



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 09:54 AM EDT

PDB ID : 3E3L / pdb_00003e3l
Title : The R-state Glycogen Phosphorylase
Authors : Leonidas, D.D.; Zographos, S.E.; Oikonomakos, N.G.
Deposited on : 2008-08-07
Resolution : 2.59 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
Mogul : 2022.3.0, CSD as543be (2022)
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

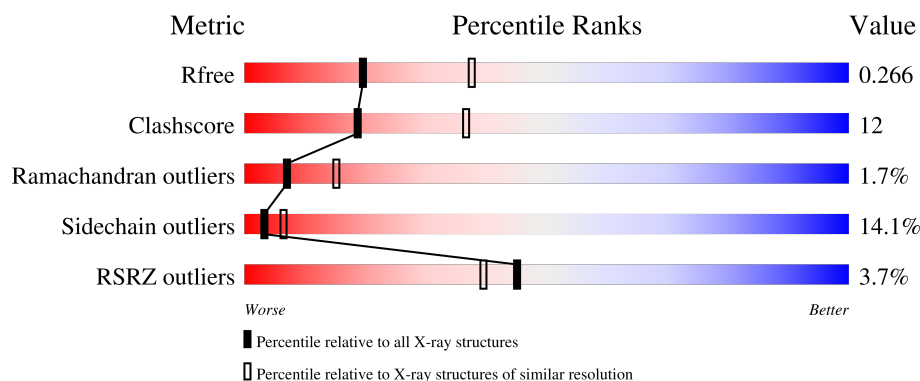
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	842	 2% 65% 26% 5% .
1	B	842	 % 68% 24% 5% .
1	C	842	 2% 68% 23% 5% .
1	D	842	 8% 57% 31% 6% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 26533 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 Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	810	Total	C	N	O	P	S	0	0	0
			6601	4206	1164	1201	1	29			
1	B	811	Total	C	N	O	P	S	0	0	0
			6608	4208	1165	1205	1	29			
1	C	807	Total	C	N	O	P	S	0	0	0
			6578	4192	1161	1195	1	29			
1	D	806	Total	C	N	O	P	S	0	0	0
			6576	4190	1159	1197	1	29			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

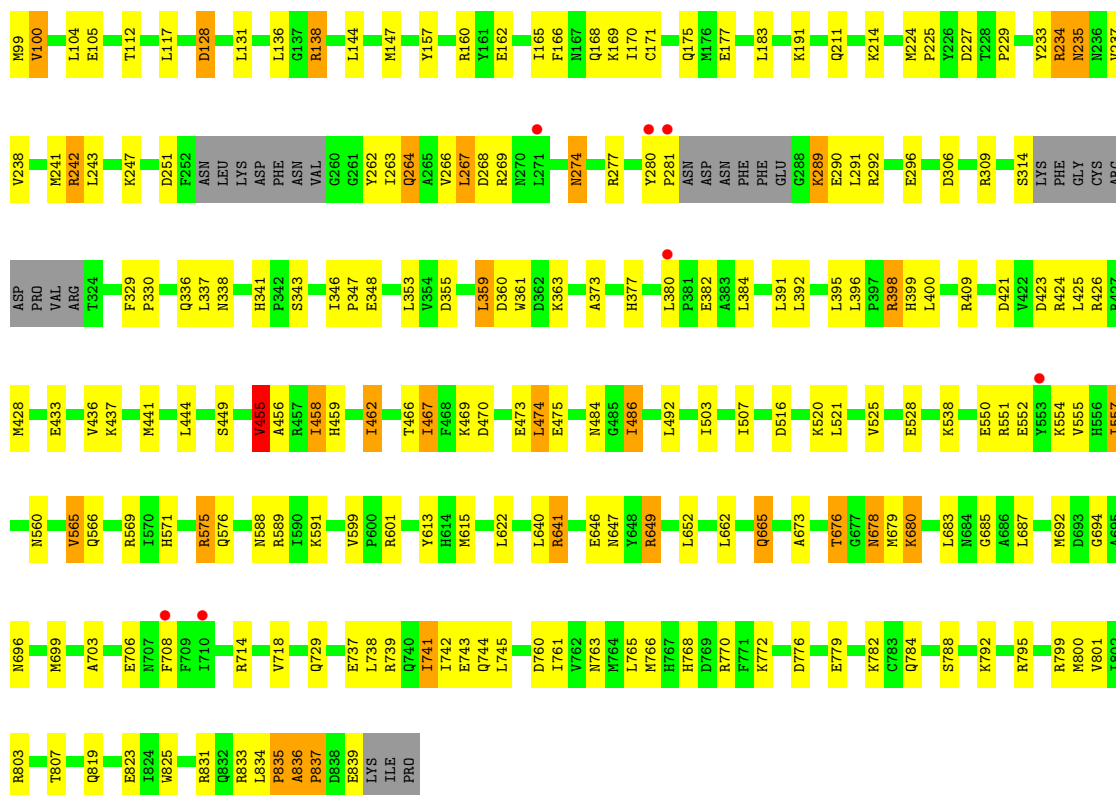
Continued on next page...

Continued from previous page...

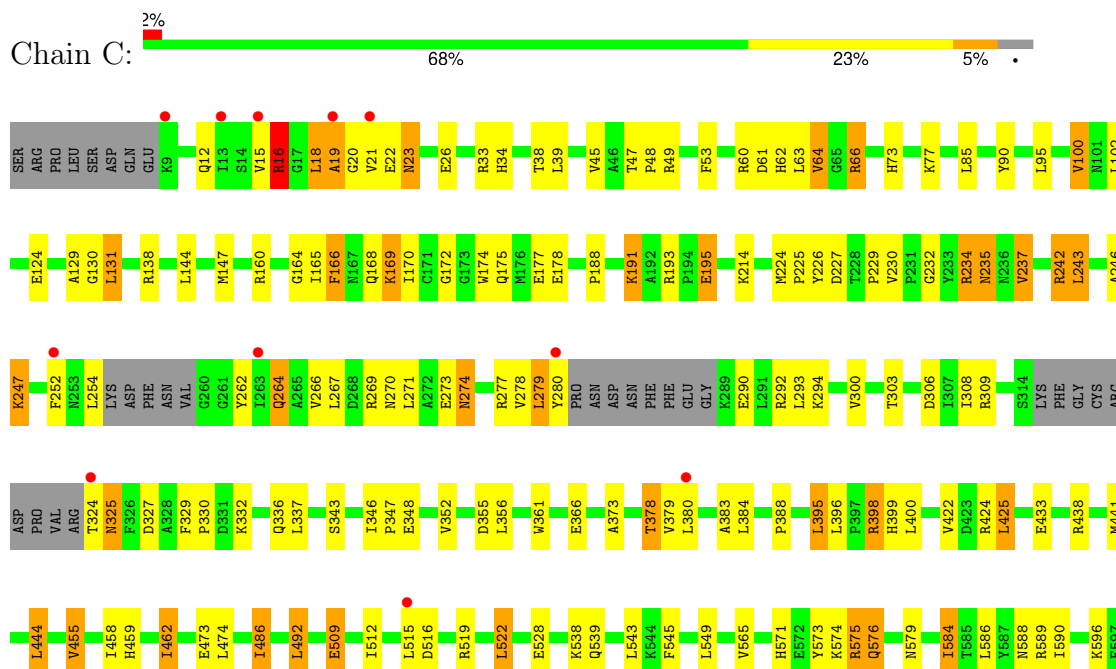
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		
3	B	35	Total	O	0	0
			35	35		
3	C	26	Total	O	0	0
			26	26		
3	D	26	Total	O	0	0
			26	26		

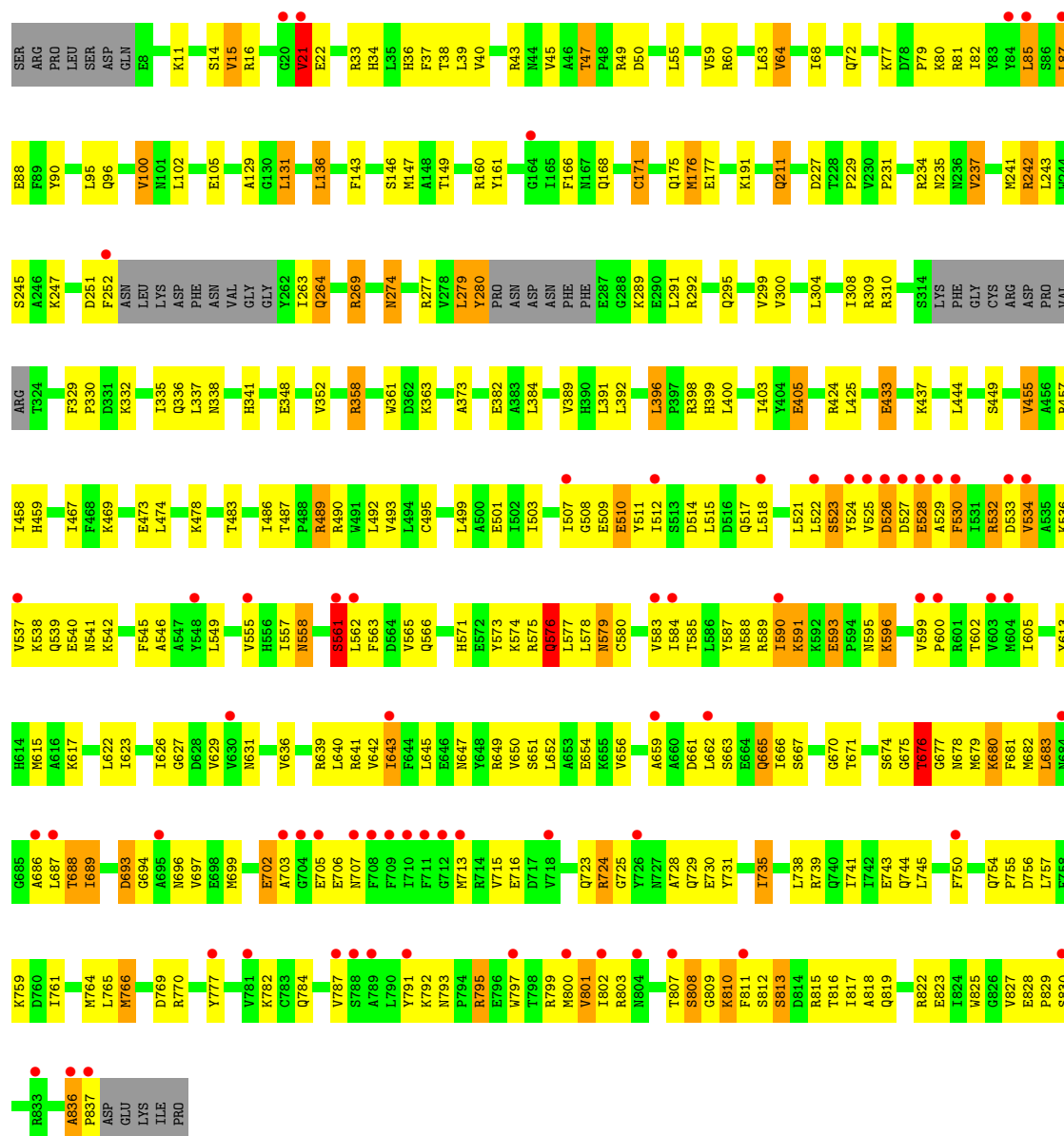


• Molecule 1: Glycogen phosphorylase, muscle form





• Molecule 1: Glycogen phosphorylase, muscle form



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.89Å 189.92Å 88.16Å 90.00° 109.27° 90.00°	Depositor
Resolution (Å)	29.59 – 2.59 29.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.59-2.59) 99.3 (29.59-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.92 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.266 0.207 , 0.266	Depositor DCC
R_{free} test set	5654 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26533	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: LLP, SO4

