



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:39 PM UTC

PDB ID : 2QLL / pdb_00002qll
Title : Human liver glycogen phosphorylase- GL complex
Authors : Pautsch, A.; Streicher, R.; Wissdorf, O.; Stadler, N.
Deposited on : 2007-07-13
Resolution : 2.56 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

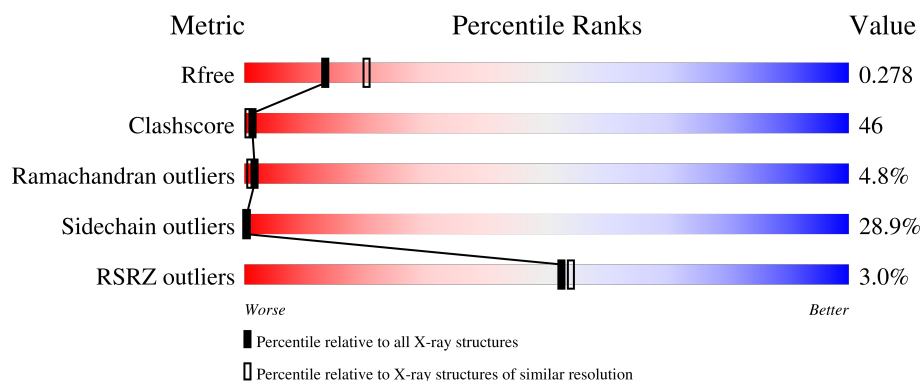
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	847	
2	B	4	

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
3	PLP	A	999	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6734 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, liver form.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	806	6529	4189	1115	1195	1	29	0	0	0

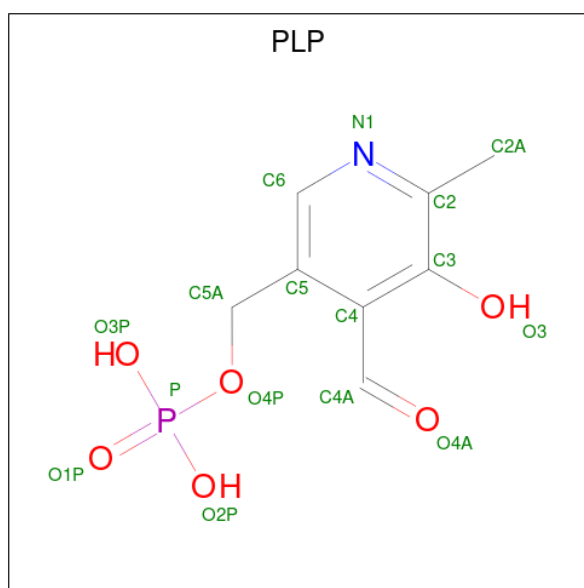
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	SEP	SER	modified residue	UNP P06737

- Molecule 2 is a protein called protein targeting to glycogen - GL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	4	36	25	4	7	0	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

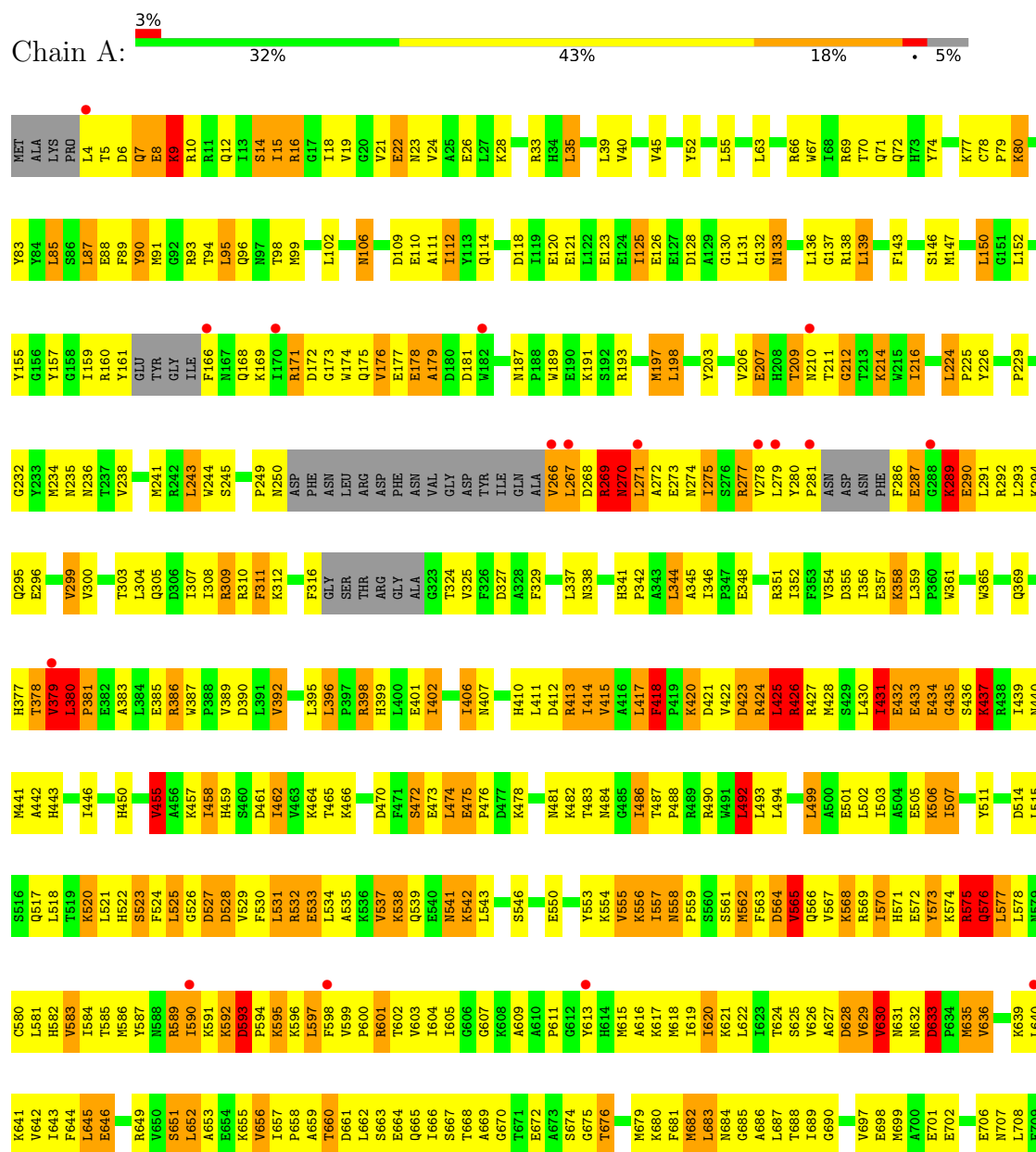
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	153	Total	O	0	0
			153	153		
4	B	1	Total	O	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glycogen phosphorylase, liver form





- Molecule 2: protein targeting to glycogen - GL



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.99Å 123.99Å 125.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.50 – 2.56 19.50 – 2.56	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.50-2.56) 97.3 (19.50-2.56)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.92 (at 2.56Å)	Xtriage
Refinement program	REFMAC, BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.203 , 0.276 (Not available) , 0.278	Depositor DCC
R_{free} test set	1769 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 84.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6734	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: PLP, SEP

