



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:48 am GMT

PDB ID : 3UA4
Title : Crystal Structure of Protein Arginine Methyltransferase PRMT5
Authors : Sun, L.; Wang, M.; Lv, Z.; Yang, N.; Liu, Y.; Bao, S.; Gong, W.; Xu, R.M.
Deposited on : 2011-10-21
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

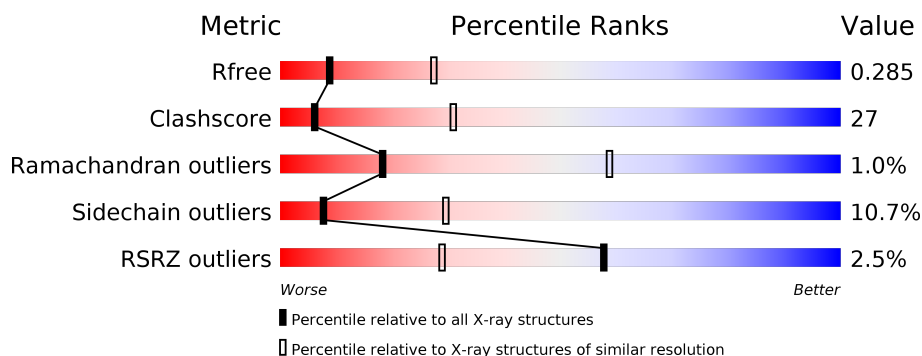
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	745	<div> <div>2%</div> <div>45%</div> <div>37%</div> <div>•</div> <div>14%</div> </div>
1	B	745	<div> <div>3%</div> <div>41%</div> <div>38%</div> <div>6%</div> <div>16%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	B	743	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10345 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 Protein arginine N-methyltransferase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	640	Total	C	N	O	S	0	0	0
			5143	3291	875	957	20			
1	B	628	Total	C	N	O	S	1	0	0
			5049	3238	854	937	20			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP P46580
A	-1	ALA	-	EXPRESSION TAG	UNP P46580
A	0	SER	-	EXPRESSION TAG	UNP P46580
A	735	LEU	-	EXPRESSION TAG	UNP P46580
A	736	GLU	-	EXPRESSION TAG	UNP P46580
A	737	HIS	-	EXPRESSION TAG	UNP P46580
A	738	HIS	-	EXPRESSION TAG	UNP P46580
A	739	HIS	-	EXPRESSION TAG	UNP P46580
A	740	HIS	-	EXPRESSION TAG	UNP P46580
A	741	HIS	-	EXPRESSION TAG	UNP P46580
A	742	HIS	-	EXPRESSION TAG	UNP P46580
B	-2	MET	-	EXPRESSION TAG	UNP P46580
B	-1	ALA	-	EXPRESSION TAG	UNP P46580
B	0	SER	-	EXPRESSION TAG	UNP P46580
B	735	LEU	-	EXPRESSION TAG	UNP P46580
B	736	GLU	-	EXPRESSION TAG	UNP P46580
B	737	HIS	-	EXPRESSION TAG	UNP P46580
B	738	HIS	-	EXPRESSION TAG	UNP P46580
B	739	HIS	-	EXPRESSION TAG	UNP P46580
B	740	HIS	-	EXPRESSION TAG	UNP P46580
B	741	HIS	-	EXPRESSION TAG	UNP P46580
B	742	HIS	-	EXPRESSION TAG	UNP P46580

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		

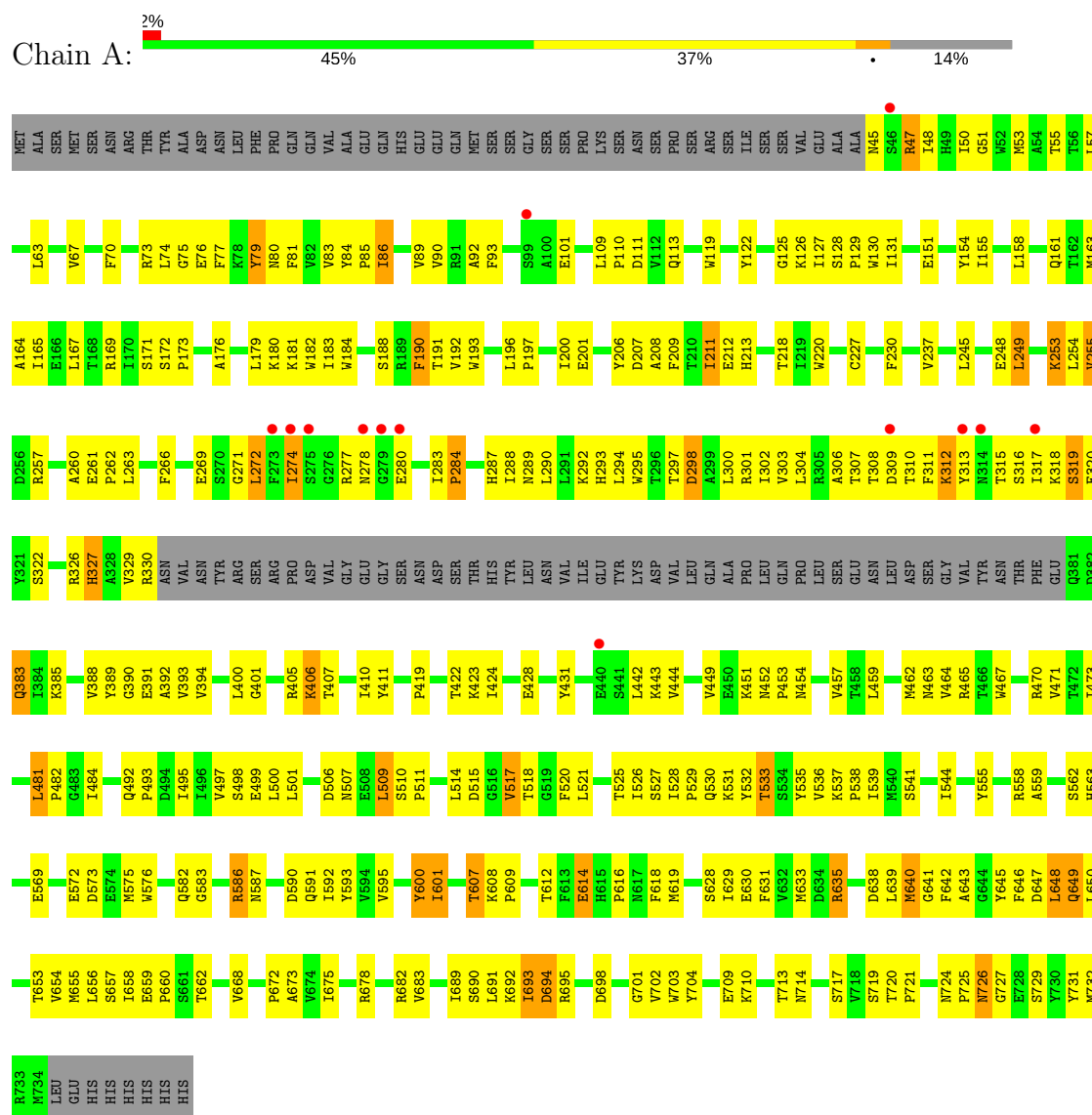
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		
3	B	73	Total	O	0	0
			73	73		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Protein arginine N-methyltransferase 5



- Molecule 1: Protein arginine N-methyltransferase 5





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.56Å 129.49Å 149.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.02 – 3.00 30.02 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.02-3.00) 99.4 (30.02-3.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.232 , 0.288 0.227 , 0.285	Depositor DCC
R_{free} test set	1817 reflections (4.62%)	DCC
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 87.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10345	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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

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

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	0.28	0/5272	0.47	0/7161
1	B	0.27	0/5176	0.47	0/7031
All	All	0.27	0/10448	0.47	0/14192

There are no bond length outliers.

