A:63:PHE:CD2	2.56	0.40
1:A:597:ARG:HB2	1:A:644:ALA:HA	2.04	0.40
1:A:60:SER:HB3	1:A:164:THR:HB	2.03	0.40
1:A:443:THR:HG21	1:A:757:VAL:HA	2.03	0.40
1:B:21:ILE:O	1:B:24:ALA:HB3	2.20	0.40
1:A:204:LEU:HA	1:A:204:LEU:HD23	1.87	0.40
1:A:572:THR:OG1	1:A:615:GLU:HA	2.22	0.40
1:B:193:LEU:HD21	1:B:237:ALA:HB2	2.02	0.40
1:B:349:GLU:HB2	1:B:357:LYS:HE2	2.03	0.40
1:B:532:VAL:C	1:B:534:PRO:HD3	2.46	0.40
1:B:499:GLU:CG	1:B:502:ARG:HD2	2.48	0.40
1:B:675:VAL:HG12	1:B:676:VAL:N	2.36	0.40
1:A:284:LEU:HD23	1:A:321:LYS:HG2	2.02	0.40
1:A:603:LEU:HD23	1:A:603:LEU:HA	1.82	0.40
1:A:683:LYS:C	1:A:685:ASP:N	2.78	0.40
1:B:197:LEU:HD11	1:B:237:ALA:HA	2.04	0.40
1:B:239:ASP:HA	1:B:269:PRO:HG3	2.04	0.40
1:B:746:TRP:HB2	1:B:747:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

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	750/789 (95%)	663 (88%)	75 (10%)	12 (2%)	7	27
1	B	739/789 (94%)	660 (89%)	70 (10%)	9 (1%)	10	34
All	All	1489/1578 (94%)	1323 (89%)	145 (10%)	21 (1%)	9	30

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	SER
1	A	361	SER
1	A	464	LYS
1	B	325	LYS
1	B	361	SER
1	B	464	LYS
1	B	766	LYS
1	A	110	ALA
1	A	325	LYS
1	A	544	PRO
1	A	689	ILE
1	A	738	ASP
1	B	184	SER
1	B	738	ASP
1	A	90	PRO
1	B	90	PRO
1	B	544	PRO
1	A	255	PHE
1	A	684	ASP
1	B	528	GLY
1	A	528	GLY

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	510/681 (75%)	500 (98%)	10 (2%)	48	80
1	B	513/681 (75%)	501 (98%)	12 (2%)	44	78
All	All	1023/1362 (75%)	1001 (98%)	22 (2%)	45	78

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	PHE
1	A	160	LEU
1	A	362	PHE
1	A	402	THR
1	A	430	THR
1	A	483	VAL
1	A	543	ARG
1	A	652	THR
1	A	660	TYR
1	A	699	ILE
1	B	134	PHE
1	B	160	LEU
1	B	251	LEU
1	B	362	PHE
1	B	402	THR
1	B	430	THR
1	B	483	VAL
1	B	543	ARG
1	B	652	THR
1	B	660	TYR
1	B	735	VAL
1	B	767	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	136	HIS
1	A	231	GLN
1	A	376	ASN
1	A	497	HIS
1	A	639	GLN
1	A	653	GLN
1	A	736	ASN
1	B	51	GLN
1	B	61	ASN
1	B	128	HIS
1	B	376	ASN
1	B	497	HIS
1	B	653	GLN
1	B	736	ASN

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](#)

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	756/789 (95%)	-0.16	9 (1%) 76 68	27, 58, 93, 144	0
1	B	747/789 (94%)	-0.15	11 (1%) 72 63	23, 55, 92, 145	0
All	All	1503/1578 (95%)	-0.16	20 (1%) 75 66	23, 57, 92, 145	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	660	TYR	4.3
1	A	684	ASP	3.9
1	B	293	ASP	3.6
1	A	660	TYR	3.6
1	A	713	SER	3.2
1	A	687	ASN	2.7
1	A	741	LEU	2.4
1	B	741	LEU	2.4
1	A	681	SER	2.3
1	B	713	SER	2.3
1	B	739	CYS	2.2
1	B	146	ALA	2.2
1	B	684	ASP	2.2
1	B	767	TYR	2.2
1	B	717	PHE	2.1
1	A	680	PHE	2.1
1	B	663	LEU	2.1
1	B	441	PHE	2.1
1	A	738	ASP	2.0
1	A	745	GLY	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.