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	0.61	0/6657	1.15	54/8994 (0.6%)
2	B	0.62	0/38	1.45	2/50 (4.0%)
All	All	0.61	0/6695	1.15	56/9044 (0.6%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	633	ASP	CA-C-N	14.02	133.56	119.82
1	A	633	ASP	C-N-CA	14.02	133.56	119.82
1	A	380	LEU	CA-C-N	12.43	135.38	119.84
1	A	380	LEU	C-N-CA	12.43	135.38	119.84
1	A	487	THR	CA-C-N	12.07	131.65	119.82
1	A	487	THR	C-N-CA	12.07	131.65	119.82
1	A	8	GLU	N-CA-C	-11.97	96.07	112.94
1	A	341	HIS	CA-C-N	-9.47	108.00	119.84
1	A	341	HIS	C-N-CA	-9.47	108.00	119.84
1	A	593	ASP	CA-C-N	9.05	131.15	119.84
1	A	593	ASP	C-N-CA	9.05	131.15	119.84
1	A	418	PHE	CA-C-N	8.73	130.75	119.84
1	A	418	PHE	C-N-CA	8.73	130.75	119.84
1	A	475	GLU	CA-C-N	8.18	130.07	119.84
1	A	475	GLU	C-N-CA	8.18	130.07	119.84
1	A	9	LYS	N-CA-C	-8.00	101.86	111.69
1	A	380	LEU	C-N-CD	-7.86	92.78	125.00
1	A	289	LYS	N-CA-C	-7.73	100.91	112.04
1	A	91	MET	N-CA-C	7.71	122.45	112.89
1	A	198	LEU	CA-C-N	7.55	128.66	120.13
1	A	198	LEU	C-N-CA	7.55	128.66	120.13
1	A	187	ASN	CA-C-N	-7.26	112.23	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	ASN	C-N-CA	-7.26	112.23	119.56
1	A	455	VAL	N-CA-C	6.96	118.78	112.17
1	A	754	GLN	CA-C-N	6.84	126.80	119.28
1	A	754	GLN	C-N-CA	6.84	126.80	119.28
1	A	346	ILE	CA-C-N	-6.67	112.75	119.56
1	A	346	ILE	C-N-CA	-6.67	112.75	119.56
1	A	565	VAL	N-CA-C	6.63	118.15	108.53
2	B	281	GLY	CA-C-N	6.49	127.95	119.84
2	B	281	GLY	C-N-CA	6.49	127.95	119.84
1	A	12	GLN	N-CA-C	-6.38	104.98	112.89
1	A	106	ASN	N-CA-C	6.10	118.01	111.36
1	A	379	VAL	N-CA-C	-6.09	104.57	110.42
1	A	179	ALA	N-CA-C	6.00	119.04	110.10
1	A	725	GLY	N-CA-C	-5.84	105.33	112.68
1	A	234	MET	N-CA-C	5.81	120.31	113.23
1	A	688	THR	N-CA-C	5.76	118.86	109.59
1	A	814	ASP	N-CA-C	-5.63	104.63	112.45
1	A	768	HIS	N-CA-C	5.62	119.90	111.81
1	A	24	VAL	N-CA-C	5.62	115.81	110.53
1	A	111	ALA	N-CA-C	-5.60	105.08	111.07
1	A	568	LYS	N-CA-C	-5.60	101.25	109.81
1	A	686	ALA	N-CA-C	-5.55	102.54	110.59
1	A	465	THR	N-CA-C	5.45	117.97	111.71
1	A	424	ARG	N-CA-C	-5.43	104.76	111.33
1	A	80	LYS	N-CA-C	-5.42	102.26	110.28
1	A	765	LEU	N-CA-C	-5.35	104.95	112.12
1	A	270	ASN	N-CA-C	-5.34	108.03	114.75
1	A	312	LYS	N-CA-C	-5.32	106.05	112.54
1	A	232	GLY	N-CA-C	-5.29	105.77	112.54
1	A	475	GLU	C-N-CD	-5.23	103.55	125.00
1	A	392	VAL	N-CA-C	-5.21	104.53	111.05
1	A	378	THR	N-CA-C	5.13	117.11	108.96
1	A	417	LEU	N-CA-C	5.09	117.56	111.71
1	A	431	ILE	N-CA-C	5.01	115.12	108.11

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	6529	0	6551	603	0
2	B	36	0	27	0	0
3	A	15	0	6	5	0
4	A	153	0	0	9	0
4	B	1	0	0	0	0
All	All	6734	0	6584	603	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 46.