There are no bond angle outliers.

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	5143	0	5096	272	0
1	B	5049	0	5005	285	0
2	B	6	0	8	0	0
3	A	74	0	0	5	0
3	B	73	0	0	2	0
All	All	10345	0	10109	553	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 27.

All (553) 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:724:ASN:HD21	1:B:730:TYR:HB3	1.10	1.15
1:A:533:THR:HB	1:A:612:THR:HG22	1.23	1.08
1:A:635:ARG:HH11	1:A:635:ARG:HG2	1.16	1.07
1:A:74:LEU:HB3	1:A:79:TYR:HE1	1.20	1.07
1:B:198:SER:HB2	1:B:202:LYS:HD3	1.48	0.96
1:A:47:ARG:H	1:A:47:ARG:HD3	1.32	0.94
1:A:422:THR:HG22	1:A:467:TRP:HE1	1.30	0.93
1:B:383:GLN:HE21	1:B:383:GLN:H	1.02	0.93
1:A:449:VAL:HG21	1:A:481:LEU:HD11	1.53	0.91
1:A:608:LYS:HG3	1:A:609:PRO:HD2	1.51	0.89
1:A:635:ARG:NH1	1:A:635:ARG:HG2	1.84	0.86
1:B:383:GLN:N	1:B:383:GLN:HE21	1.73	0.86
1:A:630:GLU:HA	1:A:689:ILE:O	1.78	0.84
1:A:691:LEU:HD21	1:A:693:ILE:HD11	1.59	0.83
1:B:94:TRP:CH2	1:B:96:PRO:HB3	2.15	0.82
1:A:74:LEU:HB3	1:A:79:TYR:CE1	2.11	0.82
1:B:536:VAL:HG22	1:B:642:PHE:HB3	1.61	0.81
1:A:532:TYR:HB3	1:A:648:LEU:HD12	1.62	0.81
1:A:179:LEU:O	1:A:183:ILE:HG12	1.79	0.81
1:B:409:VAL:HG22	1:B:445:LYS:HB3	1.64	0.80
1:B:87:GLY:HA2	1:B:107:ILE:HG23	1.62	0.80
1:B:724:ASN:ND2	1:B:730:TYR:HB3	1.95	0.79
1:A:277:ARG:HB2	1:A:280:GLU:HG3	1.66	0.78
1:A:635:ARG:CG	1:A:635:ARG:HH11	1.97	0.78
1:B:89:VAL:HG13	1:B:93:PHE:HD2	1.49	0.78
1:B:266:PHE:HB2	1:B:302:ILE:HG12	1.65	0.77
1:B:408:VAL:HG23	1:B:442:LEU:HD11	1.63	0.77
1:A:521:LEU:HD22	1:A:525:THR:HG21	1.66	0.77
1:A:312:LYS:HG2	1:A:317:ILE:HG22	1.66	0.76
1:A:529:PRO:HG2	1:A:648:LEU:HD11	1.67	0.76
1:B:697:VAL:HG13	1:B:702:VAL:HG22	1.68	0.76
1:A:86:ILE:HG13	1:A:155:ILE:HG12	1.68	0.76
1:B:89:VAL:HG13	1:B:93:PHE:CD2	2.20	0.76
1:B:537:LYS:HE2	1:B:602:PRO:HB3	1.68	0.75
1:B:529:PRO:HB3	1:B:650:LEU:HD23	1.69	0.75
1:B:312:LYS:HE3	1:B:312:LYS:N	2.02	0.74
1:B:492:GLN:HB3	1:B:522:LYS:HG3	1.69	0.74
1:B:271:GLY:O	1:B:272:LEU:HD13	1.86	0.74
1:A:315:THR:HG23	1:A:318:LYS:HE3	1.70	0.73
1:A:392:ALA:HB2	1:A:654:VAL:HG11	1.70	0.73
1:B:87:GLY:HA3	1:B:91:ARG:HD3	1.70	0.73
1:B:392:ALA:HA	1:B:654:VAL:HG21	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ILE:HG13	1:A:320:GLU:OE1	1.89	0.72
1:B:436:ARG:HH11	1:B:442:LEU:HB2	1.54	0.72
1:A:649:GLN:HA	1:A:655:MET:CB	2.19	0.72
1:B:698:ASP:HB2	1:B:703:TRP:HZ3	1.54	0.72
1:B:94:TRP:HZ2	1:B:102:ASN:HB3	1.54	0.71
1:B:508:GLU:O	1:B:509:LEU:HB2	1.89	0.71
1:A:501:LEU:HD11	1:A:648:LEU:HD22	1.71	0.71
1:B:383:GLN:NE2	1:B:383:GLN:H	1.84	0.71
1:B:405:ARG:HH21	1:B:405:ARG:HB2	1.55	0.71
1:A:48:ILE:HG21	1:A:326:ARG:HG2	1.72	0.71
1:B:155:ILE:HD13	1:B:160:LEU:HD12	1.72	0.70
1:A:206:TYR:HE2	1:A:211:ILE:HD13	1.55	0.70
1:A:89:VAL:HG13	1:A:93:PHE:CD2	2.26	0.70
1:B:532:TYR:CE1	1:B:613:PHE:HB2	2.26	0.69
1:B:70:PHE:HE2	1:B:74:LEU:HD11	1.57	0.69
1:A:406:LYS:HD2	1:A:406:LYS:H	1.58	0.69
1:B:635:ARG:HG2	1:B:635:ARG:HH11	1.58	0.69
1:B:91:ARG:HA	1:B:105:PRO:HB2	1.75	0.68
1:A:310:THR:C	1:A:312:LYS:H	1.95	0.68
1:B:449:VAL:HA	1:B:474:ILE:HG23	1.75	0.68
1:A:501:LEU:CD1	1:A:648:LEU:HD22	2.25	0.67
1:B:711:LYS:HA	1:B:716:GLU:O	1.94	0.67
1:A:196:LEU:HD11	1:A:220:TRP:HB2	1.77	0.67
1:A:646:PHE:O	1:A:658:ILE:HG22	1.95	0.67
1:B:531:LYS:HZ1	1:B:614:GLU:HB3	1.60	0.67
1:A:313:TYR:HD2	1:A:316:SER:HB3	1.59	0.67
1:A:600:TYR:O	1:A:601:ILE:HD12	1.95	0.67
1:B:86:ILE:CD1	1:B:155:ILE:HG12	2.25	0.66
1:B:411:TYR:HD2	1:B:493:PRO:HB3	1.61	0.66
1:B:700:THR:O	1:B:734:MET:HG2	1.95	0.66
1:A:419:PRO:O	1:A:423:LYS:HB2	1.97	0.65
1:B:510:SER:HB3	1:B:532:TYR:OH	1.97	0.65
1:A:555:TYR:O	1:A:558:ARG:HG2	1.96	0.65
1:B:56:THR:HA	1:B:59:VAL:HG23	1.79	0.65
1:A:422:THR:CG2	1:A:467:TRP:HE1	2.05	0.65
1:B:68:ALA:HB2	1:B:114:LEU:CD1	2.27	0.65
1:B:481:LEU:HA	1:B:484:ILE:HG12	1.79	0.64
1:B:411:TYR:CD2	1:B:493:PRO:HB3	2.31	0.64
1:A:500:LEU:O	1:A:510:SER:HB2	1.98	0.64
1:A:196:LEU:HB3	1:A:197:PRO:HD2	1.78	0.64
1:A:127:ILE:HG23	1:A:131:ILE:HD12	1.77	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LEU:HD22	1:A:405:ARG:HH11	1.62	0.64
1:A:501:LEU:HD11	1:A:648:LEU:HD13	1.80	0.64
1:B:600:TYR:O	1:B:601:ILE:HD12	1.97	0.64
1:B:689:ILE:HD11	1:B:710:LYS:HG3	1.80	0.64
1:A:274:ILE:H	1:A:274:ILE:HD13	1.62	0.63
1:A:531:LYS:HB3	1:A:649:GLN:HG2	1.79	0.63
1:A:92:ALA:O	1:A:129:PRO:HD2	1.97	0.63
1:B:495:ILE:HG12	1:B:526:ILE:HG13	1.81	0.63
1:A:649:GLN:HA	1:A:655:MET:HB2	1.79	0.63
1:B:215:ASP:HB2	1:B:248:GLU:OE1	1.99	0.62
1:B:501:LEU:HD22	1:B:648:LEU:HD13	1.81	0.62
1:B:711:LYS:HE2	1:B:717:SER:HB2	1.81	0.62
1:B:70:PHE:CE2	1:B:74:LEU:HD11	2.34	0.62
1:B:593:TYR:O	1:B:673:ALA:HA	1.99	0.62
1:B:635:ARG:HG2	1:B:635:ARG:NH1	2.12	0.62
1:A:698:ASP:HB2	1:A:703:TRP:HZ3	1.64	0.62
1:B:529:PRO:HA	1:B:650:LEU:HA	1.81	0.62
1:A:53:MET:HG3	1:A:83:VAL:HB	1.81	0.62
1:A:151:GLU:O	1:A:155:ILE:HG13	2.00	0.62
1:A:86:ILE:HD11	1:A:154:TYR:HB3	1.81	0.62
1:A:400:LEU:HB3	1:A:405:ARG:HE	1.65	0.62
1:B:531:LYS:NZ	1:B:614:GLU:HB3	2.15	0.61