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	0.62	1/6721 (0.0%)	0.93	4/9091 (0.0%)
1	B	0.61	1/6728 (0.0%)	0.93	3/9100 (0.0%)
1	C	0.62	1/6697 (0.0%)	0.93	6/9058 (0.1%)
1	D	0.63	0/6695	0.95	10/9055 (0.1%)
All	All	0.62	3/26841 (0.0%)	0.93	23/36304 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	795	ARG	CZ-NH1	6.14	1.41	1.32
1	A	657	ILE	CA-CB	6.04	1.57	1.54
1	B	64	VAL	CA-CB	5.07	1.60	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	565	VAL	N-CA-C	7.20	118.27	107.75
1	A	565	VAL	N-CA-C	6.95	118.13	108.12
1	C	754	GLN	CA-C-N	6.47	126.70	119.32
1	C	754	GLN	C-N-CA	6.47	126.70	119.32
1	B	565	VAL	N-CA-C	6.20	116.79	108.11
1	D	467	ILE	N-CA-C	5.87	116.52	110.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	455	VAL	CB-CA-C	5.78	117.29	110.93
1	A	676	THR	N-CA-C	5.75	118.49	111.82
1	A	262	TYR	N-CA-C	5.70	116.81	108.14
1	B	555	VAL	N-CA-C	5.61	115.63	106.72
1	D	15	VAL	CB-CA-C	-5.49	104.85	112.04
1	D	529	ALA	N-CA-C	5.49	119.80	113.38
1	C	528	GLU	N-CA-C	5.37	117.21	111.36
1	D	676	THR	CB-CA-C	5.28	116.30	109.28
1	D	526	ASP	N-CA-C	5.26	117.44	111.02
1	C	16	ARG	N-CA-C	5.19	121.86	110.80
1	A	280	TYR	N-CA-C	5.18	116.64	108.55
1	C	735	ILE	CA-C-N	5.16	124.34	118.97
1	C	735	ILE	C-N-CA	5.16	124.34	118.97
1	D	675	GLY	N-CA-C	-5.14	104.99	111.72
1	D	528	GLU	N-CA-C	5.09	117.06	108.96
1	D	643	ILE	N-CA-C	5.08	115.43	108.12
1	D	105	GLU	N-CA-C	5.01	116.55	111.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	VAL	Peptide

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	6601	0	6554	159	0
1	B	6608	0	6554	123	0
1	C	6578	0	6537	146	0
1	D	6576	0	6528	211	0
2	A	15	0	0	1	0
2	B	15	0	0	0	0
2	C	10	0	0	0	0
2	D	20	0	0	1	0
3	A	23	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	35	0	0	0	0
3	C	26	0	0	0	0
3	D	26	0	0	0	0
All	All	26533	0	26173	627	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 12.