All (603) 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:744:GLN:HG2	1:A:749:PHE:HD2	1.07	1.15
1:A:744:GLN:HG2	1:A:749:PHE:CD2	1.95	1.02
1:A:197:MET:HE2	1:A:224:LEU:HD22	1.39	1.01
1:A:566:GLN:HE22	1:A:576:GLN:HA	1.22	1.01
1:A:738:LEU:HG	1:A:742:ILE:HG12	1.44	0.99
1:A:723:LYS:HA	1:A:723:LYS:HE2	1.40	0.98
1:A:732:TYR:HE1	1:A:739:LYS:HA	1.28	0.98
1:A:748:GLY:HA3	1:A:755:PRO:HB3	1.47	0.97
1:A:241:MET:HE3	1:A:243:LEU:HD22	1.46	0.97
1:A:707:ASN:HD21	1:A:803:LYS:HE2	1.27	0.96
1:A:793:ASN:HD22	1:A:794:PRO:HD2	1.34	0.93
1:A:754:GLN:HG2	1:A:757:LEU:HB2	1.49	0.93
1:A:428:MET:HE3	1:A:470:ASP:HB3	1.51	0.92
1:A:541:ASN:N	1:A:541:ASN:HD22	1.67	0.92
1:A:171:ARG:HG2	1:A:176:VAL:HG11	1.54	0.90
1:A:616:ALA:HA	1:A:619:ILE:HD13	1.53	0.89
1:A:732:TYR:CE1	1:A:739:LYS:HA	2.07	0.88
1:A:541:ASN:HD22	1:A:541:ASN:H	1.23	0.87
1:A:622:LEU:HD12	1:A:761:ILE:HD13	1.58	0.85
1:A:428:MET:HE3	1:A:470:ASP:CB	2.06	0.85
1:A:751:SER:HB3	1:A:758:PHE:HE2	1.41	0.85
1:A:566:GLN:NE2	1:A:576:GLN:HA	1.90	0.84
1:A:574:LYS:HB2	1:A:576:GLN:NE2	1.93	0.84
1:A:355:ASP:OD1	1:A:398:ARG:HD3	1.78	0.83
1:A:324:THR:HB	1:A:327:ASP:OD1	1.79	0.83
1:A:732:TYR:CE1	1:A:739:LYS:HG2	2.13	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:LYS:HZ2	1:A:635:MET:HE3	1.45	0.82
1:A:566:GLN:HB2	1:A:664:GLU:HB2	1.62	0.81
1:A:241:MET:HE3	1:A:243:LEU:CD2	2.10	0.81
1:A:96:GLN:HB3	1:A:494:LEU:HD11	1.62	0.81
1:A:574:LYS:HE2	1:A:672:GLU:OE2	1.81	0.80
1:A:136:LEU:HD11	1:A:338:ASN:ND2	1.96	0.80
1:A:503:ILE:CG2	1:A:507:ILE:HD11	2.12	0.80
1:A:52:TYR:OH	1:A:126:GLU:HG3	1.83	0.79
1:A:562:MET:HB2	1:A:791:TYR:CE2	2.16	0.79
1:A:676:THR:HG22	1:A:680:LYS:HE3	1.64	0.79
1:A:521:LEU:HB3	1:A:802:LEU:HD11	1.64	0.79
1:A:146:SER:O	1:A:150:LEU:HB2	1.84	0.78
1:A:577:LEU:HD21	1:A:622:LEU:HD13	1.64	0.78
1:A:584:ILE:HG21	1:A:741:VAL:HG13	1.66	0.78
1:A:23:ASN:ND2	1:A:26:GLU:H	1.81	0.77
1:A:392:VAL:HG21	1:A:439:ILE:HD12	1.66	0.77
1:A:591:LYS:HZ2	1:A:635:MET:CE	1.98	0.77
1:A:458:ILE:O	1:A:462:ILE:HD12	1.85	0.77
1:A:506:LYS:HG3	1:A:530:PHE:CE1	2.21	0.76
1:A:23:ASN:HD21	1:A:26:GLU:H	1.35	0.75
1:A:139:LEU:HD11	1:A:484:ASN:HD21	1.51	0.75
1:A:492:LEU:HG	1:A:683:LEU:HD13	1.69	0.75
1:A:433:GLU:HA	1:A:437:LYS:HB3	1.68	0.74
1:A:507:ILE:HG21	1:A:520:LYS:HB2	1.70	0.74
1:A:782:LYS:HD2	1:A:782:LYS:O	1.87	0.74
1:A:538:LYS:O	1:A:542:LYS:HB2	1.88	0.74
1:A:584:ILE:HG22	1:A:741:VAL:HG22	1.67	0.74
1:A:763:ASN:O	1:A:767:TYR:HB2	1.88	0.74
1:A:723:LYS:HA	1:A:723:LYS:CE	2.17	0.73
1:A:565:VAL:CG1	1:A:660:THR:HB	2.17	0.73
1:A:669:ALA:HB1	1:A:715:ILE:HG12	1.70	0.73
1:A:738:LEU:CG	1:A:742:ILE:HG12	2.17	0.73
1:A:615:MET:HG3	1:A:619:ILE:HD11	1.70	0.72
1:A:531:LEU:HD21	1:A:799:THR:CG2	2.19	0.72
1:A:615:MET:O	1:A:619:ILE:HD12	1.89	0.72
1:A:581:LEU:HB3	1:A:777:TYR:HE1	1.53	0.72
1:A:303:THR:O	1:A:307:ILE:HD12	1.90	0.72
1:A:305:GLN:HG3	4:A:1022:HOH:O	1.90	0.72
1:A:575:ARG:C	1:A:576:GLN:HG2	2.15	0.72
1:A:16:ARG:HG3	1:A:16:ARG:HH11	1.54	0.71
1:A:558:ASN:HB3	1:A:561:SER:HB2	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:O	1:A:406:ILE:HD12	1.91	0.71
1:A:793:ASN:ND2	1:A:794:PRO:HD2	2.06	0.71
1:A:410:HIS:O	1:A:414:ILE:HD13	1.91	0.71
1:A:748:GLY:HA3	1:A:755:PRO:CB	2.20	0.70
1:A:777:TYR:O	1:A:781:VAL:HG23	1.91	0.70
1:A:582:HIS:CD2	1:A:784:GLN:HG3	2.26	0.70
1:A:616:ALA:HA	1:A:619:ILE:CD1	2.21	0.70
1:A:723:LYS:HE2	1:A:723:LYS:CA	2.20	0.70
1:A:225:PRO:HD3	1:A:244:TRP:CZ3	2.26	0.70
1:A:279:LEU:HG	1:A:280:TYR:HD2	1.57	0.69
1:A:412:ASP:O	1:A:415:VAL:HG23	1.92	0.69
1:A:687:LEU:HD21	1:A:801:VAL:HA	1.74	0.69
1:A:292:ARG:O	1:A:296:GLU:HG3	1.92	0.69
1:A:779:ALA:O	1:A:783:CYS:HB2	1.93	0.69
1:A:279:LEU:HG	1:A:280:TYR:CD2	2.27	0.69
1:A:541:ASN:H	1:A:541:ASN:ND2	1.87	0.69
1:A:707:ASN:HD21	1:A:803:LYS:CE	2.04	0.68
1:A:589:ARG:HG2	1:A:589:ARG:HH11	1.57	0.68
1:A:728:ALA:HB3	1:A:766:PHE:HD2	1.58	0.68
1:A:572:GLU:HG3	1:A:613:TYR:OH	1.93	0.68
1:A:721:LEU:HD23	1:A:721:LEU:O	1.92	0.68
1:A:80:LYS:HE2	1:A:825:TRP:O	1.93	0.68
1:A:828:GLU:OE1	1:A:829:PRO:HD2	1.94	0.68
1:A:7:GLN:OE1	1:A:7:GLN:N	2.26	0.68
1:A:728:ALA:HB3	1:A:766:PHE:CD2	2.28	0.68
1:A:506:LYS:HG3	1:A:530:PHE:HE1	1.59	0.68
1:A:633:ASP:OD2	1:A:635:MET:HB2	1.93	0.68
1:A:55:LEU:HD13	1:A:112:ILE:HD11	1.75	0.68
1:A:573:TYR:CZ	1:A:574:LYS:HE3	2.28	0.67
1:A:627:ALA:O	1:A:631:ASN:ND2	2.27	0.67
1:A:177:GLU:OE1	1:A:611:PRO:HB3	1.95	0.67
1:A:760:ASP:OD2	1:A:760:ASP:N	2.28	0.67
1:A:206:VAL:HG21	1:A:401:GLU:OE1	1.95	0.67
1:A:522:HIS:HD2	1:A:525:LEU:HD21	1.59	0.67
1:A:93:ARG:O	1:A:490:ARG:NH2	2.25	0.66
1:A:542:LYS:HA	1:A:659:ALA:HB1	1.77	0.66
1:A:16:ARG:HG3	1:A:16:ARG:NH1	2.10	0.66
1:A:515:LEU:HD23	1:A:809:GLY:HA2	1.76	0.66
1:A:542:LYS:HE3	1:A:661:ASP:OD2	1.96	0.66
1:A:752:PRO:O	1:A:755:PRO:HD3	1.96	0.66
1:A:736:PRO:HG2	1:A:737:GLU:H	1.61	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:LEU:HG	1:A:742:ILE:CG1	2.22	0.66
1:A:522:HIS:CD2	1:A:525:LEU:HD21	2.32	0.65
1:A:584:ILE:HG12	1:A:750:PHE:CZ	2.31	0.65
1:A:577:LEU:HD21	1:A:622:LEU:CD1	2.25	0.65
1:A:666:ILE:HG22	1:A:690:GLY:HA2	1.78	0.65
1:A:522:HIS:HA	1:A:525:LEU:HD22	1.77	0.65
1:A:793:ASN:HD22	1:A:794:PRO:CD	2.08	0.65
1:A:782:LYS:HD2	1:A:782:LYS:C	2.21	0.65
1:A:398:ARG:O	1:A:402:ILE:HD12	1.97	0.64
1:A:531:LEU:HD21	1:A:799:THR:HG22	1.77	0.64
1:A:635:MET:O	1:A:639:LYS:NZ	2.31	0.64
1:A:580:CYS:O	1:A:583:VAL:HB	1.96	0.64
1:A:304:LEU:HD12	1:A:348:GLU:HG2	1.79	0.64
1:A:503:ILE:HG23	1:A:507:ILE:HD11	1.80	0.64
1:A:157:TYR:OH	1:A:310:ARG:NH2	2.30	0.64
1:A:203:TYR:CE2	1:A:395:LEU:HD12	2.33	0.64
1:A:426:ARG:NH1	1:A:426:ARG:HG3	2.13	0.64
1:A:710:ILE:HG22	1:A:711:PHE:N	2.13	0.64
1:A:622:LEU:HD12	1:A:761:ILE:CD1	2.27	0.63
1:A:622:LEU:O	1:A:626:VAL:HG23	1.97	0.63
1:A:517:GLN:HG2	4:A:1004:HOH:O	1.97	0.63
1:A:761:ILE:HG22	1:A:765:LEU:CD2	2.28	0.63
1:A:174:TRP:CE3	1:A:621:LYS:HB2	2.33	0.63
1:A:268:ASP:C	1:A:270:ASN:H	2.07	0.63
1:A:626:VAL:O	1:A:630:VAL:HG13	1.97	0.63
1:A:6:ASP:O	1:A:9:LYS:HB2	1.98	0.63
1:A:69:ARG:HH11	1:A:72:GLN:HE22	1.46	0.63
1:A:656:VAL:CG2	1:A:657:ILE:N	2.62	0.63
1:A:63:LEU:HD21	1:A:229:PRO:HB2	1.79	0.63
1:A:352:ILE:O	1:A:356:ILE:HB	1.99	0.63
1:A:413:ARG:HH11	1:A:417:LEU:HD11	1.63	0.63
1:A:828:GLU:OE1	1:A:828:GLU:HA	1.98	0.63
1:A:810:LYS:O	1:A:815:ARG:NH1	2.28	0.63
1:A:52:TYR:CZ	1:A:126:GLU:HG3	2.33	0.63
1:A:568:LYS:HE3	1:A:665:GLN:OE1	1.98	0.63
1:A:455:VAL:H	1:A:459:HIS:HD2	1.45	0.62
1:A:589:ARG:HG2	1:A:589:ARG:NH1	2.12	0.62
1:A:683:LEU:HD23	1:A:808:SER:OG	1.99	0.62
1:A:152:LEU:HD22	1:A:827:VAL:HG13	1.81	0.62
1:A:680:LYS:NZ	3:A:999:PLP:C4A	2.62	0.62
1:A:653:ALA:O	1:A:657:ILE:HG13	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:ILE:HG22	1:A:746:ASP:N	2.14	0.62