1:A:274:ILE:HG12	1:A:274:ILE:O	2.00	0.61
1:A:533:THR:HG23	1:A:647:ASP:OD1	2.00	0.61
1:B:724:ASN:HD21	1:B:730:TYR:CB	2.00	0.61
1:A:310:THR:HG23	1:A:310:THR:O	2.00	0.61
1:A:50:ILE:O	1:A:79:TYR:HB2	2.01	0.61
1:A:691:LEU:CD2	1:A:693:ILE:HD11	2.29	0.61
1:B:255:VAL:HG12	1:B:294:LEU:HD11	1.82	0.61
1:B:57:LEU:HD12	1:B:306:ALA:HB1	1.83	0.61
1:B:68:ALA:HB2	1:B:114:LEU:HD11	1.82	0.61
1:A:529:PRO:CG	1:A:648:LEU:HD11	2.31	0.60
1:A:292:LYS:HA	1:A:329:VAL:HG12	1.84	0.60
1:B:714:ASN:N	1:B:714:ASN:OD1	2.35	0.60
1:B:677:LEU:HD23	1:B:723:GLN:OE1	2.02	0.60
1:A:47:ARG:H	1:A:47:ARG:CD	2.11	0.60
1:B:395:GLY:HA2	1:B:398:LYS:HD3	1.83	0.60
1:A:527:SER:HB3	1:A:616:PRO:HD3	1.84	0.59
1:A:206:TYR:CE2	1:A:211:ILE:HD13	2.37	0.59
1:A:406:LYS:HD2	1:A:407:THR:H	1.67	0.59
1:A:128:SER:HB3	1:A:130:TRP:NE1	2.18	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:GLN:CD	1:A:383:GLN:H	2.06	0.59
1:A:391:GLU:O	1:A:394:VAL:HG22	2.03	0.59
1:B:195:GLN:HG3	1:B:267:VAL:HG21	1.85	0.59
1:A:169:ARG:HD3	3:A:806:HOH:O	2.01	0.59
1:B:86:ILE:HG21	1:B:155:ILE:CD1	2.32	0.59
1:B:383:GLN:N	1:B:383:GLN:NE2	2.48	0.59
1:B:481:LEU:O	1:B:481:LEU:HD23	2.03	0.59
1:A:633:MET:HG2	1:A:683:VAL:HG21	1.85	0.58
1:A:180:LYS:HB2	1:A:227:CYS:HA	1.85	0.58
1:A:642:PHE:CD2	1:A:691:LEU:HD22	2.37	0.58
1:B:314:ASN:HB3	1:B:317:ILE:HG13	1.84	0.58
1:B:171:SER:C	1:B:173:PRO:HD3	2.24	0.58
1:A:600:TYR:HD2	1:A:600:TYR:H	1.52	0.58
1:B:69:THR:O	1:B:73:ARG:HG3	2.02	0.58
1:B:690:SER:HB2	1:B:709:GLU:HB2	1.84	0.58
1:B:196:LEU:HB3	1:B:197:PRO:HD2	1.85	0.58
1:A:407:THR:HA	1:A:443:LYS:O	2.04	0.58
1:B:182:TRP:O	1:B:186:ARG:HG2	2.04	0.58
1:B:189:ARG:HD3	1:B:234:TYR:CE1	2.39	0.58
1:B:418:GLY:N	1:B:419:PRO:HD3	2.19	0.58
1:A:562:SER:HB2	3:A:751:HOH:O	2.04	0.57
1:B:698:ASP:HB2	1:B:703:TRP:CZ3	2.36	0.57
1:A:248:GLU:HA	1:A:254:LEU:HD12	1.86	0.57
1:B:236:GLN:HB3	1:B:264:ALA:HB2	1.87	0.57
1:B:443:LYS:HE3	1:B:470:ARG:NH2	2.20	0.57
1:B:521:LEU:HD22	1:B:525:THR:HG21	1.86	0.57
1:A:591:GLN:HB2	1:A:593:TYR:CE1	2.39	0.57
1:B:326:ARG:C	1:B:328:ALA:H	2.08	0.57
1:B:668:VAL:O	1:B:668:VAL:HG12	2.05	0.57
1:A:207:ASP:C	1:A:209:PHE:H	2.08	0.57
1:B:492:GLN:HB2	1:B:522:LYS:HE2	1.86	0.57
1:A:410:ILE:HG21	1:A:424:ILE:HD13	1.87	0.56
1:B:474:ILE:HD11	1:B:484:ILE:HD12	1.87	0.56
1:A:538:PRO:HD3	1:A:631:PHE:CE1	2.41	0.56
1:B:172:SER:N	1:B:173:PRO:HD3	2.20	0.56
1:B:541:SER:HB2	1:B:600:TYR:HB2	1.87	0.56
1:A:592:ILE:HD12	1:A:675:ILE:HG13	1.88	0.55
1:B:562:SER:HB2	3:B:778:HOH:O	2.06	0.55
1:A:191:THR:HG22	1:A:192:VAL:N	2.22	0.55
1:B:646:PHE:CE2	1:B:658:ILE:HB	2.40	0.55
1:A:254:LEU:HA	1:A:257:ARG:HD2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:ILE:HD11	1:B:497:VAL:HG12	1.89	0.55
1:A:254:LEU:O	1:A:257:ARG:HD3	2.06	0.55
1:A:517:VAL:O	1:A:517:VAL:HG13	2.05	0.55
1:A:63:LEU:HD11	1:A:70:PHE:CD1	2.42	0.55
1:A:544:ILE:HB	1:A:640:MET:HE2	1.89	0.55
1:B:381:GLN:OE1	1:B:381:GLN:HA	2.07	0.55
1:B:425:LEU:HD12	1:B:467:TRP:CD1	2.41	0.55
1:B:692:LYS:HB2	1:B:707:HIS:CD2	2.41	0.55
1:B:284:PRO:HG2	1:B:287:HIS:CG	2.42	0.55
1:B:245:LEU:HD13	1:B:287:HIS:CD2	2.42	0.55
1:A:127:ILE:CG2	1:A:131:ILE:HD12	2.37	0.54
1:A:51:GLY:HA3	1:A:81:PHE:CE1	2.42	0.54
1:B:63:LEU:HD11	1:B:70:PHE:CD1	2.42	0.54
1:A:520:PHE:O	1:A:520:PHE:CG	2.60	0.54
1:A:497:VAL:HG22	1:A:528:ILE:CG2	2.37	0.54
1:A:511:PRO:O	1:A:515:ASP:HB2	2.07	0.54
1:A:648:LEU:O	1:A:655:MET:HB2	2.07	0.54
1:A:649:GLN:HA	1:A:655:MET:HB3	1.88	0.54
1:B:181:LYS:HD2	1:B:576:TRP:CZ2	2.42	0.54
1:A:255:VAL:HG12	1:A:294:LEU:HD11	1.89	0.54
1:A:582:GLN:NE2	1:A:587:ASN:HB2	2.23	0.54
1:B:312:LYS:HE3	1:B:312:LYS:H	1.72	0.54
1:B:518:THR:HA	1:B:521:LEU:HD12	1.88	0.54
1:A:451:LYS:HG3	1:A:452:ASN:N	2.21	0.54
1:B:450:GLU:O	1:B:475:GLU:HA	2.06	0.54
1:B:52:TRP:O	1:B:82:VAL:HG23	2.08	0.54
1:B:537:LYS:HB2	1:B:607:THR:HG22	1.90	0.54
1:A:70:PHE:O	1:A:74:LEU:HG	2.08	0.54
1:B:86:ILE:HD11	1:B:151:GLU:HG2	1.89	0.54
1:B:193:TRP:CH2	1:B:301:ARG:HD3	2.43	0.54
1:B:193:TRP:HH2	1:B:301:ARG:HD3	1.73	0.54
1:A:51:GLY:HA3	1:A:81:PHE:CZ	2.43	0.53
1:A:586:ARG:HD2	1:A:678:ARG:NH2	2.23	0.53
1:B:433:ASN:N	1:B:433:ASN:OD1	2.41	0.53
1:A:260:ALA:HB1	1:B:541:SER:HA	1.89	0.53
1:A:410:ILE:HD12	1:A:444:VAL:HG11	1.90	0.53
1:A:532:TYR:HB3	1:A:648:LEU:CD1	2.36	0.53
1:B:635:ARG:HH11	1:B:635:ARG:CG	2.19	0.53
1:A:257:ARG:HH21	1:B:636:ASN:HB2	1.74	0.53
1:A:659:GLU:HG2	1:A:660:PRO:HD2	1.89	0.53
1:B:423:LYS:HE3	1:B:426:LYS:HE2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:SER:HB3	1:A:511:PRO:HD3	1.89	0.53
1:B:86:ILE:HG21	1:B:155:ILE:HD11	1.90	0.53
1:A:411:TYR:CD2	1:A:493:PRO:HB3	2.44	0.53
1:B:410:ILE:HG13	1:B:495:ILE:HB	1.90	0.53
1:B:44:ALA:N	1:B:47:ARG:HD3	2.24	0.53
1:B:86:ILE:HD12	1:B:155:ILE:HG12	1.91	0.53
1:A:308:THR:OG1	1:A:310:THR:HG22	2.09	0.53
1:A:312:LYS:HG2	1:A:317:ILE:CG2	2.36	0.53
1:A:515:ASP:O	1:A:518:THR:HG23	2.09	0.53
1:B:611:PHE:CE2	1:B:695:ARG:HB2	2.43	0.53
1:A:81:PHE:HB2	1:A:122:TYR:O	2.09	0.53