All (627) 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:615:MET:HE1	1:A:761:ILE:HG12	1.24	1.10
1:A:712:GLY:H	1:A:779:GLU:HG2	1.22	1.03
1:A:682:MET:HE3	1:A:808:SER:HB2	1.36	1.03
1:B:641:ARG:HG3	1:B:641:ARG:HH11	1.24	0.98
1:A:20:GLY:O	1:A:21:VAL:HG13	1.65	0.96
1:D:707:ASN:HA	1:D:800:MET:SD	2.09	0.93
1:C:274:ASN:H	1:C:274:ASN:HD22	1.18	0.92
1:D:146:SER:OG	1:D:813:SER:HB2	1.66	0.92
1:D:588:ASN:HD21	1:D:744:GLN:HE22	1.00	0.91
1:B:615:MET:HE1	1:B:761:ILE:HG12	1.50	0.90
1:C:138:ARG:O	1:C:138:ARG:HD3	1.70	0.90
1:B:455:VAL:H	1:B:459:HIS:HD2	1.18	0.88
1:C:66:ARG:HG3	1:C:66:ARG:HH11	1.39	0.87
1:B:676:THR:HG22	1:B:680:LLP:H4'1	1.58	0.86
1:A:93:ARG:O	1:A:490:ARG:NH2	2.08	0.86
1:A:262:TYR:HB3	1:A:264:GLN:NE2	1.91	0.86
1:A:227:ASP:OD1	1:A:242:ARG:HD3	1.76	0.85
1:C:516:ASP:O	1:C:519:ARG:HG2	1.76	0.85
1:C:455:VAL:CG1	1:C:674:SER:HB2	2.09	0.83
1:A:87:LEU:HD21	1:A:292:ARG:NH2	1.94	0.83
1:A:703:ALA:HA	1:A:807:THR:HG21	1.60	0.82
1:A:426:ARG:HH21	1:D:755:PRO:HD3	1.45	0.81
1:D:455:VAL:HG12	1:D:674:SER:HB2	1.63	0.81
1:C:274:ASN:H	1:C:274:ASN:ND2	1.79	0.81
1:D:495:CYS:HB2	1:D:654:GLU:O	1.81	0.81
1:C:703:ALA:HA	1:C:807:THR:HG21	1.63	0.80
1:B:486:ILE:HD11	1:B:676:THR:HG23	1.64	0.79
1:C:739:ARG:O	1:C:743:GLU:HG2	1.82	0.79
1:B:687:LEU:HD13	1:B:800:MET:HE2	1.64	0.79
1:D:791:TYR:HA	1:D:797:TRP:CD1	2.17	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ARG:HG2	1:A:457:ARG:HH11	1.46	0.79
1:D:836:ALA:HB1	1:D:837:PRO:HA	1.65	0.79
1:D:739:ARG:O	1:D:743:GLU:HG2	1.83	0.78
1:A:682:MET:CE	1:A:808:SER:HB2	2.12	0.78
1:A:615:MET:CE	1:A:761:ILE:HG12	2.11	0.78
1:B:641:ARG:HH11	1:B:641:ARG:CG	1.96	0.78
1:A:168:GLN:HE21	1:A:647:ASN:H	1.28	0.77
1:D:588:ASN:HD21	1:D:744:GLN:NE2	1.81	0.77
1:B:47:THR:HG22	1:B:49:ARG:H	1.50	0.76
1:B:227:ASP:OD1	1:B:242:ARG:HD3	1.84	0.76
1:D:813:SER:O	1:D:817:ILE:HG12	1.85	0.76
1:A:682:MET:HE3	1:A:808:SER:CB	2.15	0.76
1:A:741:ILE:HA	1:A:744:GLN:HE21	1.51	0.76
1:B:703:ALA:HA	1:B:807:THR:HG21	1.66	0.76
1:A:110:GLU:HG3	1:A:114:GLN:HE21	1.50	0.75
1:D:588:ASN:ND2	1:D:744:GLN:HE22	1.80	0.75
1:C:168:GLN:HG3	1:C:175:GLN:HG3	1.67	0.75
1:D:455:VAL:CG1	1:D:674:SER:HB2	2.15	0.75
1:D:665:GLN:HB3	1:D:696:ASN:HD21	1.52	0.75
1:A:766:MET:HE2	1:A:766:MET:HA	1.69	0.74
1:A:262:TYR:HB3	1:A:264:GLN:HE22	1.53	0.74
1:A:455:VAL:H	1:A:459:HIS:HD2	1.35	0.74
1:C:615:MET:HE2	1:C:764:MET:HE2	1.69	0.74
1:C:47:THR:HG23	1:C:48:PRO:HD2	1.70	0.74
1:C:274:ASN:HD22	1:C:274:ASN:N	1.82	0.74
1:C:588:ASN:HD21	1:C:744:GLN:HE22	1.37	0.73
1:D:800:MET:C	1:D:802:ILE:H	1.96	0.73
1:C:741:ILE:HA	1:C:744:GLN:HE21	1.54	0.73
1:D:455:VAL:H	1:D:459:HIS:HD2	1.36	0.73
1:A:739:ARG:O	1:A:743:GLU:HG2	1.89	0.72
1:B:455:VAL:H	1:B:459:HIS:CD2	2.06	0.72
1:C:60:ARG:O	1:C:64:VAL:HG13	1.90	0.72
1:A:85:LEU:HD21	1:A:303:THR:HG21	1.70	0.71
1:B:729:GLN:HG2	1:C:724:ARG:HA	1.73	0.71
1:C:574:LYS:HB2	1:C:576:GLN:HE22	1.53	0.71
1:A:47:THR:HG22	1:A:49:ARG:H	1.57	0.70
1:A:712:GLY:N	1:A:779:GLU:HG2	2.01	0.70
1:B:168:GLN:HE21	1:B:647:ASN:H	1.39	0.70
1:C:235:ASN:H	1:C:235:ASN:HD22	1.38	0.70
1:A:438:ARG:HH11	1:A:438:ARG:CG	2.05	0.70
1:A:582:HIS:HD2	1:A:781:VAL:HG12	1.54	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:HH21	1:B:277:ARG:HH22	1.36	0.70
1:B:336:GLN:NE2	1:B:373:ALA:HB3	2.08	0.69
1:A:756:ASP:HB2	1:A:759:LYS:HG3	1.75	0.68
1:C:227:ASP:OD1	1:C:242:ARG:HD3	1.94	0.68
1:C:308:ILE:HD12	1:C:352:VAL:HG11	1.75	0.68
1:C:224:MET:HE2	1:C:226:TYR:CE1	2.28	0.68
1:A:21:VAL:HG21	1:A:26:GLU:HG3	1.74	0.68
1:C:47:THR:HG22	1:C:49:ARG:H	1.58	0.67
1:C:378:THR:HG21	1:C:383:ALA:HB3	1.76	0.67
1:B:458:ILE:O	1:B:462:ILE:HG12	1.95	0.67
1:A:168:GLN:NE2	1:A:647:ASN:H	1.93	0.66
1:A:703:ALA:CA	1:A:807:THR:HG21	2.25	0.66
1:D:800:MET:O	1:D:802:ILE:N	2.27	0.66
1:B:741:ILE:HA	1:B:744:GLN:HE21	1.60	0.66
1:C:252:PHE:HZ	1:C:269:ARG:HB2	1.59	0.66
1:D:801:VAL:HG12	1:D:801:VAL:O	1.95	0.66
1:C:144:LEU:HD23	1:C:147:MET:CE	2.26	0.65
1:C:336:GLN:NE2	1:C:373:ALA:HB3	2.10	0.65
1:D:681:PHE:O	1:D:686:ALA:HB3	1.96	0.65
1:A:250:ASN:HB3	1:A:252:PHE:HE2	1.62	0.65
1:B:100:VAL:O	1:B:234:ARG:NH1	2.29	0.65
1:D:689:ILE:HG23	1:D:689:ILE:O	1.97	0.65
1:A:365:TRP:O	1:A:369:VAL:HG23	1.96	0.65
1:B:157:TYR:OH	1:B:306:ASP:OD2	2.13	0.65
1:B:280:TYR:HD1	1:B:281:PRO:HA	1.62	0.64
1:A:138:ARG:O	1:A:138:ARG:HD3	1.98	0.64
1:B:306:ASP:OD1	1:B:309:ARG:NH1	2.31	0.64
1:D:14:SER:OG	1:D:16:ARG:HG2	1.97	0.64
1:D:627:GLY:HA2	1:D:642:VAL:HB	1.80	0.64
1:D:539:GLN:C	1:D:541:ASN:H	2.06	0.64
1:C:262:TYR:HB2	1:C:264:GLN:OE1	1.97	0.64
1:D:60:ARG:O	1:D:64:VAL:HG12	1.98	0.63
1:D:615:MET:HE1	1:D:761:ILE:HG12	1.81	0.63
1:A:795:ARG:O	1:A:799:ARG:HG3	1.99	0.63
1:C:579:ASN:HD22	1:C:579:ASN:C	2.06	0.63
1:D:211:GLN:HG3	1:D:358:ARG:NH2	2.13	0.63
1:C:21:VAL:HG22	1:C:22:GLU:HG2	1.80	0.63
1:C:378:THR:CG2	1:C:383:ALA:HB3	2.29	0.63
1:C:455:VAL:H	1:C:459:HIS:HD2	1.45	0.63
1:D:455:VAL:N	1:D:459:HIS:HD2	1.97	0.63
1:C:676:THR:HG22	1:C:680:LLP:H5'1	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:CYS:O	1:A:449:SER:OG	2.17	0.62
1:D:741:ILE:HA	1:D:744:GLN:HE21	1.64	0.62
1:D:661:ASP:HB3	1:D:797:TRP:CH2	2.34	0.62
1:D:590:ILE:HG22	1:D:590:ILE:O	1.98	0.62
1:B:575:ARG:NH2	1:B:776:ASP:HB2	2.15	0.62
1:D:574:LYS:HB3	1:D:576:GLN:NE2	2.15	0.62
1:D:507:ILE:HD12	1:D:517:GLN:HG2	1.81	0.62
1:B:34:HIS:HE1	1:B:61:ASP:OD2	1.83	0.61
1:A:49:ARG:HA	1:A:125:ILE:HG21	1.83	0.61
1:C:225:PRO:HB2	1:C:242:ARG:HD2	1.82	0.61
1:B:687:LEU:HD13	1:B:800:MET:CE	2.30	0.61
1:B:803:ARG:O	1:B:807:THR:HG22	2.01	0.61
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.82	0.61
1:B:15:VAL:HA	1:B:18:LEU:HD22	1.81	0.61
1:C:687:LEU:HD13	1:C:800:MET:HE2	1.83	0.60
1:D:801:VAL:O	1:D:801:VAL:CG1	2.49	0.60
1:C:424:ARG:NH2	1:C:473:GLU:OE1	2.35	0.60
1:A:110:GLU:HG3	1:A:114:GLN:NE2	2.17	0.60
1:A:582:HIS:CD2	1:A:781:VAL:HG12	2.36	0.60
1:A:549:LEU:O	1:A:552:GLU:O	2.20	0.59
1:D:566:GLN:HE22	1:D:576:GLN:HA	1.66	0.59
1:C:509:GLU:HG2	1:C:512:ILE:HD12	1.82	0.59
1:D:563:PHE:HD2	1:D:659:ALA:O	1.85	0.59
1:D:599:VAL:HG12	1:D:600:PRO:O	2.03	0.59
1:A:680:LLP:NZ	1:A:680:LLP:O3	2.36	0.59
1:B:225:PRO:HB2	1:B:242:ARG:HD2	1.84	0.59
1:D:600:PRO:HB3	1:D:639:ARG:HA	1.83	0.59
1:A:630:VAL:HG21	1:A:642:VAL:HG23	1.83	0.59
1:C:165:ILE:O	1:C:166:PHE:O	2.21	0.59
1:D:662:LEU:HD23	1:D:687:LEU:O	2.02	0.59
1:D:670:GLY:H	1:D:693:ASP:CG	2.10	0.59
1:A:296:GLU:OE2	1:A:385:GLU:OE2	2.21	0.58
1:A:9:LYS:H	1:A:9:LYS:HD2	1.69	0.58
1:D:580:CYS:O	1:D:584:ILE:HG13	2.03	0.58
1:C:574:LYS:HB2	1:C:576:GLN:NE2	2.18	0.58
1:A:679:MET:HE2	1:A:811:PHE:CD1	2.38	0.58
1:D:676:THR:HG22	1:D:680:LLP:H5'1	1.84	0.58
1:D:21:VAL:CG2	1:D:22:GLU:N	2.67	0.58
1:D:791:TYR:C	1:D:793:ASN:H	2.10	0.58
1:C:270:ASN:O	1:C:274:ASN:ND2	2.37	0.58
1:D:348:GLU:OE1	1:D:399:HIS:HE1	1.87	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.85	0.57
1:D:227:ASP:OD1	1:D:242:ARG:HD3	2.03	0.57
1:D:573:TYR:HD2	1:D:671:THR:HG1	1.52	0.57
1:A:311:PHE:CG	1:A:311:PHE:O	2.57	0.57
1:D:235:ASN:CG	1:D:237:VAL:HG13	2.30	0.57
1:C:33:ARG:HE	1:D:33:ARG:NE	2.03	0.57
1:A:336:GLN:HG2	1:A:825:TRP:HE1	1.70	0.57
1:C:279:LEU:HD22	1:C:280:TYR:H	1.70	0.57
1:D:129:ALA:HB1	1:D:131:LEU:HD22	1.87	0.57
1:D:651:SER:HA	1:D:654:GLU:HG2	1.86	0.57
1:A:110:GLU:O	1:A:114:GLN:HG2	2.05	0.57
1:B:105:GLU:OE1	1:B:105:GLU:HA	2.04	0.57
1:B:224:MET:HE2	1:B:247:LYS:HE3	1.85	0.57
1:D:764:MET:HE2	1:D:769:ASP:HA	1.86	0.57
1:A:426:ARG:CZ	1:A:426:ARG:HB2	2.33	0.57
1:A:457:ARG:HH11	1:A:457:ARG:CG	2.18	0.57
1:D:87:LEU:HD13	1:D:341:HIS:HB3	1.87	0.57
1:C:64:VAL:HG22	1:D:37:PHE:HD1	1.70	0.56
1:A:87:LEU:HD21	1:A:292:ARG:HH22	1.68	0.56
1:D:579:ASN:HD22	1:D:605:ILE:HD11	1.70	0.56
1:D:702:GLU:OE2	1:D:702:GLU:HA	2.04	0.56
1:A:815:ARG:NH1	1:A:816:THR:HA	2.19	0.56
1:D:584:ILE:HG22	1:D:741:ILE:HG22	1.86	0.56
1:A:554:LYS:HD3	1:A:554:LYS:N	2.20	0.56
1:B:343:SER:OG	1:B:441:MET:HE3	2.04	0.56
1:B:391:LEU:O	1:B:395:LEU:HD23	2.06	0.56
1:D:663:SER:HB2	1:D:681:PHE:HB3	1.88	0.56
1:D:455:VAL:H	1:D:459:HIS:CD2	2.21	0.56
1:D:595:ASN:O	1:D:596:LYS:C	2.48	0.56
1:D:47:THR:HG22	1:D:50:ASP:H	1.69	0.56
1:A:336:GLN:NE2	1:A:373:ALA:HB3	2.21	0.55
1:D:336:GLN:HE21	1:D:825:TRP:HE1	1.54	0.55
1:D:574:LYS:HB3	1:D:576:GLN:HE22	1.70	0.55
1:A:824:ILE:HG22	1:A:825:TRP:CD1	2.41	0.55
1:A:782:LYS:HE3	1:A:782:LYS:HA	1.88	0.55
1:D:702:GLU:OE2	1:D:702:GLU:CA	2.54	0.55
1:A:486:ILE:CD1	1:A:676:THR:O	2.55	0.55
1:B:678:ASN:HB3	1:B:679:MET:HG3	1.89	0.55
1:D:21:VAL:HG22	1:D:22:GLU:N	2.22	0.55
1:D:703:ALA:O	1:D:707:ASN:ND2	2.40	0.55
1:B:227:ASP:OD1	1:B:242:ARG:CD	2.54	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ALA:C	1:C:247:LYS:HG2	2.32	0.55
1:D:149:THR:HG21	1:D:489:ARG:HH12	1.70	0.55
1:B:280:TYR:CD1	1:B:281:PRO:HA	2.41	0.55
1:C:756:ASP:HB2	1:C:759:LYS:HD2	1.89	0.55
1:B:346:ILE:HB	1:B:347:PRO:HD3	1.89	0.54
1:B:718:VAL:HG13	1:B:772:LYS:HZ2	1.72	0.54
1:C:486:ILE:HD11	1:C:680:LLP:HE2	1.88	0.54
1:A:166:PHE:CD2	1:A:177:GLU:HB3	2.42	0.54
1:A:679:MET:HE2	1:A:811:PHE:HD1	1.72	0.54
1:A:361:TRP:CZ3	1:A:409:ARG:HD2	2.43	0.54
1:A:455:VAL:HG13	1:A:674:SER:HB2	1.89	0.54
1:B:168:GLN:NE2	1:B:647:ASN:H	2.03	0.54
1:D:160:ARG:HB2	1:D:243:LEU:HB3	1.88	0.54
1:D:575:ARG:C	1:D:577:LEU:N	2.65	0.54
1:C:599:VAL:HG21	1:C:788:SER:O	2.07	0.54
1:D:241:MET:HG2	1:D:243:LEU:HD13	1.89	0.54
1:A:88:GLU:HB3	1:A:132:GLY:HA2	1.90	0.54
1:B:136:LEU:HD23	1:B:338:ASN:ND2	2.23	0.54
1:D:689:ILE:HD12	1:D:784:GLN:OE1	2.07	0.54
1:B:685:GLY:HA2	1:B:801:VAL:HG13	1.89	0.54
1:B:474:LEU:HD13	1:B:475:GLU:HG3	1.90	0.53
1:C:252:PHE:CZ	1:C:269:ARG:HB2	2.41	0.53
1:D:274:ASN:HB2	1:D:277:ARG:HD3	1.89	0.53
1:C:271:LEU:HA	1:C:274:ASN:HD21	1.73	0.53
1:D:558:ASN:O	1:D:561:SER:HB2	2.08	0.53
1:D:636:VAL:O	1:D:639:ARG:HG3	2.08	0.53
1:C:34:HIS:HE1	1:C:61:ASP:OD2	1.91	0.53
1:C:306:ASP:OD1	1:C:309:ARG:NH1	2.41	0.53
1:A:456:ALA:C	1:A:481:ASN:HD21	2.15	0.53
1:C:232:GLY:HA3	1:C:235:ASN:HD21	1.74	0.53
1:D:68:ILE:O	1:D:72:GLN:HG3	2.08	0.53
1:B:112:THR:HG22	1:B:117:LEU:O	2.08	0.53
1:B:588:ASN:HD21	1:B:744:GLN:HE22	1.54	0.53
1:D:589:ARG:C	1:D:591:LYS:H	2.15	0.53
1:C:522:LEU:HD22	1:C:806:ALA:HB1	1.90	0.53
1:C:66:ARG:HH11	1:C:66:ARG:CG	2.16	0.53
1:C:680:LLP:NZ	1:C:680:LLP:O3	2.42	0.53
1:C:764:MET:HA	1:C:768:HIS:CE1	2.44	0.53
1:A:264:GLN:H	1:A:264:GLN:HE21	1.56	0.53
1:B:738:LEU:O	1:B:742:ILE:HG12	2.08	0.53
1:C:343:SER:OG	1:C:441:MET:HE3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:LEU:HD22	1:D:338:ASN:HD21	1.73	0.53
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.49	0.52
1:B:834:LEU:O	1:B:835:PRO:O	2.27	0.52
1:C:455:VAL:HG12	1:C:674:SER:HB2	1.89	0.52
1:D:171:CYS:SG	1:D:176:MET:HG3	2.49	0.52
1:D:533:ASP:HA	1:D:536:LYS:HB3	1.91	0.52
1:B:641:ARG:HG3	1:B:641:ARG:NH1	2.05	0.52
1:D:589:ARG:O	1:D:591:LYS:N	2.33	0.52
1:D:63:LEU:HD13	1:D:229:PRO:HG2	1.92	0.52
1:B:353:LEU:O	1:B:359:LEU:HB2	2.08	0.52
1:A:237:VAL:HG12	1:A:834:LEU:HD13	1.92	0.52
1:A:575:ARG:NH2	1:A:776:ASP:HB2	2.23	0.52
1:C:455:VAL:H	1:C:459:HIS:CD2	2.26	0.52
1:C:235:ASN:H	1:C:235:ASN:ND2	2.06	0.52
1:C:324:THR:O	1:C:325:ASN:C	2.53	0.52
1:C:670:GLY:H	1:C:693:ASP:CG	2.17	0.52
1:D:146:SER:HG	1:D:813:SER:HB2	1.74	0.52
1:D:274:ASN:HD22	1:D:274:ASN:C	2.18	0.52
1:A:676:THR:HG23	1:A:680:LLP:H4'1	1.92	0.52
1:A:554:LYS:HD3	1:A:554:LYS:H	1.75	0.52
1:B:466:THR:OG1	1:B:467:ILE:HD12	2.10	0.52
1:C:168:GLN:HE21	1:C:647:ASN:H	1.56	0.52
1:D:663:SER:OG	1:D:688:THR:HG23	2.10	0.52
1:B:96:GLN:HA	1:B:99:MET:HE2	1.91	0.52
1:D:308:ILE:HD13	1:D:352:VAL:HG11	1.92	0.52
1:D:728:ALA:HB3	1:D:766:MET:O	2.10	0.52
1:C:224:MET:SD	1:C:247:LYS:HE3	2.49	0.51
1:C:590:ILE:HG12	1:C:598:VAL:HG11	1.92	0.51
1:D:503:ILE:HG23	1:D:521:LEU:HD11	1.92	0.51
1:D:815:ARG:O	1:D:819:GLN:HG3	2.10	0.51
1:A:703:ALA:CB	1:A:807:THR:HG21	2.41	0.51
1:B:241:MET:HG2	1:B:243:LEU:HD13	1.91	0.51
1:D:584:ILE:HG23	1:D:750:PHE:HZ	1.76	0.51
1:A:486:ILE:HD11	1:A:676:THR:O	2.10	0.51
1:D:336:GLN:NE2	1:D:825:TRP:HE1	2.09	0.51
1:A:687:LEU:HD12	1:A:797:TRP:CE2	2.45	0.51
1:B:168:GLN:HG3	1:B:175:GLN:HG3	1.93	0.51
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.94	0.51
1:B:16:ARG:HG3	1:B:17:GLY:H	1.76	0.51
1:B:426:ARG:CZ	1:C:755:PRO:HD2	2.40	0.51
1:D:580:CYS:SG	1:D:623:ILE:HG12	2.51	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:GLN:HE22	1:B:576:GLN:HA	1.76	0.51
1:D:143:PHE:HB3	1:D:147:MET:HE2	1.92	0.51
1:B:433:GLU:OE2	1:B:437:LYS:HE2	2.11	0.51
1:C:138:ARG:HD3	1:C:138:ARG:C	2.36	0.51
1:C:355:ASP:OD2	1:C:398:ARG:HD3	2.11	0.51
1:B:575:ARG:HH22	1:B:776:ASP:HB2	1.75	0.50
1:D:508:GLY:O	1:D:510:GLU:N	2.45	0.50
1:D:575:ARG:C	1:D:577:LEU:H	2.19	0.50
1:A:232:GLY:HA3	1:A:235:ASN:HD21	1.74	0.50
1:A:379:VAL:HG21	1:A:670:GLY:O	2.10	0.50
1:B:699:MET:HE2	1:B:708:PHE:HZ	1.76	0.50
1:B:680:LLP:NZ	1:B:680:LLP:O3	2.44	0.50
1:A:23:ASN:HB3	1:A:26:GLU:HG2	1.92	0.50
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.94	0.50
1:D:571:HIS:CD2	1:D:613:TYR:HE2	2.29	0.50
1:A:78:ASP:OD2	1:A:332:LYS:NZ	2.44	0.50
1:A:573:TYR:HB3	1:A:771:PHE:CE1	2.47	0.50
1:C:169:LYS:NZ	1:C:178:GLU:OE1	2.45	0.50
1:D:263:ILE:HG13	1:D:263:ILE:O	2.12	0.50
1:D:336:GLN:HE22	1:D:373:ALA:HB3	1.76	0.50
1:D:63:LEU:HD21	1:D:231:PRO:HB3	1.94	0.50
1:A:575:ARG:HD3	1:A:666:ILE:O	2.12	0.50
1:B:34:HIS:HD2	1:B:38:THR:OG1	1.95	0.50
1:A:661:ASP:HB3	1:A:797:TRP:CH2	2.47	0.50
1:C:34:HIS:HD2	1:C:38:THR:OG1	1.95	0.50
1:C:324:THR:O	1:C:325:ASN:O	2.30	0.50
1:A:20:GLY:O	1:A:21:VAL:CG1	2.51	0.49
1:A:386:ARG:HG2	1:A:440:ASN:HA	1.93	0.49
1:A:456:ALA:C	1:A:481:ASN:ND2	2.70	0.49
1:D:280:TYR:OH	1:D:291:LEU:HD12	2.12	0.49
1:D:661:ASP:HB3	1:D:797:TRP:HH2	1.74	0.49
1:A:472:TYR:C	1:A:474:LEU:H	2.20	0.49
1:B:395:LEU:HD23	1:B:395:LEU:H	1.77	0.49
1:C:160:ARG:HB2	1:C:243:LEU:HB3	1.94	0.49
1:D:818:ALA:O	1:D:822:ARG:HG3	2.12	0.49
1:A:235:ASN:HD22	1:A:236:ASN:N	2.10	0.49
1:B:348:GLU:OE1	1:B:399:HIS:CE1	2.65	0.49
1:D:21:VAL:CG2	1:D:22:GLU:H	2.25	0.49
1:D:85:LEU:HD12	1:D:335:ILE:HG23	1.93	0.49
1:C:741:ILE:HA	1:C:744:GLN:NE2	2.26	0.49