1:A:683:LEU:HD23	1:A:808:SER:CB	2.30	0.62
1:A:171:ARG:HG2	1:A:176:VAL:CG1	2.27	0.62
1:A:398:ARG:O	1:A:398:ARG:HG3	1.97	0.62
1:A:420:LYS:O	1:A:422:VAL:HG23	1.98	0.62
1:A:428:MET:HE3	1:A:470:ASP:C	2.24	0.62
1:A:735:LEU:HD21	1:A:778:GLU:CD	2.24	0.62
1:A:582:HIS:O	1:A:582:HIS:ND1	2.31	0.62
1:A:241:MET:HG2	1:A:243:LEU:HD13	1.81	0.62
1:A:735:LEU:HD21	1:A:778:GLU:OE2	2.00	0.62
1:A:790:LEU:CD2	1:A:797:TRP:HA	2.29	0.62
1:A:139:LEU:HD22	1:A:143:PHE:CE1	2.34	0.62
1:A:666:ILE:HD12	1:A:666:ILE:O	2.00	0.62
1:A:304:LEU:HD12	1:A:348:GLU:CG	2.30	0.61
1:A:578:LEU:HD12	1:A:578:LEU:O	1.99	0.61
1:A:736:PRO:O	1:A:739:LYS:HB2	1.99	0.61
1:A:174:TRP:CZ3	1:A:621:LYS:HB2	2.35	0.61
1:A:751:SER:CB	1:A:758:PHE:HE2	2.13	0.61
1:A:584:ILE:CG2	1:A:741:VAL:HG13	2.30	0.61
1:A:85:LEU:CD2	1:A:303:THR:HG21	2.29	0.61
1:A:577:LEU:HG	1:A:619:ILE:HG23	1.82	0.61
1:A:738:LEU:HD11	1:A:742:ILE:HD11	1.82	0.61
1:A:575:ARG:O	1:A:577:LEU:N	2.29	0.61
1:A:741:VAL:HA	1:A:744:GLN:HB2	1.83	0.61
1:A:14:SEP:O2P	1:A:16:ARG:NH1	2.34	0.60
1:A:599:VAL:HG11	1:A:788:SER:CB	2.31	0.60
1:A:426:ARG:HG3	1:A:426:ARG:HH11	1.65	0.60
1:A:528:ASP:OD1	1:A:795:LYS:HD2	2.01	0.60
1:A:562:MET:HB2	1:A:791:TYR:HE2	1.66	0.60
1:A:550:GLU:OE2	1:A:556:LYS:NZ	2.29	0.60
1:A:87:LEU:HD13	1:A:279:LEU:CD1	2.32	0.60
1:A:746:ASP:HB2	1:A:762:ILE:CD1	2.31	0.60
1:A:748:GLY:CA	1:A:755:PRO:HB3	2.26	0.60
1:A:344:LEU:HD22	4:A:1068:HOH:O	2.02	0.60
1:A:143:PHE:O	1:A:147:MET:HG3	2.02	0.59
1:A:413:ARG:NH1	1:A:417:LEU:HD11	2.16	0.59
1:A:584:ILE:O	1:A:587:TYR:HB3	2.02	0.59
1:A:599:VAL:CG1	1:A:788:SER:HB3	2.32	0.59
1:A:744:GLN:O	1:A:749:PHE:HB3	2.02	0.59
1:A:159:ILE:HG22	1:A:160:ARG:N	2.17	0.59
1:A:527:ASP:OD2	1:A:529:VAL:HB	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:PHE:C	1:A:760:ASP:H	2.11	0.59
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.84	0.59
1:A:407:ASN:O	1:A:410:HIS:HB3	2.02	0.59
1:A:139:LEU:HD11	1:A:484:ASN:ND2	2.18	0.58
1:A:396:LEU:HB3	1:A:399:HIS:HB2	1.84	0.58
1:A:423:ASP:O	1:A:427:ARG:HG3	2.01	0.58
1:A:553:TYR:OH	1:A:646:GLU:N	2.30	0.58
1:A:486:ILE:O	1:A:488:PRO:HD3	2.03	0.58
1:A:599:VAL:HG11	1:A:788:SER:HB3	1.84	0.58
1:A:197:MET:CE	1:A:224:LEU:HD22	2.26	0.58
1:A:499:LEU:HD22	1:A:503:ILE:CD1	2.34	0.58
1:A:433:GLU:HG3	1:A:437:LYS:HD2	1.84	0.58
1:A:714:ARG:O	1:A:718:VAL:HG23	2.03	0.58
1:A:738:LEU:CD1	1:A:742:ILE:HD11	2.34	0.58
1:A:751:SER:HB3	1:A:758:PHE:CE2	2.30	0.58
1:A:756:ASP:O	1:A:759:LYS:HB2	2.04	0.58
1:A:193:ARG:HB2	1:A:225:PRO:HG2	1.86	0.58
1:A:557:ILE:O	1:A:559:PRO:HD3	2.03	0.58
1:A:754:GLN:HG2	1:A:757:LEU:CB	2.28	0.58
1:A:506:LYS:N	1:A:506:LYS:HD2	2.16	0.57
1:A:586:MET:O	1:A:590:ILE:HG13	2.04	0.57
1:A:746:ASP:C	1:A:748:GLY:H	2.12	0.57
1:A:96:GLN:HB3	1:A:494:LEU:CD1	2.33	0.57
1:A:177:GLU:OE2	1:A:617:LYS:NZ	2.35	0.57
1:A:203:TYR:CZ	1:A:395:LEU:HD12	2.39	0.57
1:A:417:LEU:HB2	1:A:418:PHE:CE1	2.39	0.57
1:A:761:ILE:HG22	1:A:765:LEU:HD23	1.87	0.57
1:A:442:ALA:O	1:A:446:ILE:HG13	2.04	0.57
1:A:731:TYR:O	1:A:735:LEU:HB2	2.02	0.57
1:A:35:LEU:HG	1:A:35:LEU:O	2.04	0.57
1:A:433:GLU:CG	1:A:437:LYS:HD2	2.35	0.57
1:A:118:ASP:HB3	4:A:1105:HOH:O	2.04	0.57
1:A:713:MET:HB3	1:A:717:ASP:HB3	1.86	0.57
1:A:735:LEU:HD21	1:A:778:GLU:OE1	2.04	0.57
1:A:266:VAL:C	1:A:267:LEU:HG	2.29	0.57
1:A:531:LEU:HD21	1:A:799:THR:HG23	1.86	0.57
1:A:506:LYS:NZ	1:A:530:PHE:HD1	2.03	0.56
1:A:562:MET:HE1	1:A:787:VAL:HG12	1.87	0.56
1:A:636:VAL:O	1:A:639:LYS:HD2	2.05	0.56
1:A:128:ASP:OD2	1:A:651:SER:OG	2.23	0.56
1:A:676:THR:HG22	3:A:999:PLP:C4A	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ARG:HG2	4:A:1076:HOH:O	2.06	0.56
1:A:492:LEU:HG	1:A:683:LEU:CD1	2.34	0.56
1:A:575:ARG:O	1:A:576:GLN:HG2	2.06	0.56
1:A:629:VAL:HG12	1:A:630:VAL:N	2.19	0.56
1:A:707:ASN:HD22	1:A:803:LYS:HB3	1.69	0.56
1:A:597:LEU:HD23	1:A:597:LEU:C	2.29	0.56
1:A:538:LYS:NZ	1:A:684:ASN:O	2.31	0.56
1:A:450:HIS:HE1	4:A:1117:HOH:O	1.89	0.56
1:A:584:ILE:HG23	1:A:750:PHE:HZ	1.70	0.56
1:A:15:ILE:HG22	1:A:18:ILE:HD11	1.88	0.55
1:A:566:GLN:HB2	1:A:664:GLU:CB	2.35	0.55
1:A:832:LEU:HG	1:A:832:LEU:O	2.04	0.55
1:A:793:ASN:HD22	1:A:793:ASN:C	2.14	0.55
1:A:6:ASP:OD2	1:A:6:ASP:N	2.39	0.55
1:A:591:LYS:NZ	1:A:635:MET:HE3	2.19	0.55
1:A:506:LYS:CG	1:A:530:PHE:HE1	2.18	0.55
1:A:584:ILE:CD1	1:A:745:ILE:HD11	2.36	0.55
1:A:225:PRO:HD3	1:A:244:TRP:HZ3	1.69	0.55
1:A:645:LEU:HD22	1:A:652:LEU:HD11	1.89	0.55
1:A:33:ARG:HD2	4:A:1134:HOH:O	2.06	0.55
1:A:619:ILE:HD12	1:A:619:ILE:H	1.70	0.55
1:A:168:GLN:NE2	1:A:607:GLY:O	2.39	0.55
1:A:354:VAL:O	1:A:358:LYS:HA	2.06	0.55
1:A:522:HIS:C	1:A:524:PHE:H	2.14	0.55
1:A:687:LEU:CD2	1:A:801:VAL:HG22	2.37	0.54
1:A:748:GLY:HA2	1:A:755:PRO:HA	1.89	0.54
1:A:764:MET:HE2	1:A:768:HIS:O	2.08	0.54
1:A:15:ILE:HA	1:A:18:ILE:HG12	1.89	0.54
1:A:434:GLU:HG3	1:A:435:GLY:H	1.72	0.54
1:A:392:VAL:HG21	1:A:439:ILE:CD1	2.36	0.54
1:A:565:VAL:HG13	1:A:660:THR:HB	1.89	0.54
1:A:698:GLU:O	1:A:702:GLU:HG2	2.07	0.54
1:A:721:LEU:CD2	1:A:726:TYR:HB2	2.37	0.54
1:A:816:THR:O	1:A:820:TYR:HD2	1.91	0.54
1:A:110:GLU:O	1:A:114:GLN:HG3	2.08	0.54
1:A:118:ASP:OD2	1:A:121:GLU:HG3	2.07	0.54
1:A:275:ILE:O	1:A:295:GLN:HG2	2.08	0.54
1:A:731:TYR:HB3	1:A:735:LEU:HD12	1.90	0.53
1:A:85:LEU:HD21	1:A:303:THR:HG21	1.90	0.53
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.89	0.53
1:A:287:GLU:HA	1:A:290:GLU:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ASP:O	1:A:9:LYS:HD3	2.09	0.53
1:A:160:ARG:HG2	1:A:160:ARG:HH11	1.73	0.53
1:A:455:VAL:HG23	1:A:674:SER:HB2	1.90	0.53
1:A:486:ILE:HD11	1:A:676:THR:HG23	1.90	0.53
1:A:685:GLY:HA2	1:A:805:ILE:HD11	1.89	0.53
1:A:761:ILE:O	1:A:765:LEU:HB2	2.08	0.53
1:A:716:ASP:O	1:A:719:ALA:N	2.41	0.53
1:A:574:LYS:HB2	1:A:576:GLN:HE21	1.71	0.53
1:A:622:LEU:HD23	1:A:622:LEU:C	2.34	0.53
1:A:757:LEU:O	1:A:760:ASP:OD2	2.27	0.53
1:A:198:LEU:HD22	1:A:305:GLN:NE2	2.23	0.53
1:A:526:GLY:O	1:A:528:ASP:N	2.41	0.53
1:A:531:LEU:CD2	1:A:799:THR:HG23	2.39	0.53
1:A:379:VAL:HG13	1:A:380:LEU:HD23	1.90	0.53
1:A:663:SER:HG	1:A:665:GLN:HE21	1.52	0.53
1:A:70:THR:HG22	1:A:74:TYR:CE2	2.44	0.53
1:A:713:MET:HE1	1:A:775:ALA:CB	2.39	0.53
1:A:89:PHE:O	1:A:131:LEU:HB2	2.09	0.52
1:A:389:VAL:HG13	1:A:437:LYS:O	2.10	0.52
1:A:515:LEU:O	1:A:518:LEU:HG	2.10	0.52
1:A:575:ARG:HD3	1:A:666:ILE:O	2.09	0.52
1:A:562:MET:HB2	1:A:791:TYR:CD2	2.44	0.52
1:A:742:ILE:HD13	1:A:742:ILE:N	2.24	0.52
1:A:615:MET:O	1:A:618:MET:HB2	2.09	0.52
1:A:83:TYR:CD1	1:A:157:TYR:HE1	2.27	0.52
1:A:769:ASP:OD2	1:A:772:LYS:N	2.43	0.52
1:A:627:ALA:HB2	1:A:642:VAL:CG1	2.40	0.52
1:A:410:HIS:HE1	1:A:428:MET:O	1.93	0.52
1:A:754:GLN:O	1:A:757:LEU:HB3	2.10	0.52