1:B:642:PHE:CD2	1:B:691:LEU:HD22	2.44	0.53
1:B:541:SER:HB2	1:B:600:TYR:CB	2.38	0.53
1:B:94:TRP:CZ3	1:B:96:PRO:HB3	2.43	0.53
1:B:86:ILE:HD13	1:B:155:ILE:HG12	1.91	0.53
1:A:720:THR:HB	1:A:721:PRO:HD2	1.91	0.52
1:A:77:PHE:CZ	1:A:315:THR:HG22	2.44	0.52
1:A:184:TRP:O	1:A:559:ALA:HB3	2.09	0.52
1:A:47:ARG:HD3	1:A:47:ARG:N	2.13	0.52
1:B:406:LYS:HD2	1:B:407:THR:HG22	1.90	0.52
1:A:537:LYS:HD3	1:A:607:THR:HG22	1.91	0.52
1:B:390:GLY:O	1:B:394:VAL:HG13	2.10	0.52
1:B:445:LYS:HE2	1:B:447:TYR:CE2	2.43	0.52
1:B:51:GLY:HA2	1:B:81:PHE:O	2.10	0.52
1:A:86:ILE:HG22	1:A:126:LYS:O	2.09	0.52
1:B:446:LEU:O	1:B:471:VAL:HG23	2.10	0.52
1:A:501:LEU:HD11	1:A:648:LEU:CD2	2.39	0.52
1:B:569:GLU:CD	1:B:579:LYS:HE2	2.29	0.52
1:A:111:ASP:HB3	1:A:158:LEU:HD23	1.92	0.52
1:A:167:LEU:HD13	3:A:755:HOH:O	2.10	0.52
1:A:310:THR:C	1:A:312:LYS:N	2.62	0.52
1:B:220:TRP:CD2	1:B:237:VAL:HB	2.45	0.52
1:A:284:PRO:O	1:A:288:ILE:HG12	2.10	0.51
1:A:85:PRO:HB2	1:A:92:ALA:HB2	1.92	0.51
1:B:273:PHE:CD2	1:B:282:SER:HB2	2.46	0.51
1:B:391:GLU:O	1:B:394:VAL:HG22	2.10	0.51
1:A:327:HIS:HA	1:A:330:ARG:HG2	1.91	0.51
1:A:645:TYR:HB3	1:A:658:ILE:HG23	1.93	0.51
1:A:70:PHE:CE2	1:A:74:LEU:HD11	2.45	0.51
1:B:77:PHE:CE2	1:B:318:LYS:HD3	2.45	0.51
1:B:86:ILE:HD11	1:B:151:GLU:CG	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:HIS:HD2	1:A:591:GLN:OE1	1.93	0.51
1:A:709:GLU:HG2	1:A:719:SER:HB3	1.93	0.51
1:A:73:ARG:O	1:A:76:GLU:HB2	2.10	0.51
1:A:533:THR:O	1:A:646:PHE:HA	2.11	0.51
1:A:628:SER:O	1:A:629:ILE:HD13	2.11	0.51
1:B:208:ALA:HA	1:B:211:ILE:HG12	1.93	0.51
1:A:535:TYR:CD1	1:A:609:PRO:HA	2.47	0.50
1:B:77:PHE:CD2	1:B:318:LYS:HD3	2.46	0.50
1:A:274:ILE:HD13	1:A:274:ILE:N	2.26	0.50
1:A:51:GLY:HA2	1:A:81:PHE:O	2.11	0.50
1:B:423:LYS:HE3	1:B:426:LYS:CE	2.42	0.50
1:B:495:ILE:HD13	1:B:526:ILE:HD11	1.92	0.50
1:B:649:GLN:HA	1:B:655:MET:HB2	1.92	0.50
1:A:642:PHE:CZ	1:A:691:LEU:HB2	2.46	0.50
1:B:152:LEU:HB3	1:B:182:TRP:CE2	2.47	0.50
1:B:74:LEU:HB3	1:B:79:TYR:HE1	1.77	0.50
1:A:319:SER:O	1:A:322:SER:HB2	2.11	0.50
1:A:463:ASN:HA	1:A:467:TRP:HB2	1.93	0.50
1:A:724:ASN:OD1	1:A:727:GLY:HA2	2.11	0.50
1:B:405:ARG:HD3	1:B:405:ARG:H	1.76	0.50
1:B:615:HIS:HA	1:B:616:PRO:C	2.31	0.50
1:A:533:THR:HB	1:A:612:THR:CG2	2.17	0.49
1:A:249:LEU:HD13	1:A:290:LEU:HD11	1.94	0.49
1:B:422:THR:O	1:B:426:LYS:HB3	2.11	0.49
1:A:583:GLY:HA3	3:A:760:HOH:O	2.12	0.49
1:B:272:LEU:HD21	1:B:287:HIS:CE1	2.47	0.49
1:B:77:PHE:CE2	1:B:315:THR:HG22	2.47	0.49
1:A:459:LEU:HB3	1:A:473:ILE:HD12	1.94	0.49
1:B:649:GLN:O	1:B:649:GLN:HG3	2.12	0.49
1:B:240:THR:HA	1:B:267:VAL:HB	1.94	0.49
1:B:544:ILE:HB	1:B:640:MET:HE2	1.94	0.49
1:B:387:ASP:HA	1:B:423:LYS:NZ	2.28	0.49
1:B:492:GLN:CB	1:B:522:LYS:HG3	2.42	0.49
1:B:55:THR:HG22	1:B:57:LEU:H	1.77	0.49
1:B:695:ARG:HG3	1:B:704:TYR:HE2	1.77	0.49
1:A:422:THR:HG22	1:A:467:TRP:NE1	2.12	0.49
1:A:57:LEU:HD12	1:A:306:ALA:HB1	1.95	0.49
1:B:615:HIS:HA	1:B:617:ASN:N	2.28	0.49
1:A:657:SER:HB3	1:A:662:THR:O	2.13	0.48
1:A:127:ILE:HD12	1:A:127:ILE:N	2.28	0.48
1:B:271:GLY:C	1:B:272:LEU:HD22	2.33	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:THR:HA	1:B:59:VAL:CG2	2.42	0.48
1:A:207:ASP:OD2	1:A:209:PHE:HB3	2.13	0.48
1:A:317:ILE:HG13	1:A:320:GLU:CD	2.34	0.48
1:A:184:TRP:CE2	1:A:230:PHE:HD1	2.32	0.48
1:B:201:GLU:HA	1:B:206:TYR:CE2	2.48	0.48
1:B:249:LEU:O	1:B:290:LEU:HD13	2.14	0.48
1:A:527:SER:HB3	1:A:616:PRO:CD	2.44	0.48
1:B:210:THR:HG22	1:B:210:THR:O	2.14	0.48
1:B:481:LEU:N	1:B:482:PRO:CD	2.77	0.48
1:A:220:TRP:CE2	1:A:237:VAL:HB	2.49	0.48
1:A:308:THR:C	1:A:310:THR:H	2.17	0.48
1:A:541:SER:HB2	1:A:600:TYR:HA	1.96	0.48
1:A:590:ASP:HB2	1:A:729:SER:HB2	1.96	0.48
1:B:496:ILE:HG13	1:B:496:ILE:O	2.14	0.48
1:A:451:LYS:HG3	1:A:452:ASN:H	1.79	0.48
1:B:389:TYR:O	1:B:393:VAL:HG23	2.13	0.48
1:B:675:ILE:HD12	1:B:675:ILE:N	2.29	0.48
1:B:420:ILE:HD11	1:B:497:VAL:CG1	2.44	0.47
1:B:689:ILE:CD1	1:B:710:LYS:HG3	2.42	0.47
1:A:608:LYS:CG	1:A:609:PRO:HD2	2.34	0.47
1:B:703:TRP:CD1	1:B:727:GLY:N	2.82	0.47
1:A:312:LYS:CG	1:A:317:ILE:HG22	2.39	0.47
1:A:86:ILE:C	1:A:86:ILE:HD13	2.35	0.47
1:B:647:ASP:HA	1:B:657:SER:HB2	1.95	0.47
1:A:173:PRO:O	1:A:176:ALA:HB3	2.15	0.47
1:A:297:THR:O	1:A:300:LEU:HD13	2.14	0.47
1:A:646:PHE:H	1:A:658:ILE:HG22	1.80	0.47
1:B:155:ILE:HD12	1:B:163:MET:HB2	1.96	0.47
1:B:407:THR:HA	1:B:443:LYS:O	2.14	0.47
1:B:659:GLU:CD	1:B:660:PRO:HD2	2.35	0.47
1:A:593:TYR:O	1:A:673:ALA:HA	2.14	0.47
1:A:601:ILE:HD11	1:B:259:LYS:HE3	1.97	0.47
1:A:89:VAL:HG13	1:A:93:PHE:HD2	1.77	0.47
1:B:220:TRP:CE2	1:B:237:VAL:HB	2.49	0.47
1:B:707:HIS:C	1:B:707:HIS:CD2	2.88	0.47
1:B:50:ILE:O	1:B:79:TYR:HB2	2.15	0.47
1:A:165:ILE:HG23	1:A:165:ILE:O	2.14	0.47
1:B:227:CYS:HB2	3:B:783:HOH:O	2.15	0.47
1:A:220:TRP:CD2	1:A:237:VAL:HB	2.50	0.47
1:A:269:GLU:HB3	1:A:307:THR:HG21	1.97	0.47
1:A:388:VAL:HG12	1:A:650:LEU:HD11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:VAL:HG23	1:B:458:THR:HG23	1.96	0.46