1:C:336:GLN:HE21	1:C:825:TRP:HE1	1.59	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:GLU:HA	1:B:183:LEU:HD12	1.94	0.49
1:C:676:THR:HG22	1:C:680:LLP:H4'1	1.94	0.49
1:D:584:ILE:HG23	1:D:750:PHE:CZ	2.47	0.49
1:A:142:CYS:SG	1:A:487:THR:HG22	2.52	0.49
1:D:545:PHE:O	1:D:549:LEU:HB2	2.12	0.49
1:A:24:VAL:O	1:A:28:LYS:HG3	2.12	0.49
1:A:227:ASP:OD1	1:A:242:ARG:CD	2.56	0.49
1:A:241:MET:HG2	1:A:243:LEU:HD13	1.95	0.49
1:A:740:GLN:O	1:A:744:GLN:HG3	2.12	0.49
1:A:731:TYR:CE1	1:A:775:ALA:HA	2.48	0.49
1:B:528:GLU:OE1	1:B:795:ARG:NH1	2.45	0.49
1:C:346:ILE:HB	1:C:347:PRO:HD3	1.95	0.49
1:D:96:GLN:O	1:D:100:VAL:HG13	2.13	0.49
1:A:474:LEU:O	1:A:475:GLU:HG3	2.12	0.49
1:D:405:GLU:OE1	1:D:405:GLU:HA	2.13	0.48
1:C:63:LEU:HD13	1:C:229:PRO:HG2	1.95	0.48
1:A:340:THR:OG1	1:A:385:GLU:HB2	2.13	0.48
1:D:389:VAL:HG22	1:D:437:LYS:O	2.12	0.48
1:A:309:ARG:NH2	2:A:902:SO4:O1	2.46	0.48
1:C:23:ASN:HB3	1:C:26:GLU:HB2	1.94	0.48
1:C:193:ARG:HB2	1:C:225:PRO:HG2	1.96	0.48
1:A:455:VAL:H	1:A:459:HIS:CD2	2.22	0.48
1:D:168:GLN:NE2	1:D:647:ASN:H	2.12	0.48
1:A:47:THR:HG22	1:A:49:ARG:N	2.26	0.48
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.78	0.48
1:A:568:LYS:NZ	1:A:680:LLP:OP1	2.47	0.48
1:D:424:ARG:NH2	1:D:473:GLU:OE1	2.47	0.48
1:D:85:LEU:CD1	1:D:335:ILE:HG23	2.44	0.48
1:D:836:ALA:CB	1:D:837:PRO:HA	2.37	0.48
1:A:103:ALA:HB2	1:A:234:ARG:HE	1.78	0.48
1:C:170:ILE:HA	1:C:174:TRP:O	2.14	0.48
1:C:336:GLN:NE2	1:C:825:TRP:HE1	2.12	0.48
1:D:348:GLU:OE1	1:D:399:HIS:CE1	2.67	0.48
1:B:428:MET:SD	1:B:470:ASP:HB3	2.54	0.47
1:C:124:GLU:CD	1:C:655:LYS:HZ1	2.22	0.47
1:C:378:THR:HG22	1:C:380:LEU:H	1.79	0.47
1:D:146:SER:HB2	1:D:817:ILE:HG13	1.96	0.47
1:B:739:ARG:O	1:B:743:GLU:HG2	2.14	0.47
1:D:589:ARG:C	1:D:591:LYS:N	2.72	0.47
1:A:724:ARG:C	1:D:729:GLN:HG2	2.40	0.47
1:D:549:LEU:HD23	1:D:557:ILE:HG21	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ASN:OD1	1:B:377:HIS:CE1	2.68	0.47
1:C:751:SER:O	1:C:752:PRO:C	2.57	0.47
1:C:727:ASN:HD21	1:C:729:GLN:HB3	1.79	0.47
1:A:526:ASP:OD1	1:A:799:ARG:NH1	2.48	0.47
1:B:274:ASN:HA	1:B:277:ARG:HB2	1.95	0.47
1:C:130:GLY:O	1:C:164:GLY:HA2	2.14	0.47
1:C:269:ARG:NH1	1:C:273:GLU:OE1	2.43	0.47
1:C:274:ASN:HA	1:C:277:ARG:HB2	1.97	0.47
1:B:507:ILE:HG21	1:B:520:LYS:HB3	1.96	0.47
1:A:23:ASN:HD22	1:A:23:ASN:HA	1.58	0.47
1:A:727:ASN:HD21	1:D:725:GLY:HA3	1.80	0.47
1:B:128:ASP:OD2	1:B:649:ARG:HG3	2.15	0.46
1:B:373:ALA:HA	1:B:449:SER:HB3	1.97	0.46
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.97	0.46
1:B:138:ARG:HD3	1:B:138:ARG:O	2.16	0.46
1:B:144:LEU:HD23	1:B:147:MET:HE3	1.96	0.46
1:C:336:GLN:HG2	1:C:825:TRP:HE1	1.79	0.46
1:D:511:TYR:O	1:D:514:ASP:C	2.57	0.46
1:A:380:LEU:HD12	1:A:380:LEU:HA	1.86	0.46
1:A:438:ARG:HH11	1:A:438:ARG:HG2	1.78	0.46
1:D:546:ALA:HA	1:D:549:LEU:HB3	1.98	0.46
1:D:563:PHE:CD1	1:D:602:THR:OG1	2.68	0.46
1:C:325:ASN:C	1:C:327:ASP:N	2.74	0.46
1:B:336:GLN:HG2	1:B:825:TRP:HE1	1.79	0.46
1:B:336:GLN:HE22	1:B:373:ALA:HB3	1.79	0.46
1:B:462:ILE:HG12	1:B:462:ILE:H	1.62	0.46
1:C:774:PHE:C	1:C:776:ASP:H	2.24	0.46
1:D:43:ARG:NH1	2:D:900:SO4:O1	2.44	0.46
1:D:87:LEU:HD13	1:D:341:HIS:CB	2.44	0.46
1:A:464:LYS:HG2	1:A:472:TYR:CD1	2.51	0.46
1:D:663:SER:HB3	1:D:688:THR:HA	1.98	0.46
1:D:836:ALA:HB1	1:D:837:PRO:CA	2.40	0.46
1:D:530:PHE:C	1:D:532:ARG:N	2.72	0.46
1:D:662:LEU:HD22	1:D:689:ILE:HG22	1.98	0.46
1:B:235:ASN:H	1:B:235:ASN:HD22	1.64	0.46
1:B:665:GLN:HB3	1:B:696:ASN:HD21	1.81	0.46
1:D:699:MET:HA	1:D:811:PHE:CZ	2.51	0.46
1:C:677:GLY:HA2	1:C:680:LLP:HD3	1.97	0.46
1:D:458:ILE:HD11	1:D:694:GLY:H	1.81	0.46
1:C:47:THR:CG2	1:C:48:PRO:HD2	2.43	0.45
1:D:47:THR:HG23	1:D:49:ARG:H	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:631:ASN:HA	1:D:641:ARG:NH1	2.31	0.45
1:A:450:HIS:O	1:A:478:LYS:HG3	2.16	0.45
1:A:781:VAL:O	1:A:785:GLU:HG3	2.16	0.45
1:D:665:GLN:HG2	1:D:678:ASN:OD1	2.16	0.45
1:C:66:ARG:HG3	1:C:66:ARG:NH1	2.19	0.45
1:C:336:GLN:HE22	1:C:373:ALA:HB3	1.79	0.45
1:A:47:THR:HG23	1:A:48:PRO:HD2	1.98	0.45
1:A:438:ARG:CG	1:A:438:ARG:NH1	2.72	0.45
1:A:804:ASN:O	1:A:807:THR:HG22	2.15	0.45
1:B:348:GLU:OE1	1:B:399:HIS:HE1	2.00	0.45
1:B:503:ILE:HG23	1:B:521:LEU:HD11	1.99	0.45
1:C:575:ARG:HD2	1:C:668:THR:H	1.81	0.45
1:D:309:ARG:HH11	1:D:309:ARG:HB3	1.82	0.45
1:D:563:PHE:CD2	1:D:659:ALA:O	2.68	0.45
1:D:557:ILE:HG22	1:D:557:ILE:O	2.15	0.45
1:B:557:ILE:HD13	1:B:557:ILE:HA	1.83	0.45
1:C:388:PRO:HA	1:C:438:ARG:HG2	1.98	0.45
1:C:571:HIS:ND1	1:C:573:TYR:HD1	2.15	0.45
1:C:618:MET:HB3	1:C:761:ILE:HD11	1.98	0.45
1:D:602:THR:HG22	1:D:641:ARG:HB2	1.99	0.45
1:A:550:GLU:HG2	1:A:555:VAL:O	2.16	0.45
1:C:279:LEU:CD2	1:C:280:TYR:H	2.30	0.45
1:A:89:PHE:O	1:A:131:LEU:HB3	2.17	0.45
1:A:348:GLU:OE1	1:A:399:HIS:HE1	2.00	0.45
1:B:47:THR:HG23	1:B:48:PRO:HD2	1.98	0.45
1:B:738:LEU:HD12	1:B:741:ILE:HD11	1.99	0.45
1:A:21:VAL:HG21	1:A:26:GLU:CG	2.43	0.45
1:A:454:GLY:HA3	1:A:460:SER:OG	2.17	0.45
1:C:129:ALA:HB1	1:C:131:LEU:HD22	1.99	0.45
1:C:274:ASN:ND2	1:C:274:ASN:N	2.47	0.45
1:C:325:ASN:C	1:C:327:ASP:H	2.25	0.45
1:C:455:VAL:HG13	1:C:674:SER:HB2	1.96	0.45
1:C:584:ILE:H	1:C:584:ILE:HG13	1.67	0.45
1:B:601:ARG:NH2	1:B:784:GLN:OE1	2.46	0.45
1:D:810:LYS:O	1:D:815:ARG:NE	2.34	0.45
1:A:580:CYS:O	1:A:584:ILE:HG13	2.17	0.44
1:C:571:HIS:ND1	1:C:573:TYR:CD1	2.85	0.44
1:A:465:LYS:O	1:A:469:LYS:HD2	2.18	0.44
1:B:16:ARG:HG3	1:B:17:GLY:N	2.33	0.44
1:A:235:ASN:HD22	1:A:235:ASN:C	2.26	0.44
1:B:456:ALA:HB3	1:B:673:ALA:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ARG:NH1	1:C:309:ARG:HB3	2.32	0.44
1:D:489:ARG:H	1:D:489:ARG:HE	1.65	0.44
1:B:575:ARG:HH22	1:B:776:ASP:CB	2.29	0.44
1:B:599:VAL:HG21	1:B:788:SER:O	2.17	0.44
1:C:329:PHE:HB3	1:C:330:PRO:HD3	1.99	0.44
1:A:810:LYS:HG2	1:A:810:LYS:O	2.16	0.44
1:B:615:MET:CE	1:B:761:ILE:HG12	2.34	0.44
1:C:235:ASN:HD22	1:C:235:ASN:N	2.04	0.44
1:C:729:GLN:O	1:C:732:TYR:HB3	2.16	0.44
1:C:799:ARG:O	1:C:803:ARG:HG3	2.18	0.44
1:D:735:ILE:H	1:D:735:ILE:HG12	1.46	0.44
1:C:290:GLU:HG2	1:C:294:LYS:HD2	1.99	0.44
1:B:329:PHE:HB3	1:B:330:PRO:HD3	2.00	0.44
1:D:295:GLN:O	1:D:299:VAL:HG12	2.17	0.44
1:D:803:ARG:HE	1:D:803:ARG:HB2	1.63	0.44
1:A:396:LEU:HB3	1:A:399:HIS:HB2	1.99	0.44
1:B:136:LEU:CD2	1:B:338:ASN:ND2	2.80	0.44
1:B:836:ALA:HB1	1:B:837:PRO:HA	2.00	0.44
1:D:493:VAL:HG21	1:D:512:ILE:HG21	2.00	0.44
1:A:753:LYS:N	1:A:753:LYS:HD2	2.33	0.43
1:B:42:ASP:C	1:B:42:ASP:OD2	2.61	0.43
1:D:289:LYS:HG3	1:D:291:LEU:H	1.83	0.43
1:C:195:GLU:H	1:C:195:GLU:HG3	1.50	0.43
1:C:492:LEU:HG	1:C:683:LEU:HD22	1.99	0.43
1:D:677:GLY:O	1:D:681:PHE:HD1	2.00	0.43
1:D:754:GLN:HG2	1:D:757:LEU:HD13	2.00	0.43
1:D:495:CYS:HB3	1:D:654:GLU:HB2	2.01	0.43
1:D:699:MET:HA	1:D:811:PHE:HZ	1.82	0.43
1:A:457:ARG:CG	1:A:457:ARG:NH1	2.80	0.43
1:A:817:ILE:HD13	1:A:817:ILE:HA	1.89	0.43
1:B:263:ILE:O	1:B:266:VAL:HG23	2.19	0.43
1:B:355:ASP:OD2	1:B:398:ARG:HD3	2.19	0.43
1:B:835:PRO:HB2	1:B:836:ALA:H	1.62	0.43
1:D:34:HIS:HD2	1:D:38:THR:OG1	2.01	0.43
1:D:396:LEU:HB3	1:D:399:HIS:HB2	2.00	0.43
1:A:682:MET:HE2	1:A:682:MET:HB3	1.87	0.43
1:A:766:MET:HE1	1:A:774:PHE:HE2	1.83	0.43
1:C:235:ASN:CG	1:C:237:VAL:HG13	2.43	0.43
1:B:63:LEU:HD13	1:B:229:PRO:HG2	2.00	0.43
1:C:676:THR:CG2	1:C:680:LLP:H4'1	2.48	0.43
1:A:19:ALA:HB1	1:A:30:ASN:HD21	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:PRO:O	1:A:386:ARG:NH2	2.52	0.43
1:D:136:LEU:HD22	1:D:338:ASN:ND2	2.34	0.43
1:D:578:LEU:HB3	1:D:666:ILE:HD12	2.01	0.43
1:A:138:ARG:HD3	1:A:138:ARG:C	2.43	0.43
1:B:267:LEU:H	1:B:267:LEU:HG	1.68	0.43
1:B:424:ARG:NH2	1:B:473:GLU:OE1	2.52	0.43
1:B:795:ARG:O	1:B:799:ARG:HG3	2.19	0.43
1:C:53:PHE:CE1	1:C:188:PRO:HG3	2.53	0.43
1:D:627:GLY:O	1:D:631:ASN:ND2	2.52	0.43
1:D:645:LEU:HD11	1:D:656:VAL:HG21	2.00	0.43
1:A:836:ALA:HA	1:A:837:PRO:HA	1.89	0.43
1:C:458:ILE:O	1:C:462:ILE:HG23	2.19	0.43
1:D:309:ARG:HB3	1:D:309:ARG:NH1	2.33	0.43
1:D:329:PHE:HB3	1:D:330:PRO:HD3	2.01	0.43
1:D:682:MET:HE2	1:D:682:MET:HB3	1.94	0.43
1:D:730:GLU:HG3	1:D:731:TYR:N	2.34	0.43
1:A:359:LEU:HD12	1:A:363:LYS:HG2	2.00	0.42
1:A:423:ASP:O	1:A:426:ARG:NH1	2.49	0.42
1:A:575:ARG:HH22	1:A:776:ASP:HB2	1.84	0.42
1:B:455:VAL:HG13	1:B:484:ASN:ND2	2.34	0.42
1:B:641:ARG:CG	1:B:641:ARG:NH1	2.65	0.42
1:D:264:GLN:HA	1:D:264:GLN:OE1	2.18	0.42
1:D:373:ALA:HA	1:D:449:SER:HB3	2.01	0.42
1:A:571:HIS:H	1:A:576:GLN:NE2	2.16	0.42
1:B:60:ARG:O	1:B:64:VAL:HG13	2.19	0.42
1:C:309:ARG:HB3	1:C:309:ARG:HH11	1.84	0.42
1:C:422:VAL:O	1:C:425:LEU:HB2	2.18	0.42
1:C:615:MET:HE2	1:C:764:MET:CE	2.44	0.42
1:C:738:LEU:O	1:C:739:ARG:C	2.62	0.42
1:C:741:ILE:H	1:C:741:ILE:HG12	1.60	0.42
1:D:274:ASN:C	1:D:274:ASN:ND2	2.76	0.42
1:D:800:MET:C	1:D:802:ILE:N	2.62	0.42
1:B:34:HIS:CE1	1:B:61:ASP:OD2	2.68	0.42
1:B:233:TYR:CZ	1:B:234:ARG:HD3	2.55	0.42
1:D:593:GLU:CD	1:D:593:GLU:N	2.78	0.42
1:D:650:VAL:O	1:D:650:VAL:CG1	2.66	0.42
1:D:739:ARG:NH1	1:D:739:ARG:HB2	2.34	0.42
1:B:361:TRP:CZ3	1:B:409:ARG:HD2	2.54	0.42
1:C:759:LYS:O	1:C:763:ASN:HB2	2.19	0.42
1:D:499:LEU:N	1:D:537:VAL:HG11	2.35	0.42
1:D:587:TYR:O	1:D:591:LYS:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ASN:C	1:A:800:MET:HE3	2.45	0.42
1:C:19:ALA:HA	1:C:20:GLY:HA3	1.73	0.42
1:D:536:LYS:C	1:D:538:LYS:H	2.28	0.42
1:D:741:ILE:O	1:D:745:LEU:HG	2.20	0.42
1:A:12:GLN:HE22	1:B:28:LYS:NZ	2.17	0.42
1:A:81:ARG:HG2	1:A:155:TYR:HE2	1.84	0.42
1:C:515:LEU:HD22	1:C:812:SER:HB2	2.01	0.42
1:D:517:GLN:CG	1:D:517:GLN:O	2.67	0.42
1:D:542:LYS:O	1:D:546:ALA:CB	2.68	0.42
1:A:714:ARG:O	1:A:718:VAL:HG23	2.19	0.42
1:D:517:GLN:HG2	1:D:517:GLN:O	2.19	0.42
1:D:683:LEU:HD23	1:D:683:LEU:HA	1.83	0.42
1:C:689:ILE:HA	1:C:709:PHE:O	2.20	0.42
1:D:483:THR:O	1:D:816:THR:HG23	2.19	0.42
1:D:487:THR:HG23	1:D:490:ARG:HB3	2.01	0.42
1:D:665:GLN:HE21	1:D:678:ASN:HA	1.85	0.42
1:D:738:LEU:HB2	1:D:777:TYR:CE2	2.55	0.42
1:D:791:TYR:C	1:D:793:ASN:N	2.78	0.42
1:D:791:TYR:CA	1:D:797:TRP:CD1	2.97	0.42
1:A:600:PRO:HA	1:A:639:ARG:O	2.20	0.42
1:B:292:ARG:HH21	1:B:341:HIS:CD2	2.38	0.42
1:B:760:ASP:HA	1:B:763:ASN:HB2	2.01	0.42
1:C:378:THR:O	1:C:459:HIS:HE1	2.01	0.42
1:D:562:LEU:HD23	1:D:563:PHE:N	2.35	0.42
1:A:503:ILE:HG12	1:A:521:LEU:HD21	2.02	0.41
1:C:172:GLY:O	1:C:621:LYS:NZ	2.53	0.41
1:C:293:LEU:HD23	1:C:395:LEU:HD21	2.02	0.41
1:D:515:LEU:HD23	1:D:809:GLY:HA2	2.01	0.41
1:D:527:ASP:O	1:D:532:ARG:NH2	2.36	0.41
1:A:37:PHE:CD1	1:B:64:VAL:HG22	2.55	0.41
1:B:289:LYS:HZ2	1:B:290:GLU:H	1.68	0.41
1:D:252:PHE:HD2	1:D:269:ARG:HG2	1.86	0.41
1:D:542:LYS:HE3	1:D:563:PHE:CG	2.55	0.41
1:D:822:ARG:NH1	1:D:828:GLU:OE2	2.51	0.41
1:C:73:HIS:CD2	1:C:834:LEU:HD11	2.55	0.41
1:D:536:LYS:C	1:D:538:LYS:N	2.78	0.41
1:D:803:ARG:O	1:D:807:THR:HG22	2.20	0.41
1:C:626:ILE:O	1:C:630:VAL:HG13	2.20	0.41
1:D:143:PHE:CG	1:D:817:ILE:HD11	2.56	0.41
1:D:571:HIS:ND1	1:D:573:TYR:HD1	2.18	0.41
1:D:715:VAL:O	1:D:715:VAL:HG12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:795:ARG:O	1:D:799:ARG:HG3	2.21	0.41
1:A:100:VAL:O	1:A:234:ARG:NH1	2.53	0.41
1:A:467:ILE:H	1:A:467:ILE:HD12	1.85	0.41
1:D:21:VAL:O	1:D:22:GLU:C	2.63	0.41
1:D:168:GLN:HG3	1:D:175:GLN:HG3	2.03	0.41
1:A:85:LEU:CD2	1:A:303:THR:HG21	2.44	0.41
1:C:64:VAL:CG2	1:D:37:PHE:HD1	2.32	0.41
1:D:665:GLN:NE2	1:D:678:ASN:OD1	2.53	0.41
1:A:129:ALA:HB1	1:A:131:LEU:HD22	2.03	0.41
1:A:230:VAL:HG22	1:A:230:VAL:O	2.20	0.41
1:A:579:ASN:C	1:A:579:ASN:HD22	2.28	0.41
1:A:807:THR:O	1:A:807:THR:HG23	2.21	0.41
1:B:157:TYR:CE2	1:B:242:ARG:HG2	2.56	0.41
1:C:805:ILE:O	1:C:805:ILE:HG22	2.21	0.41
1:D:55:LEU:O	1:D:59:VAL:HG23	2.21	0.41
1:A:136:LEU:HD11	1:A:338:ASN:ND2	2.35	0.41
1:A:260:GLY:O	1:A:261:GLY:C	2.64	0.41
1:A:495:CYS:HB3	1:A:654:GLU:HB2	2.01	0.41
1:B:67:TRP:HA	1:B:238:VAL:HB	2.03	0.41
1:B:262:TYR:HB3	1:B:264:GLN:HE22	1.85	0.41
1:B:819:GLN:O	1:B:823:GLU:HB2	2.21	0.41
1:C:100:VAL:O	1:C:234:ARG:NH1	2.53	0.41
1:C:727:ASN:O	1:C:730:GLU:HG2	2.21	0.41
1:D:534:VAL:C	1:D:536:LYS:H	2.29	0.41
1:D:791:TYR:HD1	1:D:797:TRP:CE2	2.38	0.41
1:C:433:GLU:OE1	1:C:433:GLU:HA	2.21	0.41
1:D:79:PRO:O	1:D:80:LYS:C	2.63	0.41
1:D:235:ASN:OD1	1:D:237:VAL:HG13	2.21	0.41
1:D:363:LYS:HA	1:D:363:LYS:HD2	1.89	0.41
1:A:34:HIS:CD2	1:A:38:THR:OG1	2.73	0.40
1:B:292:ARG:O	1:B:296:GLU:HG3	2.20	0.40
1:B:550:GLU:C	1:B:552:GLU:H	2.29	0.40
1:B:571:HIS:H	1:B:576:GLN:NE2	2.18	0.40
1:C:348:GLU:OE1	1:C:399:HIS:HE1	2.04	0.40
1:D:161:TYR:CZ	1:D:279:LEU:HG	2.55	0.40
1:B:170:ILE:HG12	1:B:646:GLU:HG3	2.03	0.40
1:B:458:ILE:HD11	1:B:694:GLY:CA	2.51	0.40
1:B:571:HIS:O	1:B:576:GLN:NE2	2.54	0.40
1:B:591:LYS:HA	1:B:591:LYS:HD3	1.86	0.40
1:C:21:VAL:HG23	1:C:62:HIS:CD2	2.56	0.40
1:C:85:LEU:HD11	1:C:303:THR:HG21	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:GLN:HG3	1:C:825:TRP:HZ2	1.86	0.40
1:C:545:PHE:O	1:C:549:LEU:HB2	2.21	0.40
1:C:717:ASP:OD1	1:C:717:ASP:N	2.54	0.40
1:D:36:HIS:O	1:D:40:VAL:HA	2.20	0.40
1:D:274:ASN:HA	1:D:277:ARG:HB2	2.02	0.40
1:D:211:GLN:HG3	1:D:358:ARG:HH22	1.84	0.40
1:D:808:SER:O	1:D:811:PHE:N	2.48	0.40
1:D:828:GLU:C	1:D:829:PRO:O	2.63	0.40
1:A:515:LEU:HD23	1:A:809:GLY:HA2	2.03	0.40
1:B:274:ASN:HD22	1:B:274:ASN:C	2.30	0.40
1:C:53:PHE:CD1	1:C:188:PRO:HG3	2.56	0.40
1:C:782:LYS:O	1:C:785:GLU:HB2	2.21	0.40
1:D:665:GLN:NE2	1:D:678:ASN:HA	2.35	0.40
1:A:250:ASN:HB3	1:A:252:PHE:CE2	2.49	0.40
1:A:269:ARG:HH21	1:B:277:ARG:NH2	2.12	0.40
1:A:305:GLN:O	1:A:309:ARG:HB2	2.21	0.40
1:C:191:LYS:C	1:C:191:LYS:HD3	2.46	0.40
1:C:347:PRO:HD3	1:C:444:LEU:HD11	2.03	0.40
1:D:399:HIS:O	1:D:403:ILE:HG13	2.22	0.40
1:D:433:GLU:H	1:D:433:GLU:HG2	1.72	0.40
1:D:523:SER:HB2	1:D:524:TYR:CE1	2.56	0.40
1:D:571:HIS:CD2	1:D:613:TYR:CE2	3.09	0.40
1:D:584:ILE:HD11	1:D:626:ILE:HD11	2.03	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	801/842 (95%)	745 (93%)	43 (5%)	13 (2%)	7	16
1	B	802/842 (95%)	754 (94%)	37 (5%)	11 (1%)	9	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	798/842 (95%)	746 (94%)	43 (5%)	9 (1%)	11	25
1	D	797/842 (95%)	698 (88%)	78 (10%)	21 (3%)	4	7
All	All	3198/3368 (95%)	2943 (92%)	201 (6%)	54 (2%)	7	15