1:A:683:LEU:HD23	1:A:808:SER:HB2	1.91	0.51
1:A:710:ILE:O	1:A:711:PHE:HB3	2.09	0.51
1:A:160:ARG:HD3	1:A:226:TYR:CD2	2.45	0.51
1:A:395:LEU:O	1:A:396:LEU:HD13	2.10	0.51
1:A:407:ASN:ND2	1:A:431:ILE:HG23	2.25	0.51
1:A:570:ILE:HB	1:A:609:ALA:HB2	1.91	0.51
1:A:173:GLY:O	1:A:621:LYS:HA	2.10	0.51
1:A:601:ARG:O	1:A:640:LEU:HA	2.10	0.51
1:A:636:VAL:HA	1:A:639:LYS:HD2	1.91	0.51
1:A:63:LEU:CD2	1:A:229:PRO:HB2	2.40	0.51
1:A:575:ARG:HG2	1:A:578:LEU:HD23	1.92	0.51
1:A:718:VAL:O	1:A:722:ASP:OD2	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TYR:HB2	1:A:137:GLY:C	2.36	0.51
1:A:161:TYR:CD2	1:A:161:TYR:N	2.78	0.51
1:A:171:ARG:CG	1:A:176:VAL:HG11	2.35	0.51
1:A:386:ARG:NH1	1:A:386:ARG:HG3	2.26	0.51
1:A:633:ASP:O	1:A:636:VAL:HG23	2.11	0.51
1:A:506:LYS:NZ	1:A:530:PHE:CD1	2.78	0.51
1:A:529:VAL:O	1:A:532:ARG:HB2	2.11	0.51
1:A:656:VAL:HG22	1:A:657:ILE:N	2.25	0.51
1:A:780:TYR:CZ	1:A:784:GLN:NE2	2.79	0.51
1:A:424:ARG:O	1:A:427:ARG:HB2	2.11	0.50
1:A:522:HIS:CA	1:A:525:LEU:HD22	2.41	0.50
1:A:543:LEU:O	1:A:546:SER:HB2	2.11	0.50
1:A:732:TYR:OH	1:A:743:ASP:OD2	2.28	0.50
1:A:550:GLU:HG2	1:A:555:VAL:O	2.12	0.50
1:A:781:VAL:O	1:A:785:ASP:OD1	2.29	0.50
1:A:96:GLN:CB	1:A:494:LEU:HD11	2.39	0.50
1:A:430:LEU:HD22	1:A:443:HIS:HB3	1.93	0.50
1:A:558:ASN:O	1:A:561:SER:N	2.42	0.50
1:A:655:LYS:O	1:A:658:PRO:HD2	2.11	0.50
1:A:428:MET:CE	1:A:470:ASP:HB3	2.33	0.50
1:A:434:GLU:CG	1:A:435:GLY:H	2.23	0.50
1:A:457:LYS:HG3	1:A:698:GLU:OE2	2.11	0.50
1:A:567:VAL:HG23	1:A:567:VAL:O	2.11	0.50
1:A:272:ALA:O	1:A:275:ILE:HB	2.11	0.50
1:A:407:ASN:HD22	1:A:431:ILE:HG23	1.77	0.50
1:A:727:GLU:O	1:A:730:GLU:OE2	2.30	0.50
1:A:593:ASP:N	1:A:594:PRO:CD	2.75	0.50
1:A:713:MET:HB2	1:A:718:VAL:HG22	1.93	0.50
1:A:280:TYR:N	1:A:281:PRO:CD	2.74	0.49
1:A:176:VAL:HG22	1:A:176:VAL:O	2.12	0.49
1:A:386:ARG:HH11	1:A:386:ARG:CG	2.25	0.49
1:A:395:LEU:C	1:A:396:LEU:HD13	2.37	0.49
1:A:550:GLU:O	1:A:554:LYS:HA	2.12	0.49
1:A:16:ARG:HH11	1:A:16:ARG:CG	2.20	0.49
1:A:139:LEU:CD2	1:A:143:PHE:CE1	2.95	0.49
1:A:584:ILE:HD13	1:A:745:ILE:CD1	2.43	0.49
1:A:296:GLU:OE2	1:A:385:GLU:OE2	2.29	0.49
1:A:378:THR:OG1	1:A:380:LEU:HB2	2.12	0.49
1:A:769:ASP:OD1	1:A:773:VAL:HG23	2.13	0.49
1:A:411:LEU:O	1:A:415:VAL:HG22	2.13	0.49
1:A:426:ARG:HH11	1:A:426:ARG:CG	2.24	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ILE:HG21	1:A:639:LYS:HD3	1.94	0.49
1:A:666:ILE:CG2	1:A:690:GLY:HA2	2.42	0.49
1:A:515:LEU:O	1:A:809:GLY:HA3	2.12	0.49
1:A:539:GLN:O	1:A:543:LEU:N	2.43	0.49
1:A:599:VAL:HG13	1:A:599:VAL:O	2.13	0.49
1:A:613:TYR:CE1	1:A:615:MET:HB3	2.48	0.49
1:A:754:GLN:N	1:A:755:PRO:HD3	2.28	0.49
1:A:250:ASN:O	1:A:269:ARG:NH2	2.46	0.48
1:A:645:LEU:HD13	1:A:652:LEU:HD13	1.94	0.48
1:A:682:MET:HE2	1:A:804:ASN:O	2.12	0.48
1:A:159:ILE:HG12	1:A:299:VAL:HG13	1.94	0.48
1:A:203:TYR:CZ	1:A:395:LEU:CD1	2.95	0.48
1:A:616:ALA:O	1:A:620:ILE:HG13	2.13	0.48
1:A:530:PHE:HA	1:A:533:GLU:HG3	1.95	0.48
1:A:711:PHE:CD1	1:A:712:GLY:N	2.81	0.48
1:A:738:LEU:CD1	1:A:742:ILE:HG12	2.43	0.48
1:A:572:GLU:HB3	1:A:771:PHE:CE2	2.48	0.48
1:A:590:ILE:HD12	1:A:636:VAL:HG12	1.94	0.48
1:A:710:ILE:CG2	1:A:711:PHE:N	2.76	0.48
1:A:420:LYS:O	1:A:422:VAL:N	2.47	0.48
1:A:486:ILE:CD1	1:A:676:THR:HG23	2.43	0.48
1:A:582:HIS:NE2	1:A:784:GLN:HG3	2.26	0.48
1:A:751:SER:HB2	1:A:754:GLN:O	2.13	0.48
1:A:564:ASP:OD1	1:A:664:GLU:OE2	2.31	0.48
1:A:706:GLU:HG2	1:A:707:ASN:N	2.29	0.48
1:A:738:LEU:HD21	1:A:774:PHE:HD1	1.79	0.48
1:A:482:LYS:NZ	1:A:823:ASN:HB2	2.29	0.48
1:A:561:SER:HA	1:A:600:PRO:HB2	1.94	0.48
1:A:615:MET:C	1:A:619:ILE:HD12	2.39	0.48
1:A:620:ILE:O	1:A:624:THR:HG23	2.13	0.48
1:A:98:THR:O	1:A:102:LEU:HG	2.14	0.48
1:A:575:ARG:C	1:A:577:LEU:H	2.19	0.48
1:A:656:VAL:HG22	1:A:657:ILE:H	1.77	0.48
1:A:746:ASP:HB2	1:A:762:ILE:HD12	1.95	0.48
1:A:578:LEU:HD11	1:A:780:TYR:CD2	2.49	0.47
1:A:308:ILE:HD13	1:A:329:PHE:CE1	2.50	0.47
1:A:6:ASP:C	1:A:8:GLU:H	2.23	0.47
1:A:645:LEU:HD23	1:A:645:LEU:HA	1.65	0.47
1:A:736:PRO:HG2	1:A:737:GLU:HG3	1.96	0.47
1:A:580:CYS:O	1:A:583:VAL:N	2.45	0.47
1:A:627:ALA:HB2	1:A:642:VAL:HG12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLN:NE2	1:A:99:MET:CE	2.77	0.47
1:A:522:HIS:CD2	1:A:525:LEU:CD2	2.98	0.47
1:A:713:MET:HE1	1:A:775:ALA:HB3	1.96	0.47
1:A:736:PRO:CG	1:A:737:GLU:H	2.24	0.47
1:A:85:LEU:HD22	1:A:303:THR:HG21	1.95	0.47
1:A:481:ASN:O	1:A:482:LYS:HD3	2.15	0.47
1:A:578:LEU:HD11	1:A:780:TYR:HD2	1.77	0.47
1:A:580:CYS:SG	1:A:622:LEU:HD22	2.54	0.47
1:A:22:GLU:OE1	1:A:66:ARG:NH2	2.41	0.47
1:A:558:ASN:CB	1:A:561:SER:HB2	2.42	0.47
1:A:797:TRP:O	1:A:800:MET:N	2.47	0.47
1:A:69:ARG:NH1	1:A:72:GLN:HE22	2.10	0.47
1:A:286:PHE:O	1:A:289:LYS:HB2	2.15	0.47
1:A:425:LEU:O	1:A:427:ARG:N	2.48	0.47
1:A:727:GLU:C	1:A:729:LYS:H	2.22	0.47
1:A:782:LYS:NZ	1:A:786:LYS:HG2	2.30	0.47
1:A:440:ASN:C	1:A:440:ASN:HD22	2.21	0.47
1:A:78:CYS:SG	1:A:316:PHE:CD2	3.05	0.47
1:A:414:ILE:N	1:A:414:ILE:CD1	2.77	0.47
1:A:575:ARG:C	1:A:577:LEU:N	2.73	0.47
1:A:652:LEU:HD23	1:A:652:LEU:HA	1.73	0.47
1:A:732:TYR:CD1	1:A:739:LYS:HG2	2.49	0.47
1:A:506:LYS:HZ2	1:A:530:PHE:HD1	1.63	0.46
1:A:713:MET:CE	1:A:775:ALA:HB3	2.45	0.46
1:A:759:LYS:O	1:A:763:ASN:ND2	2.48	0.46
1:A:235:ASN:O	1:A:236:ASN:HB2	2.14	0.46
1:A:514:ASP:O	1:A:517:GLN:HB2	2.15	0.46
1:A:629:VAL:O	1:A:631:ASN:N	2.48	0.46
1:A:483:THR:O	1:A:815:ARG:NH2	2.46	0.46
1:A:676:THR:CG2	1:A:680:LYS:HE3	2.38	0.46
1:A:88:GLU:HG3	1:A:137:GLY:CA	2.45	0.46
1:A:178:GLU:HG3	1:A:179:ALA:N	2.30	0.46
1:A:600:PRO:HA	1:A:639:LYS:O	2.15	0.46
1:A:687:LEU:HD21	1:A:801:VAL:HG22	1.98	0.46
1:A:724:LYS:O	1:A:724:LYS:HD3	2.16	0.46
1:A:749:PHE:CD1	1:A:749:PHE:C	2.92	0.46
1:A:398:ARG:HG3	1:A:402:ILE:HD12	1.98	0.46
1:A:601:ARG:O	1:A:640:LEU:HD12	2.16	0.46
1:A:434:GLU:CG	1:A:435:GLY:N	2.78	0.46
1:A:537:VAL:O	1:A:541:ASN:ND2	2.48	0.46
1:A:571:HIS:CD2	1:A:613:TYR:CE2	3.03	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:CD1	1:A:377:HIS:CE1	2.97	0.46
1:A:88:GLU:HB3	1:A:279:LEU:CD2	2.45	0.46
1:A:378:THR:HG23	1:A:378:THR:O	2.16	0.46
1:A:499:LEU:HD22	1:A:503:ILE:HD11	1.96	0.46
1:A:768:HIS:CD2	1:A:768:HIS:H	2.33	0.46
1:A:592:LYS:HB3	1:A:592:LYS:HE3	1.31	0.46
1:A:745:ILE:CG2	1:A:746:ASP:N	2.77	0.46
1:A:515:LEU:CD2	1:A:809:GLY:HA2	2.45	0.45
1:A:645:LEU:CD1	1:A:656:VAL:HG11	2.46	0.45
1:A:676:THR:CG2	1:A:680:LYS:CE	2.94	0.45
1:A:94:THR:HG21	1:A:189:TRP:CD2	2.51	0.45
1:A:161:TYR:OH	1:A:279:LEU:HD13	2.16	0.45
1:A:772:LYS:N	1:A:772:LYS:HD3	2.32	0.45
1:A:296:GLU:O	1:A:299:VAL:HG23	2.16	0.45
1:A:535:ALA:HB2	1:A:798:ASN:OD1	2.17	0.45
1:A:636:VAL:O	1:A:639:LYS:HB2	2.17	0.45
1:A:758:PHE:C	1:A:760:ASP:N	2.75	0.45
1:A:67:TRP:HD1	1:A:238:VAL:HG12	1.80	0.45