1:A:289:ASN:O	1:A:293:HIS:HB2	2.15	0.46
1:A:51:GLY:O	1:A:303:VAL:HA	2.15	0.46
1:A:313:TYR:CD2	1:A:316:SER:HB3	2.44	0.46
1:B:94:TRP:CZ2	1:B:102:ASN:HB3	2.42	0.46
1:B:236:GLN:CB	1:B:264:ALA:HB2	2.44	0.46
1:B:407:THR:N	1:B:442:LEU:HD12	2.30	0.46
1:B:412:LEU:CD2	1:B:420:ILE:HG23	2.46	0.46
1:B:465:ARG:CZ	1:B:465:ARG:HB3	2.44	0.46
1:B:616:PRO:O	1:B:618:PHE:N	2.48	0.46
1:A:639:LEU:HD12	1:A:641:GLY:H	1.79	0.46
1:B:165:ILE:O	1:B:165:ILE:HG23	2.16	0.46
1:B:449:VAL:HG21	1:B:481:LEU:CD1	2.46	0.46
1:B:659:GLU:O	1:B:663:HIS:HB2	2.16	0.46
1:B:529:PRO:CA	1:B:650:LEU:HA	2.44	0.46
1:A:493:PRO:HG2	1:A:521:LEU:HD23	1.97	0.46
1:B:463:ASN:HA	1:B:467:TRP:HB2	1.96	0.46
1:B:74:LEU:HB3	1:B:79:TYR:CE1	2.50	0.46
1:A:172:SER:N	1:A:173:PRO:HD3	2.31	0.46
1:A:614:GLU:O	1:A:614:GLU:HG2	2.16	0.46
1:A:317:ILE:HA	1:A:320:GLU:CD	2.36	0.45
1:A:649:GLN:O	1:A:649:GLN:HG3	2.16	0.45
1:B:94:TRP:HB2	1:B:105:PRO:HG2	1.97	0.45
1:B:220:TRP:CE3	1:B:237:VAL:HB	2.51	0.45
1:B:506:ASP:HB2	1:B:695:ARG:HH21	1.81	0.45
1:A:695:ARG:HG3	1:A:704:TYR:HE2	1.82	0.45
1:B:195:GLN:HA	1:B:238:ALA:HB3	1.98	0.45
1:A:507:ASN:O	1:A:732:MET:SD	2.74	0.45
1:B:648:LEU:HD23	1:B:656:LEU:O	2.17	0.45
1:A:126:LYS:HB2	1:A:164:ALA:HB3	1.98	0.45
1:B:629:ILE:O	1:B:690:SER:HA	2.16	0.45
1:B:254:LEU:O	1:B:257:ARG:HB2	2.15	0.45
1:B:63:LEU:HD11	1:B:70:PHE:HD1	1.80	0.45
1:B:720:THR:HB	1:B:721:PRO:HD2	1.97	0.45
1:A:171:SER:C	1:A:173:PRO:HD3	2.37	0.45
1:A:572:GLU:CD	1:A:572:GLU:H	2.20	0.45
1:B:585:VAL:O	1:B:589:MET:HG2	2.17	0.45
1:A:401:GLY:HA3	1:A:431:TYR:OH	2.16	0.45
1:A:569:GLU:O	1:A:576:TRP:HA	2.16	0.45
1:B:477:ASP:C	1:B:479:ARG:H	2.20	0.45
1:A:111:ASP:HB3	1:A:158:LEU:CD2	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:ARG:HG3	1:A:704:TYR:CE2	2.52	0.45
1:A:75:GLY:HA2	1:A:79:TYR:O	2.17	0.45
1:A:245:LEU:HD13	1:A:287:HIS:CD2	2.53	0.45
1:A:312:LYS:HB3	1:A:317:ILE:HG22	1.98	0.45
1:A:675:ILE:HD12	1:A:675:ILE:N	2.32	0.44
1:B:85:PRO:HB2	1:B:92:ALA:HB2	1.98	0.44
1:B:486:LYS:HA	1:B:486:LYS:HD3	1.52	0.44
1:A:249:LEU:O	1:A:290:LEU:HD12	2.16	0.44
1:A:313:TYR:HD2	1:A:316:SER:CB	2.28	0.44
1:A:539:ILE:HD11	1:A:640:MET:HE1	2.00	0.44
1:B:688:ARG:NH1	1:B:711:LYS:HD2	2.32	0.44
1:A:640:MET:SD	1:A:640:MET:C	2.95	0.44
1:A:529:PRO:HA	1:A:650:LEU:HA	1.99	0.44
1:A:63:LEU:HD11	1:A:70:PHE:CG	2.52	0.44
1:B:134:ASP:OD1	1:B:173:PRO:HD2	2.18	0.44
1:B:647:ASP:CB	1:B:657:SER:HB2	2.48	0.44
1:A:530:GLN:HG3	1:A:650:LEU:O	2.18	0.44
1:B:468:LYS:HE3	1:B:468:LYS:H	1.83	0.44
1:B:478:MET:O	1:B:517:VAL:HG23	2.18	0.44
1:A:190:PHE:CD2	1:A:190:PHE:N	2.86	0.44
1:A:470:ARG:HA	1:A:470:ARG:HD2	1.69	0.44
1:A:497:VAL:HA	1:A:528:ILE:HG23	1.98	0.44
1:A:191:THR:CG2	1:A:192:VAL:N	2.81	0.44
1:A:283:ILE:CG2	1:A:287:HIS:HB3	2.48	0.44
1:A:155:ILE:HD12	1:A:163:MET:HG3	2.00	0.43
1:B:387:ASP:HA	1:B:423:LYS:HZ2	1.83	0.43
1:B:456:ILE:HG13	1:B:475:GLU:CG	2.47	0.43
1:B:55:THR:HG22	1:B:56:THR:N	2.33	0.43
1:B:689:ILE:HD13	1:B:710:LYS:HA	2.00	0.43
1:A:390:GLY:O	1:A:394:VAL:HG13	2.17	0.43
1:A:493:PRO:HG2	1:A:521:LEU:CD2	2.48	0.43
1:B:251:GLU:O	1:B:255:VAL:HG23	2.18	0.43
1:B:390:GLY:HA3	1:B:423:LYS:HE2	1.99	0.43
1:B:560:ILE:HG12	1:B:560:ILE:H	1.61	0.43
1:A:295:TRP:CH2	1:A:300:LEU:O	2.71	0.43
1:A:48:ILE:HG22	1:A:326:ARG:HE	1.83	0.43
1:A:454:ASN:O	1:A:457:VAL:HB	2.17	0.43
1:A:501:LEU:HD11	1:A:648:LEU:CD1	2.46	0.43
1:A:492:GLN:HA	1:A:520:PHE:CZ	2.54	0.43
1:B:53:MET:HB2	1:B:303:VAL:CG1	2.49	0.43
1:B:387:ASP:O	1:B:391:GLU:HG2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:HIS:ND1	1:B:664:THR:N	2.66	0.43
1:A:109:LEU:HD11	1:A:119:TRP:HH2	1.84	0.43
1:A:423:LYS:HD2	1:A:423:LYS:HA	1.82	0.43
1:A:452:ASN:HA	1:A:453:PRO:HD3	1.80	0.43
1:A:498:SER:O	1:A:529:PRO:HD3	2.17	0.43
1:A:539:ILE:HD11	1:A:640:MET:CE	2.48	0.43
1:B:456:ILE:HG13	1:B:475:GLU:HG3	2.00	0.43
1:A:312:LYS:HD3	1:A:318:LYS:HG2	2.01	0.43
1:A:647:ASP:HB2	1:A:657:SER:HB2	1.99	0.43
1:B:174:ARG:O	1:B:178:ILE:HG12	2.19	0.43
1:B:288:ILE:HG23	1:B:292:LYS:HE3	2.01	0.43
1:B:388:VAL:HA	1:B:391:GLU:HG2	1.99	0.43
1:A:495:ILE:HA	1:A:526:ILE:O	2.18	0.43
1:B:400:LEU:HD22	1:B:405:ARG:NH1	2.34	0.43
1:B:529:PRO:HG3	1:B:648:LEU:HD12	2.01	0.43
1:A:278:ASN:OD1	1:A:280:GLU:HG2	2.19	0.43
1:A:313:TYR:O	1:A:313:TYR:CG	2.72	0.43
1:A:406:LYS:CD	1:A:406:LYS:H	2.29	0.43
1:A:668:VAL:HG12	1:A:668:VAL:O	2.19	0.43
1:B:607:THR:CG2	1:B:660:PRO:HG2	2.49	0.43
1:B:70:PHE:O	1:B:74:LEU:HG	2.18	0.43
1:A:171:SER:OG	1:A:173:PRO:HD3	2.19	0.43
1:A:67:VAL:HG21	1:A:109:LEU:HD11	2.01	0.43
1:B:126:LYS:HZ3	1:B:166:GLU:HB2	1.84	0.43
1:B:656:LEU:HD12	1:B:657:SER:N	2.34	0.43
1:A:180:LYS:O	1:A:184:TRP:HD1	2.02	0.42
1:A:724:ASN:N	1:A:725:PRO:CD	2.82	0.42
1:B:207:ASP:C	1:B:209:PHE:H	2.21	0.42
1:B:317:ILE:HA	1:B:320:GLU:HB2	2.00	0.42
1:B:692:LYS:O	1:B:706:TRP:HA	2.19	0.42
1:B:126:LYS:NZ	1:B:166:GLU:HB2	2.34	0.42
1:B:400:LEU:HD22	1:B:405:ARG:HH12	1.84	0.42
1:B:59:VAL:HG22	1:B:89:VAL:HG11	2.00	0.42
1:A:319:SER:HA	1:A:322:SER:OG	2.19	0.42