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	514	ASP
1	A	551	ARG
1	A	835	PRO
1	B	678	ASN
1	B	835	PRO
1	C	16	ARG
1	C	19	ALA
1	C	166	PHE
1	C	325	ASN
1	D	21	VAL
1	D	509	GLU
1	D	510	GLU
1	D	590	ILE
1	D	801	VAL
1	A	166	PHE
1	A	261	GLY
1	A	421	ASP
1	A	477	HIS
1	C	18	LEU
1	C	724	ARG
1	D	166	PHE
1	D	489	ARG
1	D	724	ARG
1	D	792	LYS
1	A	473	GLU
1	B	166	PHE
1	B	211	GLN
1	B	613	TYR
1	D	576	GLN
1	D	591	LYS
1	D	596	LYS
1	D	693	ASP
1	A	836	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	421	ASP
1	C	778	GLU
1	D	251	ASP
1	D	540	GLU
1	D	561	SER
1	D	697	VAL
1	A	329	PHE
1	B	268	ASP
1	B	551	ARG
1	C	752	PRO
1	D	830	SER
1	B	836	ALA
1	C	775	ALA
1	D	523	SER
1	D	558	ASN
1	A	260	GLY
1	B	20	GLY
1	D	836	ALA
1	A	263	ILE
1	B	837	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	699/730 (96%)	600 (86%)	99 (14%)	3	6
1	B	700/730 (96%)	605 (86%)	95 (14%)	3	7
1	C	697/730 (96%)	608 (87%)	89 (13%)	4	8
1	D	697/730 (96%)	585 (84%)	112 (16%)	2	4
All	All	2793/2920 (96%)	2398 (86%)	395 (14%)	3	6