1:A:266:VAL:O	1:A:267:LEU:HG	2.15	0.45
1:A:486:ILE:HD12	1:A:486:ILE:HA	1.74	0.45
1:A:584:ILE:HD13	1:A:745:ILE:HD12	1.98	0.45
1:A:270:ASN:ND2	1:A:271:LEU:N	2.64	0.45
1:A:411:LEU:O	1:A:414:ILE:N	2.50	0.45
1:A:810:LYS:O	1:A:810:LYS:HG3	2.09	0.45
1:A:765:LEU:HG	1:A:774:PHE:CZ	2.52	0.44
1:A:762:ILE:H	1:A:762:ILE:HG12	1.56	0.44
1:A:765:LEU:HD13	1:A:765:LEU:HA	1.90	0.44
1:A:5:THR:HA	1:A:8:GLU:OE2	2.17	0.44
1:A:528:ASP:CG	1:A:795:LYS:HD2	2.41	0.44
1:A:680:LYS:HZ1	3:A:999:PLP:C4A	2.30	0.44
1:A:172:ASP:O	1:A:621:LYS:HE2	2.17	0.44
1:A:379:VAL:HG13	1:A:380:LEU:CD2	2.47	0.44
1:A:425:LEU:HD22	1:A:425:LEU:HA	1.80	0.44
1:A:573:TYR:O	1:A:667:SER:OG	2.35	0.44
1:A:710:ILE:HG22	1:A:711:PHE:H	1.79	0.44
1:A:821:ALA:HB1	1:A:827:VAL:O	2.17	0.44
1:A:564:ASP:OD2	1:A:603:VAL:HG22	2.17	0.44
1:A:790:LEU:HD21	1:A:796:ALA:C	2.43	0.44
1:A:685:GLY:CA	1:A:805:ILE:HD11	2.47	0.44
1:A:90:TYR:CD1	1:A:132:GLY:HA3	2.52	0.44
1:A:90:TYR:H	1:A:137:GLY:C	2.25	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:TRP:CZ3	1:A:406:ILE:HG12	2.53	0.44
1:A:455:VAL:H	1:A:459:HIS:CD2	2.32	0.44
1:A:584:ILE:CG2	1:A:741:VAL:HG22	2.45	0.44
1:A:464:LYS:HG3	1:A:472:SER:HB3	2.00	0.43
1:A:562:MET:CB	1:A:791:TYR:CE2	2.97	0.43
1:A:727:GLU:C	1:A:729:LYS:N	2.76	0.43
1:A:15:ILE:HA	1:A:18:ILE:CG1	2.48	0.43
1:A:118:ASP:OD1	1:A:120:GLU:HB2	2.18	0.43
1:A:118:ASP:CG	1:A:121:GLU:HG3	2.43	0.43
1:A:290:GLU:O	1:A:293:LEU:N	2.50	0.43
1:A:520:LYS:O	1:A:523:SER:HB2	2.19	0.43
1:A:584:ILE:O	1:A:587:TYR:N	2.51	0.43
1:A:711:PHE:CD1	1:A:711:PHE:C	2.95	0.43
1:A:765:LEU:HA	1:A:769:ASP:HB2	1.99	0.43
1:A:507:ILE:CG2	1:A:520:LYS:HB2	2.44	0.43
1:A:562:MET:HB3	1:A:601:ARG:HG2	2.00	0.43
1:A:311:PHE:CD2	1:A:311:PHE:C	2.97	0.43
1:A:680:LYS:HE3	3:A:999:PLP:C4A	2.49	0.43
1:A:682:MET:HG2	1:A:808:SER:HB3	2.01	0.43
1:A:782:LYS:HZ1	1:A:786:LYS:HG2	1.83	0.43
1:A:431:ILE:HD11	1:A:433:GLU:HG3	1.99	0.43
1:A:440:ASN:C	1:A:440:ASN:ND2	2.77	0.43
1:A:522:HIS:C	1:A:524:PHE:N	2.75	0.43
1:A:575:ARG:CG	1:A:578:LEU:HB3	2.48	0.43
1:A:593:ASP:H	1:A:594:PRO:HD3	1.82	0.43
1:A:733:GLU:OE1	1:A:739:LYS:HE3	2.18	0.43
1:A:136:LEU:CD1	1:A:338:ASN:ND2	2.77	0.43
1:A:561:SER:HB3	1:A:602:THR:OG1	2.19	0.43
1:A:732:TYR:CZ	1:A:739:LYS:HE2	2.52	0.43
1:A:224:LEU:O	1:A:244:TRP:HA	2.19	0.43
1:A:274:ASN:HB3	1:A:291:LEU:HD13	1.99	0.43
1:A:304:LEU:CD1	1:A:348:GLU:CG	2.97	0.43
1:A:738:LEU:CD1	1:A:742:ILE:CD1	2.96	0.43
1:A:740:LEU:HB3	1:A:741:VAL:H	1.56	0.43
1:A:660:THR:HG21	1:A:681:PHE:HE1	1.83	0.43
1:A:712:GLY:H	1:A:779:ALA:HB1	1.83	0.43
1:A:761:ILE:HG22	1:A:765:LEU:HD22	2.00	0.43
1:A:697:VAL:O	1:A:701:GLU:HG3	2.19	0.42
1:A:16:ARG:HD2	4:A:1144:HOH:O	2.18	0.42
1:A:575:ARG:HG2	1:A:578:LEU:HB3	2.00	0.42
1:A:716:ASP:HA	1:A:719:ALA:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ARG:HA	1:A:138:ARG:HD2	1.86	0.42
1:A:159:ILE:CG2	1:A:160:ARG:N	2.80	0.42
1:A:541:ASN:N	1:A:541:ASN:ND2	2.40	0.42
1:A:584:ILE:CG2	1:A:750:PHE:HZ	2.32	0.42
1:A:645:LEU:HD22	1:A:652:LEU:CD1	2.49	0.42
1:A:633:ASP:OD1	1:A:636:VAL:HG22	2.19	0.42
1:A:754:GLN:HG3	1:A:756:ASP:OD2	2.19	0.42
1:A:293:LEU:HD13	1:A:387:TRP:CD2	2.54	0.42
1:A:455:VAL:HA	1:A:482:LYS:O	2.19	0.42
1:A:15:ILE:O	1:A:19:VAL:HG12	2.20	0.42
1:A:198:LEU:HD22	1:A:305:GLN:HE21	1.84	0.42
1:A:268:ASP:O	1:A:270:ASN:N	2.51	0.42
1:A:386:ARG:NH1	1:A:386:ARG:CG	2.81	0.42
1:A:472:SER:O	1:A:476:PRO:HA	2.19	0.42
1:A:6:ASP:O	1:A:9:LYS:N	2.52	0.42
1:A:268:ASP:C	1:A:270:ASN:N	2.74	0.42
1:A:270:ASN:C	1:A:272:ALA:N	2.76	0.42
1:A:515:LEU:CG	1:A:809:GLY:HA2	2.50	0.42
1:A:630:VAL:HG21	1:A:642:VAL:HG23	2.02	0.42
1:A:718:VAL:C	1:A:720:ALA:H	2.26	0.42
1:A:774:PHE:HA	1:A:777:TYR:HB2	2.02	0.42
1:A:207:GLU:HB2	1:A:216:ILE:HD13	2.02	0.42
1:A:522:HIS:HD2	1:A:525:LEU:CD2	2.28	0.42
1:A:793:ASN:ND2	1:A:793:ASN:C	2.77	0.42
1:A:357:GLU:OE2	1:A:357:GLU:HA	2.18	0.42
1:A:571:HIS:CD2	1:A:613:TYR:HE2	2.37	0.42
1:A:577:LEU:HD23	1:A:577:LEU:HA	1.82	0.42
1:A:71:GLN:NE2	1:A:71:GLN:N	2.68	0.42
1:A:160:ARG:HG2	1:A:160:ARG:NH1	2.35	0.42
1:A:224:LEU:HA	1:A:225:PRO:HD2	1.95	0.42
1:A:511:TYR:N	4:A:1004:HOH:O	2.52	0.42
1:A:732:TYR:HA	1:A:738:LEU:HD23	2.02	0.42
1:A:772:LYS:HD3	1:A:772:LYS:H	1.85	0.42
1:A:432:GLU:O	1:A:437:LYS:HA	2.20	0.41
1:A:670:GLY:CA	1:A:715:ILE:CD1	2.98	0.41
1:A:676:THR:CG2	3:A:999:PLP:C4A	2.98	0.41
1:A:83:TYR:CD1	1:A:157:TYR:CE1	3.08	0.41
1:A:524:PHE:N	1:A:524:PHE:CD1	2.88	0.41
1:A:627:ALA:C	1:A:631:ASN:HD22	2.28	0.41
1:A:133:ASN:ND2	1:A:133:ASN:C	2.78	0.41
1:A:173:GLY:O	1:A:624:THR:HG21	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LEU:HA	1:A:381:PRO:HD2	1.51	0.41
1:A:765:LEU:HG	1:A:774:PHE:HZ	1.85	0.41
1:A:74:TYR:O	1:A:79:PRO:HD3	2.20	0.41
1:A:605:ILE:O	1:A:644:PHE:HA	2.21	0.41
1:A:628:ASP:O	1:A:632:ASN:OD1	2.39	0.41
1:A:125:ILE:HD13	1:A:125:ILE:HA	1.92	0.41
1:A:539:GLN:O	1:A:543:LEU:HG	2.20	0.41
1:A:146:SER:OG	1:A:814:ASP:OD2	2.29	0.41
1:A:585:THR:O	1:A:589:ARG:HD3	2.20	0.41
1:A:724:LYS:O	1:A:724:LYS:HE2	2.20	0.41
1:A:790:LEU:CD2	1:A:797:TRP:CA	2.98	0.41
1:A:828:GLU:HA	1:A:829:PRO:HD2	1.82	0.41
1:A:598:PHE:CD2	1:A:598:PHE:C	2.99	0.41
1:A:270:ASN:C	1:A:272:ALA:H	2.29	0.41
1:A:293:LEU:HD12	1:A:293:LEU:HA	1.95	0.41
1:A:738:LEU:CD1	1:A:742:ILE:CG1	2.98	0.41
1:A:70:THR:HB	1:A:71:GLN:NE2	2.36	0.41
1:A:206:VAL:CG1	1:A:398:ARG:HB2	2.51	0.41
1:A:270:ASN:ND2	1:A:270:ASN:C	2.78	0.41
1:A:272:ALA:O	1:A:273:GLU:C	2.63	0.41
1:A:277:ARG:C	1:A:278:VAL:HG13	2.46	0.41
1:A:300:VAL:HG13	1:A:345:ALA:HA	2.02	0.41
1:A:573:TYR:HE1	1:A:672:GLU:OE2	2.04	0.41
1:A:713:MET:CE	1:A:775:ALA:CB	2.99	0.41
1:A:294:LYS:HD3	1:A:395:LEU:HD11	2.02	0.41
1:A:486:ILE:HD11	1:A:676:THR:CG2	2.51	0.41
1:A:511:TYR:HA	1:A:514:ASP:O	2.21	0.41
1:A:670:GLY:CA	1:A:715:ILE:HD13	2.51	0.41
1:A:209:THR:HG23	1:A:212:GLY:O	2.21	0.40
1:A:580:CYS:HA	1:A:583:VAL:HB	2.03	0.40
1:A:615:MET:O	1:A:618:MET:N	2.49	0.40
1:A:571:HIS:CE1	1:A:573:TYR:H	2.39	0.40
1:A:580:CYS:C	1:A:583:VAL:H	2.29	0.40
1:A:622:LEU:C	1:A:622:LEU:CD2	2.94	0.40
1:A:538:LYS:HA	1:A:538:LYS:HD3	1.72	0.40
1:A:542:LYS:HG3	1:A:563:PHE:CD2	2.56	0.40
1:A:206:VAL:HA	1:A:214:LYS:O	2.21	0.40
1:A:361:TRP:CE3	1:A:361:TRP:O	2.74	0.40
1:A:506:LYS:HD2	1:A:506:LYS:HA	1.86	0.40
1:A:40:VAL:O	1:A:40:VAL:HG12	2.22	0.40
1:A:515:LEU:C	1:A:517:GLN:H	2.30	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:CYS:SG	1:A:622:LEU:CD2	3.09	0.40
1:A:726:TYR:CD2	1:A:726:TYR:C	2.99	0.40
1:A:757:LEU:O	1:A:757:LEU:HD12	2.21	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	795/847 (94%)	662 (83%)	95 (12%)	38 (5%)	2	1
2	B	2/4 (50%)	2 (100%)	0	0	100	100
All	All	797/851 (94%)	664 (83%)	95 (12%)	38 (5%)	2	1