1:A:698:ASP:HA	3:A:780:HOH:O	2.18	0.42
1:B:424:ILE:HG21	1:B:446:LEU:HD13	2.02	0.42
1:A:190:PHE:HD2	1:A:190:PHE:N	2.16	0.42
1:A:385:LYS:HB3	1:A:385:LYS:HE2	1.80	0.42
1:B:418:GLY:N	1:B:419:PRO:CD	2.80	0.42
1:B:425:LEU:HA	1:B:428:GLU:HG2	2.00	0.42
1:B:557:SER:O	1:B:560:ILE:HG12	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:THR:OG1	1:A:312:LYS:HA	2.20	0.42
1:A:431:TYR:CE2	1:A:442:LEU:HD23	2.54	0.42
1:A:481:LEU:N	1:A:482:PRO:HD2	2.34	0.42
1:A:630:GLU:HG2	1:A:690:SER:HA	2.00	0.42
1:A:682:ARG:HH21	1:B:221:ALA:HB1	1.83	0.42
1:B:326:ARG:C	1:B:328:ALA:N	2.72	0.42
1:B:422:THR:HA	1:B:467:TRP:HE1	1.83	0.42
1:B:495:ILE:HG12	1:B:526:ILE:CG1	2.48	0.42
1:A:501:LEU:HD13	1:A:646:PHE:HE1	1.85	0.42
1:B:383:GLN:HG2	1:B:384:ILE:N	2.34	0.42
1:B:510:SER:N	1:B:511:PRO:CD	2.83	0.42
1:A:498:SER:CB	1:A:514:LEU:HD21	2.50	0.42
1:A:84:TYR:CG	1:A:85:PRO:HD2	2.55	0.42
1:B:500:LEU:HD13	1:B:513:CYS:SG	2.59	0.42
1:A:272:LEU:HD11	1:A:284:PRO:CD	2.50	0.42
1:A:633:MET:CE	1:A:689:ILE:HG12	2.49	0.42
1:B:68:ALA:HB2	1:B:114:LEU:HD13	1.98	0.42
1:A:253:LYS:HB3	1:A:253:LYS:HE2	1.81	0.42
1:A:539:ILE:HD13	1:A:643:ALA:HB2	2.02	0.42
1:B:116:ASN:O	1:B:120:GLU:HB2	2.20	0.42
1:B:154:TYR:CE2	1:B:158:LEU:HG	2.55	0.42
1:B:263:LEU:HD12	1:B:264:ALA:N	2.34	0.42
1:B:273:PHE:CD1	1:B:273:PHE:N	2.88	0.42
1:A:263:LEU:HD21	1:A:266:PHE:CZ	2.55	0.42
1:A:269:GLU:C	1:A:271:GLY:H	2.24	0.42
1:B:492:GLN:HA	1:B:493:PRO:HD3	1.85	0.42
1:A:694:ASP:N	1:A:694:ASP:OD1	2.53	0.41
1:B:406:LYS:H	1:B:406:LYS:HD2	1.85	0.41
1:B:428:GLU:HG3	1:B:429:ARG:N	2.35	0.41
1:B:639:LEU:HD11	1:B:641:GLY:O	2.19	0.41
1:B:240:THR:HG23	1:B:267:VAL:HB	2.02	0.41
1:B:544:ILE:HB	1:B:640:MET:CE	2.50	0.41
1:A:48:ILE:HD12	1:A:298:ASP:OD1	2.20	0.41
1:A:690:SER:HB3	1:A:692:LYS:HZ3	1.85	0.41
1:B:520:PHE:C	1:B:520:PHE:CD2	2.93	0.41
1:B:501:LEU:HD21	1:B:532:TYR:CD2	2.55	0.41
1:B:648:LEU:CD2	1:B:656:LEU:HG	2.50	0.41
1:B:423:LYS:HD2	1:B:423:LYS:HA	1.84	0.41
1:B:448:ILE:HG13	1:B:471:VAL:HG21	2.02	0.41
1:B:411:TYR:HB2	1:B:496:ILE:HG22	2.02	0.41
1:B:594:VAL:HA	1:B:672:PRO:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:TRP:HH2	1:A:301:ARG:HD3	1.85	0.41
1:A:725:PRO:O	1:A:726:ASN:CB	2.68	0.41
1:A:90:VAL:HG12	1:A:90:VAL:O	2.20	0.41
1:B:187:ASN:HB3	1:B:560:ILE:HG21	2.02	0.41
1:B:572:GLU:HG2	1:B:573:ASP:OD1	2.20	0.41
1:A:616:PRO:HB2	1:A:618:PHE:CE2	2.56	0.41
1:A:70:PHE:CZ	1:A:74:LEU:HD11	2.56	0.41
1:A:701:GLY:HA3	1:A:731:TYR:CZ	2.54	0.41
1:B:201:GLU:H	1:B:201:GLU:HG2	1.63	0.41
1:B:283:ILE:HG23	1:B:287:HIS:HB3	2.02	0.41
1:B:412:LEU:HD21	1:B:415:GLY:HA2	2.02	0.41
1:B:687:ASP:OD2	1:B:712:LYS:HG2	2.19	0.41
1:B:695:ARG:HG3	1:B:704:TYR:CE2	2.56	0.41
1:A:261:GLU:HA	1:A:262:PRO:HD3	1.91	0.41
1:A:389:TYR:O	1:A:393:VAL:HG23	2.21	0.41
1:A:529:PRO:CB	1:A:648:LEU:HD11	2.50	0.41
1:A:689:ILE:HD13	1:A:710:LYS:HA	2.02	0.41
1:B:189:ARG:HH22	1:B:556:LEU:HB3	1.86	0.41
1:B:382:ASP:CG	1:B:669:SER:HB2	2.41	0.41
1:B:596:TYR:C	1:B:596:TYR:CD2	2.94	0.41
1:A:727:GLY:O	1:A:731:TYR:HB2	2.21	0.41
1:B:537:LYS:CE	1:B:602:PRO:HB3	2.45	0.41
1:B:697:VAL:HG12	1:B:698:ASP:N	2.36	0.41
1:A:302:ILE:O	1:A:302:ILE:HG22	2.21	0.41
1:A:481:LEU:N	1:A:482:PRO:CD	2.84	0.41
1:A:595:VAL:O	1:A:672:PRO:HD2	2.20	0.41
1:B:269:GLU:HA	1:B:305:ARG:HB3	2.03	0.41
1:A:245:LEU:CD1	1:A:287:HIS:CD2	3.04	0.41
1:A:253:LYS:O	1:A:253:LYS:HG2	2.21	0.41
1:B:405:ARG:HD3	1:B:405:ARG:N	2.35	0.41
1:A:245:LEU:HD13	1:A:287:HIS:NE2	2.35	0.40
1:B:500:LEU:H	1:B:501:LEU:HD12	1.86	0.40
1:A:125:GLY:O	1:A:163:MET:HG2	2.21	0.40
1:A:181:LYS:HD2	1:A:576:TRP:CZ2	2.56	0.40
1:A:509:LEU:HD21	1:A:702:VAL:HB	2.02	0.40
1:A:528:ILE:CD1	1:A:650:LEU:HB3	2.51	0.40
1:A:649:GLN:HE21	1:A:649:GLN:HB2	1.65	0.40
1:B:128:SER:HB2	1:B:131:ILE:HG13	2.02	0.40
1:B:228:GLY:O	1:B:229:ASN:HB2	2.22	0.40
1:A:101:GLU:HG3	1:A:101:GLU:O	2.22	0.40
1:A:464:VAL:HG12	1:A:465:ARG:N	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LYS:O	1:B:184:TRP:HD1	2.03	0.40
1:B:510:SER:HB3	1:B:511:PRO:HD3	2.03	0.40
1:B:493:PRO:HG3	1:B:520:PHE:CZ	2.57	0.40
1:B:558:ARG:O	1:B:577:ILE:HD12	2.22	0.40
1:B:607:THR:HG23	1:B:660:PRO:HG2	2.02	0.40
1:B:624:GLU:O	1:B:625:ARG:HD3	2.22	0.40
1:B:532:TYR:HB3	1:B:648:LEU:HB2	2.02	0.40
1:B:700:THR:C	1:B:734:MET:HG2	2.40	0.40
1:A:295:TRP:CD2	1:A:329:VAL:HG21	2.57	0.40
1:A:297:THR:H	1:A:300:LEU:HD13	1.87	0.40
1:A:313:TYR:HB3	1:A:316:SER:HB3	2.03	0.40
1:B:390:GLY:HA3	1:B:423:LYS:NZ	2.36	0.40
1:B:410:ILE:HD12	1:B:410:ILE:N	2.37	0.40
1:B:461:TYR:CZ	1:B:465:ARG:HG3	2.56	0.40
1:B:527:SER:O	1:B:530:GLN:HG3	2.21	0.40
1:B:689:ILE:HD13	1:B:689:ILE:HA	1.88	0.40
1:B:52:TRP:HB2	1:B:79:TYR:CE1	2.57	0.40
1:A:110:PRO:HD2	1:A:113:GLN:NE2	2.36	0.40
1:B:405:ARG:O	1:B:436:ARG:NH1	2.54	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	636/745 (85%)	551 (87%)	77 (12%)	8 (1%)	14	51
1	B	620/745 (83%)	538 (87%)	77 (12%)	5 (1%)	22	64
All	All	1256/1490 (84%)	1089 (87%)	154 (12%)	13 (1%)	18	59