All (395) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	10	ARG
1	A	15	VAL
1	A	16	ARG
1	A	18	LEU
1	A	23	ASN
1	A	39	LEU
1	A	63	LEU
1	A	71	GLN
1	A	76	GLU
1	A	81	ARG
1	A	82	ILE
1	A	90	TYR
1	A	91	MET
1	A	95	LEU
1	A	128	ASP
1	A	131	LEU
1	A	138	ARG
1	A	149	THR
1	A	169	LYS
1	A	177	GLU
1	A	216	VAL
1	A	224	MET
1	A	228	THR
1	A	230	VAL
1	A	235	ASN
1	A	237	VAL
1	A	242	ARG
1	A	243	LEU
1	A	251	ASP
1	A	264	GLN
1	A	268	ASP
1	A	274	ASN
1	A	279	LEU
1	A	287	GLU
1	A	292	ARG
1	A	332	LYS
1	A	333	VAL
1	A	356	LEU
1	A	369	VAL
1	A	371	THR
1	A	380	LEU
1	A	382	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	391	LEU
1	A	392	LEU
1	A	396	LEU
1	A	398	ARG
1	A	400	LEU
1	A	408	GLN
1	A	425	LEU
1	A	426	ARG
1	A	436	VAL
1	A	437	LYS
1	A	438	ARG
1	A	441	MET
1	A	444	LEU
1	A	449	SER
1	A	453	ASN
1	A	455	VAL
1	A	457	ARG
1	A	458	ILE
1	A	465	LYS
1	A	486	ILE
1	A	492	LEU
1	A	521	LEU
1	A	522	LEU
1	A	543	LEU
1	A	549	LEU
1	A	554	LYS
1	A	565	VAL
1	A	568	LYS
1	A	569	ARG
1	A	576	GLN
1	A	586	LEU
1	A	589	ARG
1	A	593	GLU
1	A	598	VAL
1	A	622	LEU
1	A	639	ARG
1	A	640	LEU
1	A	649	ARG
1	A	652	LEU
1	A	662	LEU
1	A	678	ASN
1	A	683	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	705	GLU
1	A	706	GLU
1	A	708	PHE
1	A	713	MET
1	A	714	ARG
1	A	716	GLU
1	A	743	GLU
1	A	760	ASP
1	A	765	LEU
1	A	782	LYS
1	A	797	TRP
1	A	807	THR
1	A	827	VAL
1	A	833	ARG
1	B	10	ARG
1	B	15	VAL
1	B	21	VAL
1	B	39	LEU
1	B	47	THR
1	B	64	VAL
1	B	66	ARG
1	B	69	ARG
1	B	82	ILE
1	B	85	LEU
1	B	90	TYR
1	B	91	MET
1	B	94	THR
1	B	95	LEU
1	B	100	VAL
1	B	104	LEU
1	B	128	ASP
1	B	131	LEU
1	B	138	ARG
1	B	165	ILE
1	B	169	LYS
1	B	171	CYS
1	B	177	GLU
1	B	191	LYS
1	B	214	LYS
1	B	234	ARG
1	B	235	ASN
1	B	237	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	242	ARG
1	B	251	ASP
1	B	264	GLN
1	B	267	LEU
1	B	269	ARG
1	B	274	ASN
1	B	289	LYS
1	B	291	LEU
1	B	314	SER
1	B	337	LEU
1	B	359	LEU
1	B	360	ASP
1	B	363	LYS
1	B	380	LEU
1	B	382	GLU
1	B	384	LEU
1	B	392	LEU
1	B	396	LEU
1	B	398	ARG
1	B	400	LEU
1	B	423	ASP
1	B	425	LEU
1	B	436	VAL
1	B	444	LEU
1	B	455	VAL
1	B	458	ILE
1	B	462	ILE
1	B	467	ILE
1	B	469	LYS
1	B	474	LEU
1	B	486	ILE
1	B	492	LEU
1	B	516	ASP
1	B	525	VAL
1	B	538	LYS
1	B	554	LYS
1	B	557	ILE
1	B	560	ASN
1	B	565	VAL
1	B	569	ARG
1	B	575	ARG
1	B	589	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	622	LEU
1	B	640	LEU
1	B	641	ARG
1	B	649	ARG
1	B	652	LEU
1	B	662	LEU
1	B	665	GLN
1	B	676	THR
1	B	683	LEU
1	B	692	MET
1	B	706	GLU
1	B	714	ARG
1	B	737	GLU
1	B	741	ILE
1	B	745	LEU
1	B	765	LEU
1	B	766	MET
1	B	768	HIS
1	B	770	ARG
1	B	779	GLU
1	B	782	LYS
1	B	792	LYS
1	B	831	ARG
1	B	833	ARG
1	B	839	GLU
1	C	12	GLN
1	C	15	VAL
1	C	16	ARG
1	C	18	LEU
1	C	23	ASN
1	C	39	LEU
1	C	45	VAL
1	C	64	VAL
1	C	66	ARG
1	C	77	LYS
1	C	90	TYR
1	C	95	LEU
1	C	100	VAL
1	C	102	LEU
1	C	131	LEU
1	C	169	LYS
1	C	177	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	191	LYS
1	C	195	GLU
1	C	214	LYS
1	C	230	VAL
1	C	234	ARG
1	C	235	ASN
1	C	237	VAL
1	C	242	ARG
1	C	243	LEU
1	C	247	LYS
1	C	254	LEU
1	C	264	GLN
1	C	266	VAL
1	C	267	LEU
1	C	274	ASN
1	C	278	VAL
1	C	279	LEU
1	C	292	ARG
1	C	300	VAL
1	C	332	LYS
1	C	337	LEU
1	C	356	LEU
1	C	361	TRP
1	C	366	GLU
1	C	378	THR
1	C	379	VAL
1	C	384	LEU
1	C	395	LEU
1	C	396	LEU
1	C	398	ARG
1	C	400	LEU
1	C	425	LEU
1	C	444	LEU
1	C	455	VAL
1	C	462	ILE
1	C	474	LEU
1	C	486	ILE
1	C	492	LEU
1	C	509	GLU
1	C	522	LEU
1	C	538	LYS
1	C	539	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	543	LEU
1	C	565	VAL
1	C	575	ARG
1	C	576	GLN
1	C	584	ILE
1	C	586	LEU
1	C	589	ARG
1	C	596	LYS
1	C	599	VAL
1	C	622	LEU
1	C	630	VAL
1	C	639	ARG
1	C	641	ARG
1	C	642	VAL
1	C	652	LEU
1	C	662	LEU
1	C	676	THR
1	C	678	ASN
1	C	683	LEU
1	C	714	ARG
1	C	715	VAL
1	C	741	ILE
1	C	753	LYS
1	C	760	ASP
1	C	763	ASN
1	C	765	LEU
1	C	782	LYS
1	C	788	SER
1	C	792	LYS
1	C	833	ARG
1	D	11	LYS
1	D	15	VAL
1	D	21	VAL
1	D	39	LEU
1	D	45	VAL
1	D	47	THR
1	D	64	VAL
1	D	77	LYS
1	D	81	ARG
1	D	82	ILE
1	D	85	LEU
1	D	87	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	88	GLU
1	D	90	TYR
1	D	95	LEU
1	D	100	VAL
1	D	102	LEU
1	D	131	LEU
1	D	136	LEU
1	D	171	CYS
1	D	176	MET
1	D	177	GLU
1	D	191	LYS
1	D	211	GLN
1	D	234	ARG
1	D	237	VAL
1	D	242	ARG
1	D	245	SER
1	D	247	LYS
1	D	264	GLN
1	D	269	ARG
1	D	274	ASN
1	D	279	LEU
1	D	280	TYR
1	D	292	ARG
1	D	300	VAL
1	D	304	LEU
1	D	310	ARG
1	D	332	LYS
1	D	337	LEU
1	D	358	ARG
1	D	361	TRP
1	D	382	GLU
1	D	384	LEU
1	D	391	LEU
1	D	392	LEU
1	D	396	LEU
1	D	398	ARG
1	D	400	LEU
1	D	405	GLU
1	D	425	LEU
1	D	433	GLU
1	D	444	LEU
1	D	455	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	457	ARG
1	D	469	LYS
1	D	474	LEU
1	D	478	LYS
1	D	486	ILE
1	D	492	LEU
1	D	501	GLU
1	D	518	LEU
1	D	522	LEU
1	D	525	VAL
1	D	526	ASP
1	D	528	GLU
1	D	530	PHE
1	D	532	ARG
1	D	534	VAL
1	D	555	VAL
1	D	561	SER
1	D	576	GLN
1	D	579	ASN
1	D	583	VAL
1	D	585	THR
1	D	593	GLU
1	D	617	LYS
1	D	622	LEU
1	D	629	VAL
1	D	640	LEU
1	D	643	ILE
1	D	649	ARG
1	D	652	LEU
1	D	665	GLN
1	D	667	SER
1	D	676	THR
1	D	679	MET
1	D	683	LEU
1	D	688	THR
1	D	689	ILE
1	D	702	GLU
1	D	705	GLU
1	D	706	GLU
1	D	713	MET
1	D	716	GLU
1	D	723	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	724	ARG
1	D	735	ILE
1	D	756	ASP
1	D	759	LYS
1	D	765	LEU
1	D	766	MET
1	D	770	ARG
1	D	782	LYS
1	D	787	VAL
1	D	795	ARG
1	D	808	SER
1	D	810	LYS
1	D	812	SER
1	D	813	SER
1	D	823	GLU
1	D	827	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	12	GLN
1	A	23	ASN
1	A	30	ASN
1	A	34	HIS
1	A	114	GLN
1	A	167	ASN
1	A	168	GLN
1	A	235	ASN
1	A	264	GLN
1	A	325	ASN
1	A	336	GLN
1	A	390	HIS
1	A	399	HIS
1	A	408	GLN
1	A	412	ASN
1	A	459	HIS
1	A	481	ASN
1	A	541	ASN
1	A	576	GLN
1	A	582	HIS
1	A	707	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	727	ASN
1	A	744	GLN
1	A	754	GLN
1	A	767	HIS
1	B	34	HIS
1	B	44	ASN
1	B	133	ASN
1	B	167	ASN
1	B	168	GLN
1	B	211	GLN
1	B	235	ASN
1	B	264	GLN
1	B	274	ASN
1	B	325	ASN
1	B	336	GLN
1	B	377	HIS
1	B	399	HIS
1	B	453	ASN
1	B	459	HIS
1	B	481	ASN
1	B	541	ASN
1	B	566	GLN
1	B	576	GLN
1	B	579	ASN
1	B	727	ASN
1	B	744	GLN
1	C	34	HIS
1	C	168	GLN
1	C	211	GLN
1	C	235	ASN
1	C	270	ASN
1	C	274	ASN
1	C	336	GLN
1	C	399	HIS
1	C	412	ASN
1	C	459	HIS
1	C	481	ASN
1	C	517	GLN
1	C	539	GLN
1	C	541	ASN
1	C	566	GLN
1	C	576	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	579	ASN
1	C	727	ASN
1	C	744	GLN
1	C	763	ASN
1	C	768	HIS
1	D	12	GLN
1	D	34	HIS
1	D	44	ASN
1	D	62	HIS
1	D	73	HIS
1	D	114	GLN
1	D	168	GLN
1	D	187	ASN
1	D	274	ASN
1	D	336	GLN
1	D	341	HIS
1	D	377	HIS
1	D	399	HIS
1	D	453	ASN
1	D	459	HIS
1	D	481	ASN
1	D	517	GLN
1	D	541	ASN
1	D	566	GLN
1	D	576	GLN
1	D	579	ASN
1	D	631	ASN
1	D	696	ASN
1	D	723	GLN
1	D	727	ASN
1	D	744	GLN
1	D	767	HIS
1	D	793	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are 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$
1	LLP	C	680	1	23,24,25	1.72	4 (17%)	25,32,34	1.23	3 (12%)
1	LLP	D	680	1	23,24,25	1.79	5 (21%)	25,32,34	1.42	4 (16%)
1	LLP	A	680	1	23,24,25	1.81	5 (21%)	25,32,34	1.31	3 (12%)
1	LLP	B	680	1	23,24,25	1.76	5 (21%)	25,32,34	1.31	3 (12%)