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	PRO
1	A	421	ASP
1	A	425	LEU
1	A	527	ASP
1	A	558	ASN
1	A	593	ASP
1	A	595	LYS
1	A	629	VAL
1	A	740	LEU
1	A	212	GLY
1	A	269	ARG
1	A	383	ALA
1	A	426	ARG
1	A	437	LYS
1	A	630	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	767	TYR
1	A	797	TRP
1	A	95	LEU
1	A	342	PRO
1	A	520	LYS
1	A	736	PRO
1	A	747	ASN
1	A	575	ARG
1	A	721	LEU
1	A	728	ALA
1	A	249	PRO
1	A	434	GLU
1	A	435	GLY
1	A	597	LEU
1	A	729	LYS
1	A	474	LEU
1	A	492	LEU
1	A	576	GLN
1	A	711	PHE
1	A	130	GLY
1	A	675	GLY
1	A	773	VAL
1	A	380	LEU

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	704/739 (95%)	500 (71%)	204 (29%)	0	0
2	B	3/3 (100%)	3 (100%)	0	100	100
All	All	707/742 (95%)	503 (71%)	204 (29%)	0	0

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	7	GLN
1	A	9	LYS
1	A	10	ARG
1	A	15	ILE
1	A	16	ARG
1	A	21	VAL
1	A	22	GLU
1	A	28	LYS
1	A	35	LEU
1	A	39	LEU
1	A	45	VAL
1	A	77	LYS
1	A	85	LEU
1	A	87	LEU
1	A	90	TYR
1	A	95	LEU
1	A	106	ASN
1	A	109	ASP
1	A	112	ILE
1	A	123	GLU
1	A	125	ILE
1	A	133	ASN
1	A	139	LEU
1	A	150	LEU
1	A	155	TYR
1	A	166	PHE
1	A	169	LYS
1	A	171	ARG
1	A	176	VAL
1	A	178	GLU
1	A	181	ASP
1	A	191	LYS
1	A	197	MET
1	A	207	GLU
1	A	209	THR
1	A	210	ASN
1	A	211	THR
1	A	214	LYS
1	A	216	ILE
1	A	224	LEU
1	A	243	LEU
1	A	245	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	266	VAL
1	A	267	LEU
1	A	269	ARG
1	A	270	ASN
1	A	271	LEU
1	A	275	ILE
1	A	277	ARG
1	A	287	GLU
1	A	289	LYS
1	A	290	GLU
1	A	299	VAL
1	A	309	ARG
1	A	311	PHE
1	A	325	VAL
1	A	337	LEU
1	A	344	LEU
1	A	351	ARG
1	A	358	LYS
1	A	359	LEU
1	A	369	GLN
1	A	379	VAL
1	A	380	LEU
1	A	386	ARG
1	A	390	ASP
1	A	396	LEU
1	A	398	ARG
1	A	402	ILE
1	A	406	ILE
1	A	413	ARG
1	A	414	ILE
1	A	415	VAL
1	A	418	PHE
1	A	420	LYS
1	A	423	ASP
1	A	425	LEU
1	A	426	ARG
1	A	431	ILE
1	A	432	GLU
1	A	433	GLU
1	A	436	SER
1	A	437	LYS
1	A	441	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	455	VAL
1	A	458	ILE
1	A	461	ASP
1	A	462	ILE
1	A	466	LYS
1	A	472	SER
1	A	473	GLU
1	A	474	LEU
1	A	475	GLU
1	A	478	LYS
1	A	486	ILE
1	A	492	LEU
1	A	493	LEU
1	A	499	LEU
1	A	501	GLU
1	A	502	LEU
1	A	505	GLU
1	A	506	LYS
1	A	507	ILE
1	A	523	SER
1	A	525	LEU
1	A	528	ASP
1	A	531	LEU
1	A	532	ARG
1	A	533	GLU
1	A	534	LEU
1	A	537	VAL
1	A	538	LYS
1	A	541	ASN
1	A	542	LYS
1	A	555	VAL
1	A	556	LYS
1	A	557	ILE
1	A	562	MET
1	A	564	ASP
1	A	565	VAL
1	A	569	ARG
1	A	570	ILE
1	A	573	TYR
1	A	575	ARG
1	A	576	GLN
1	A	577	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	583	VAL
1	A	589	ARG
1	A	590	ILE
1	A	592	LYS
1	A	593	ASP
1	A	595	LYS
1	A	596	LYS
1	A	601	ARG
1	A	604	ILE
1	A	620	ILE
1	A	625	SER
1	A	628	ASP
1	A	630	VAL
1	A	633	ASP
1	A	635	MET
1	A	636	VAL
1	A	641	LYS
1	A	643	ILE
1	A	645	LEU
1	A	646	GLU
1	A	649	ARG
1	A	651	SER
1	A	652	LEU
1	A	656	VAL
1	A	660	THR
1	A	662	LEU
1	A	668	THR
1	A	676	THR
1	A	679	MET
1	A	682	MET
1	A	683	LEU
1	A	689	ILE
1	A	699	MET
1	A	708	LEU
1	A	713	MET
1	A	715	ILE
1	A	717	ASP
1	A	718	VAL
1	A	721	LEU
1	A	723	LYS
1	A	724	LYS
1	A	726	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	729	LYS
1	A	733	GLU
1	A	737	GLU
1	A	740	LEU
1	A	742	ILE
1	A	744	GLN
1	A	745	ILE
1	A	751	SER
1	A	753	LYS
1	A	754	GLN
1	A	757	LEU
1	A	759	LYS
1	A	760	ASP
1	A	762	ILE
1	A	764	MET
1	A	765	LEU
1	A	768	HIS
1	A	770	ARG
1	A	772	LYS
1	A	774	PHE
1	A	778	GLU
1	A	782	LYS
1	A	786	LYS
1	A	789	GLN
1	A	790	LEU
1	A	795	LYS
1	A	803	LYS
1	A	810	LYS
1	A	815	ARG
1	A	817	ILE
1	A	822	GLN
1	A	827	VAL
1	A	828	GLU
1	A	832	LEU
1	A	833	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	71	GLN
1	A	72	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	73	HIS
1	A	133	ASN
1	A	167	ASN
1	A	250	ASN
1	A	305	GLN
1	A	369	GLN
1	A	376	ASN
1	A	399	HIS
1	A	407	ASN
1	A	408	GLN
1	A	410	HIS
1	A	440	ASN
1	A	450	HIS
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	522	HIS
1	A	541	ASN
1	A	547	GLN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	707	ASN
1	A	747	ASN
1	A	763	ASN
1	A	768	HIS
1	A	789	GLN
1	A	793	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
1	SEP	A	14	1	8,9,10	1.15	1 (12%)	7,12,14	3.25	3 (42%)