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	617	ASN
1	A	182	TRP
1	A	284	PRO
1	B	212	GLU
1	B	509	LEU
1	A	212	GLU
1	B	251	GLU
1	A	208	ALA
1	A	726	ASN
1	B	208	ALA
1	A	253	LYS
1	A	309	ASP
1	A	211	ILE

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	567/662 (86%)	511 (90%)	56 (10%)	9	34
1	B	557/662 (84%)	493 (88%)	64 (12%)	6	27
All	All	1124/1324 (85%)	1004 (89%)	120 (11%)	8	29

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	47	ARG
1	A	55	THR
1	A	79	TYR
1	A	80	ASN
1	A	86	ILE
1	A	161	GLN
1	A	188	SER
1	A	190	PHE
1	A	200	ILE
1	A	201	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	213	HIS
1	A	218	THR
1	A	249	LEU
1	A	255	VAL
1	A	272	LEU
1	A	274	ILE
1	A	298	ASP
1	A	304	LEU
1	A	311	PHE
1	A	312	LYS
1	A	319	SER
1	A	327	HIS
1	A	383	GLN
1	A	406	LYS
1	A	428	GLU
1	A	462	MET
1	A	471	VAL
1	A	481	LEU
1	A	484	ILE
1	A	499	GLU
1	A	506	ASP
1	A	509	LEU
1	A	517	VAL
1	A	533	THR
1	A	536	VAL
1	A	573	ASP
1	A	575	MET
1	A	586	ARG
1	A	600	TYR
1	A	601	ILE
1	A	607	THR
1	A	614	GLU
1	A	619	MET
1	A	635	ARG
1	A	638	ASP
1	A	640	MET
1	A	648	LEU
1	A	649	GLN
1	A	653	THR
1	A	656	LEU
1	A	693	ILE
1	A	694	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	713	THR
1	A	714	ASN
1	A	717	SER
1	B	45	ASN
1	B	56	THR
1	B	61	GLU
1	B	80	ASN
1	B	95	THR
1	B	114	LEU
1	B	117	ASP
1	B	143	LEU
1	B	151	GLU
1	B	156	CYS
1	B	163	MET
1	B	180	LYS
1	B	200	ILE
1	B	218	THR
1	B	257	ARG
1	B	263	LEU
1	B	273	PHE
1	B	291	LEU
1	B	297	THR
1	B	298	ASP
1	B	300	LEU
1	B	305	ARG
1	B	312	LYS
1	B	321	TYR
1	B	383	GLN
1	B	405	ARG
1	B	406	LYS
1	B	424	ILE
1	B	426	LYS
1	B	429	ARG
1	B	462	MET
1	B	468	LYS
1	B	472	THR
1	B	474	ILE
1	B	476	SER
1	B	486	LYS
1	B	509	LEU
1	B	520	PHE
1	B	536	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	560	ILE
1	B	585	VAL
1	B	594	VAL
1	B	596	TYR
1	B	600	TYR
1	B	614	GLU
1	B	635	ARG
1	B	638	ASP
1	B	640	MET
1	B	648	LEU
1	B	649	GLN
1	B	652	LYS
1	B	654	VAL
1	B	656	LEU
1	B	658	ILE
1	B	659	GLU
1	B	663	HIS
1	B	667	MET
1	B	679	ASP
1	B	693	ILE
1	B	707	HIS
1	B	713	THR
1	B	714	ASN
1	B	732	MET
1	B	733	ARG