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
1	LLP	C	680	1	-	0/16/17/19	0/1/1/1
1	LLP	D	680	1	-	2/16/17/19	0/1/1/1
1	LLP	A	680	1	-	0/16/17/19	0/1/1/1
1	LLP	B	680	1	-	4/16/17/19	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LLP	O3-C3	-6.31	1.22	1.36
1	D	680	LLP	O3-C3	-5.96	1.23	1.36
1	B	680	LLP	O3-C3	-5.90	1.23	1.36
1	C	680	LLP	O3-C3	-5.79	1.23	1.36
1	C	680	LLP	C2-N1	2.72	1.38	1.33
1	D	680	LLP	C2-N1	2.66	1.38	1.33
1	D	680	LLP	C4-C4'	2.64	1.52	1.46
1	B	680	LLP	C2-N1	2.62	1.38	1.33
1	A	680	LLP	C2-N1	2.43	1.38	1.33
1	D	680	LLP	CE-NZ	2.40	1.52	1.46
1	A	680	LLP	C4-C4'	2.38	1.51	1.46
1	A	680	LLP	C4'-NZ	2.31	1.34	1.27
1	A	680	LLP	CE-NZ	2.26	1.51	1.46
1	B	680	LLP	C6-N1	2.22	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	680	LLP	C4-C4'	2.21	1.51	1.46
1	B	680	LLP	C4'-NZ	2.20	1.34	1.27
1	C	680	LLP	C4'-NZ	2.19	1.34	1.27
1	C	680	LLP	C4-C4'	2.19	1.51	1.46
1	D	680	LLP	C4'-NZ	2.18	1.34	1.27