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	SEP	A	14	1	-	2/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	SEP	P-O3P	-2.07	1.47	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	SEP	OG-CB-CA	7.56	115.50	108.14
1	A	14	SEP	O2P-P-OG	2.80	113.96	106.67
1	A	14	SEP	O3P-P-OG	2.77	113.90	106.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	14	SEP	N-CA-CB-OG
1	A	14	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	14	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
3	PLP	A	999	-	15,15,16	4.31	6 (40%)	21,22,23	6.82	14 (66%)

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
3	PLP	A	999	-	-	3/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	C5-C4	-14.38	1.24	1.40
3	A	999	PLP	C6-N1	5.16	1.44	1.34
3	A	999	PLP	C5A-C5	3.55	1.60	1.50
3	A	999	PLP	O3-C3	-3.35	1.29	1.36
3	A	999	PLP	C3-C2	-2.67	1.38	1.41
3	A	999	PLP	P-O2P	2.17	1.62	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	PLP	C4A-C4-C5	-22.17	98.09	120.94
3	A	999	PLP	C5A-C5-C6	11.45	138.02	119.36
3	A	999	PLP	C4A-C4-C3	11.16	139.13	120.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	PLP	C5A-C5-C4	-7.91	107.04	122.64
3	A	999	PLP	O2P-P-O4P	-6.71	89.17	106.67
3	A	999	PLP	C3-C2-N1	-5.34	114.23	120.96
3	A	999	PLP	C6-C5-C4	-3.84	114.94	118.10
3	A	999	PLP	O3P-P-O2P	3.78	121.97	107.80
3	A	999	PLP	C4-C3-C2	3.69	125.40	119.89
3	A	999	PLP	C3-C4-C5	3.49	122.78	118.59
3	A	999	PLP	C2A-C2-C3	2.98	124.28	120.80
3	A	999	PLP	O3P-P-O4P	-2.94	99.00	106.67
3	A	999	PLP	O3P-P-O1P	2.85	121.95	110.83
3	A	999	PLP	C2A-C2-N1	2.04	121.49	117.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	PLP	C5A-O4P-P-O2P
3	A	999	PLP	C5A-O4P-P-O3P
3	A	999	PLP	C5A-O4P-P-O1P

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	PLP	5	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	805/847 (95%)	0.20	24 (2%)	52	54	27, 62, 109, 130	0
2	B	4/4 (100%)	-0.03	0	100	100	42, 44, 51, 59	0
All	All	809/851 (95%)	0.20	24 (2%)	52	54	27, 61, 109, 130	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	GLY	4.0
1	A	590	ILE	3.7
1	A	279	LEU	3.2
1	A	266	VAL	3.0
1	A	750	PHE	2.9
1	A	170	ILE	2.8
1	A	278	VAL	2.6
1	A	281	PRO	2.6
1	A	757	LEU	2.6
1	A	745	ILE	2.6
1	A	751	SER	2.5
1	A	267	LEU	2.5
1	A	4	LEU	2.4
1	A	758	PHE	2.4
1	A	756	ASP	2.3
1	A	210	ASN	2.2
1	A	182	TRP	2.2
1	A	271	LEU	2.2
1	A	166	PHE	2.2
1	A	379	VAL	2.1
1	A	640	LEU	2.0
1	A	613	TYR	2.0
1	A	598	PHE	2.0
1	A	728	ALA	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($\text{\AA}^2$)	Q<0.9
1	SEP	A	14	10/11	0.98	0.05	36,42,43,44	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($\text{\AA}^2$)	Q<0.9
3	PLP	A	999	15/16	0.93	0.07	51,56,80,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.