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

Mol	Chain	Res	Type
1	A	327	HIS
1	A	383	GLN
1	A	551	GLN
1	A	563	HIS
1	A	584	HIS
1	A	649	GLN
1	B	195	GLN
1	B	287	HIS
1	B	383	GLN
1	B	454	ASN
1	B	551	GLN
1	B	563	HIS
1	B	649	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	707	HIS
1	B	724	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	B	743	-	5,5,5	0.33	0	5,5,5	0.28	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	743	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	640/745 (85%)	-0.23	13 (2%) 65 36	14, 91, 179, 238	1 (0%)
1	B	628/745 (84%)	-0.10	19 (3%) 51 23	23, 101, 190, 251	15 (2%)
All	All	1268/1490 (85%)	-0.16	32 (2%) 58 29	14, 96, 183, 251	16 (1%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	313	TYR	4.7
1	A	275	SER	4.3
1	B	429	ARG	4.2
1	B	97	ASN	3.8
1	B	308	THR	3.5
1	B	433	ASN	3.5
1	B	47	ARG	3.4
1	A	313	TYR	3.3
1	B	432	ASN	3.1
1	B	404	GLY	3.0
1	A	280	GLU	2.9
1	B	434	THR	2.8
1	B	403	ASP	2.7
1	A	278	ASN	2.7
1	B	316	SER	2.6
1	A	440	GLU	2.6
1	B	407	THR	2.5
1	A	99	SER	2.5
1	B	402	ALA	2.5
1	A	46	SER	2.3
1	B	430	GLU	2.2
1	B	45	ASN	2.2
1	B	101	GLU	2.2
1	B	406	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	279	GLY	2.2
1	A	273	PHE	2.1
1	B	442	LEU	2.1
1	A	274	ILE	2.1
1	B	310	THR	2.1
1	A	309	ASP	2.1
1	A	317	ILE	2.0
1	A	314	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	B	743	6/6	0.91	0.45	1.42	86,91,92,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.