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	LLP	C5-C6-N1	-2.85	119.20	123.83
1	B	680	LLP	OP4-C5'-C5	2.84	114.67	109.36
1	A	680	LLP	C4-C4'-NZ	-2.78	111.22	124.04
1	B	680	LLP	C4-C4'-NZ	-2.57	112.19	124.04
1	D	680	LLP	C5'-C5-C6	-2.49	115.31	119.36
1	C	680	LLP	C5-C6-N1	-2.49	119.79	123.83
1	D	680	LLP	C5-C6-N1	-2.38	119.96	123.83
1	B	680	LLP	C5-C6-N1	-2.34	120.03	123.83
1	C	680	LLP	C4-C4'-NZ	-2.33	113.31	124.04
1	D	680	LLP	CE-NZ-C4'	-2.29	111.39	118.72
1	A	680	LLP	OP3-P-OP4	-2.27	100.74	106.67
1	D	680	LLP	OP4-C5'-C5	-2.24	105.15	109.36
1	C	680	LLP	CE-NZ-C4'	-2.22	111.60	118.72

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	680	LLP	C5'-OP4-P-OP2
1	B	680	LLP	C5'-OP4-P-OP3
1	D	680	LLP	C5'-OP4-P-OP2
1	B	680	LLP	C5'-OP4-P-OP1
1	D	680	LLP	C5'-OP4-P-OP3
1	B	680	LLP	CE-CD-CG-CB

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	680	LLP	6	0
1	D	680	LLP	1	0
1	A	680	LLP	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	680	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are 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	SO4	B	901	-	4,4,4	0.28	0	6,6,6	0.28	0
2	SO4	C	902	-	4,4,4	0.26	0	6,6,6	0.19	0
2	SO4	A	902	-	4,4,4	0.24	0	6,6,6	0.42	0
2	SO4	D	902	-	4,4,4	0.29	0	6,6,6	0.28	0
2	SO4	C	901	-	4,4,4	0.29	0	6,6,6	0.55	0
2	SO4	B	900	-	4,4,4	0.31	0	6,6,6	0.22	0
2	SO4	D	900	-	4,4,4	0.28	0	6,6,6	0.36	0
2	SO4	B	902	-	4,4,4	0.26	0	6,6,6	0.40	0
2	SO4	A	901	-	4,4,4	0.30	0	6,6,6	0.33	0
2	SO4	D	901	-	4,4,4	0.31	0	6,6,6	0.27	0
2	SO4	D	903	-	4,4,4	0.21	0	6,6,6	0.28	0
2	SO4	A	900	-	4,4,4	0.24	0	6,6,6	0.33	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	SO4	1	0
2	D	900	SO4	1	0

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	809/842 (96%)	0.34	21 (2%) 57 51	29, 46, 62, 74	0
1	B	810/842 (96%)	0.06	12 (1%) 72 68	28, 46, 66, 78	0
1	C	806/842 (95%)	0.12	16 (1%) 65 60	23, 48, 71, 83	0
1	D	805/842 (95%)	0.51	69 (8%) 16 12	34, 53, 87, 102	0
All	All	3230/3368 (95%)	0.26	118 (3%) 45 39	23, 48, 73, 102	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	530	PHE	4.6
1	B	75	TYR	4.4
1	D	709	PHE	4.2
1	A	837	PRO	4.0
1	A	836	ALA	3.9
1	C	9	LYS	3.8
1	A	261	GLY	3.7
1	D	710	ILE	3.6
1	D	534	VAL	3.4
1	C	837	PRO	3.4
1	D	164	GLY	3.4
1	D	662	LEU	3.3
1	D	529	ALA	3.3
1	D	777	TYR	3.3
1	D	781	VAL	3.2
1	D	708	PHE	3.1
1	D	525	VAL	3.1
1	D	797	TRP	3.0
1	D	789	ALA	3.0
1	D	791	TYR	3.0
1	D	630	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	280	TYR	2.9
1	D	524	TYR	2.9
1	C	252	PHE	2.9
1	D	507	ILE	2.8
1	C	15	VAL	2.8
1	D	548	TYR	2.8
1	D	704	GLY	2.8
1	D	561	SER	2.8
1	B	31	PHE	2.7
1	D	518	LEU	2.7
1	D	800	MET	2.7
1	D	527	ASP	2.7
1	B	553	TYR	2.7
1	D	659	ALA	2.7
1	A	252	PHE	2.6
1	A	75	TYR	2.6
1	B	19	ALA	2.6
1	C	21	VAL	2.6
1	D	802	ILE	2.6
1	D	804	ASN	2.6
1	D	703	ALA	2.6
1	D	522	LEU	2.5
1	C	768	HIS	2.5
1	D	707	ASN	2.5
1	D	695	ALA	2.5
1	A	21	VAL	2.5
1	D	526	ASP	2.5
1	D	85	LEU	2.5
1	D	87	LEU	2.5
1	B	281	PRO	2.4
1	D	837	PRO	2.4
1	D	590	ILE	2.4
1	B	27	LEU	2.4
1	C	797	TRP	2.4
1	B	708	PHE	2.4
1	D	603	VAL	2.4
1	C	324	THR	2.4
1	D	711	PHE	2.4
1	D	718	VAL	2.4
1	D	836	ALA	2.4
1	A	17	GLY	2.3
1	C	721	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	787	VAL	2.3
1	A	727	ASN	2.3
1	A	324	THR	2.3
1	D	512	ILE	2.3
1	C	738	LEU	2.3
1	B	380	LEU	2.3
1	B	710	ILE	2.3
1	D	562	LEU	2.3
1	A	479	PHE	2.3
1	D	21	VAL	2.3
1	A	612	GLY	2.2
1	C	263	ILE	2.2
1	C	380	LEU	2.2
1	D	713	MET	2.2
1	D	252	PHE	2.2
1	D	643	ILE	2.2
1	A	825	TRP	2.2
1	D	583	VAL	2.2
1	D	684	ASN	2.2
1	D	687	LEU	2.2
1	D	705	GLU	2.2
1	D	600	PRO	2.2
1	D	750	PHE	2.2
1	A	280	TYR	2.2
1	A	259	VAL	2.1
1	A	751	SER	2.1
1	D	599	VAL	2.1
1	D	686	ALA	2.1
1	D	726	TYR	2.1
1	D	830	SER	2.1
1	D	555	VAL	2.1
1	A	373	ALA	2.1
1	A	775	ALA	2.1
1	C	19	ALA	2.1
1	B	271	LEU	2.1
1	C	515	LEU	2.1
1	D	712	GLY	2.1
1	D	528	GLU	2.1
1	C	280	TYR	2.1
1	D	533	ASP	2.1
1	D	788	SER	2.1
1	B	24	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	537	VAL	2.0
1	D	811	PHE	2.0
1	A	16	ARG	2.0
1	A	426	ARG	2.0
1	D	20	GLY	2.0
1	C	13	ILE	2.0
1	D	84	TYR	2.0
1	D	833	ARG	2.0
1	A	260	GLY	2.0
1	D	584	ILE	2.0
1	D	807	THR	2.0
1	A	281	PRO	2.0
1	D	604	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å ²)	Q<0.9
1	LLP	D	680	24/25	0.90	0.13	51,58,62,63	0
1	LLP	B	680	24/25	0.94	0.08	37,38,40,42	0
1	LLP	C	680	24/25	0.94	0.09	40,42,48,49	0
1	LLP	A	680	24/25	0.94	0.08	28,31,36,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	SO4	A	901	5/5	0.72	0.16	82,83,83,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	900	5/5	0.74	0.13	88,89,89,90	0
2	SO4	B	900	5/5	0.82	0.17	81,81,82,83	0
2	SO4	D	902	5/5	0.83	0.14	77,77,78,78	0
2	SO4	A	902	5/5	0.84	0.13	79,80,81,81	0
2	SO4	D	901	5/5	0.84	0.14	83,84,84,85	0
2	SO4	B	901	5/5	0.84	0.15	76,77,79,79	0
2	SO4	C	901	5/5	0.85	0.15	74,76,77,77	0
2	SO4	A	900	5/5	0.91	0.11	71,72,72,73	0
2	SO4	D	903	5/5	0.91	0.12	68,69,69,70	0
2	SO4	C	902	5/5	0.96	0.12	64,64,65,65	0
2	SO4	B	902	5/5	0.97	0.12	58,58,58,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.