



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:37 AM UTC

PDB ID : 1JN0 / pdb_00001jn0
Title : Crystal structure of the non-regulatory A4 isoform of spinach chloroplast glyceraldehyde-3-phosphate dehydrogenase complexed with NADP
Authors : Fermani, S.; Ripamonti, A.; Sabatino, P.; Zanotti, G.; Scagliarini, S.; Sparla, F.; Trost, P.; Pupillo, P.
Deposited on : 2001-07-21
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

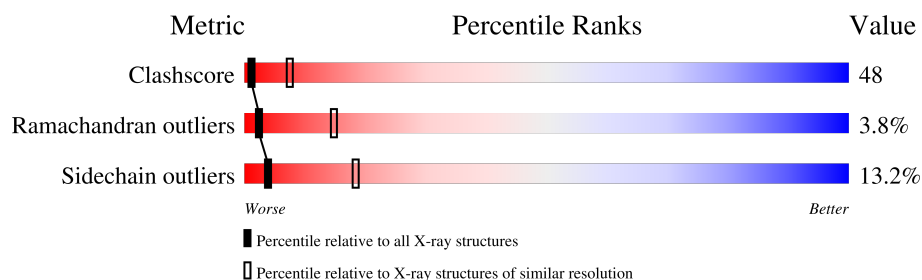
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	335	37% 49% 12% .
1	B	335	38% 48% 12% .
1	O	335	39% 45% 13% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7949 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 GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	334	Total	C	N	O	S	0	0	0
			2521	1589	439	482	11			
1	A	334	Total	C	N	O	S	0	0	0
			2521	1589	439	482	11			
1	B	334	Total	C	N	O	S	0	0	0
			2521	1589	439	482	11			

There are 6 discrepancies between the modelled and reference sequences:

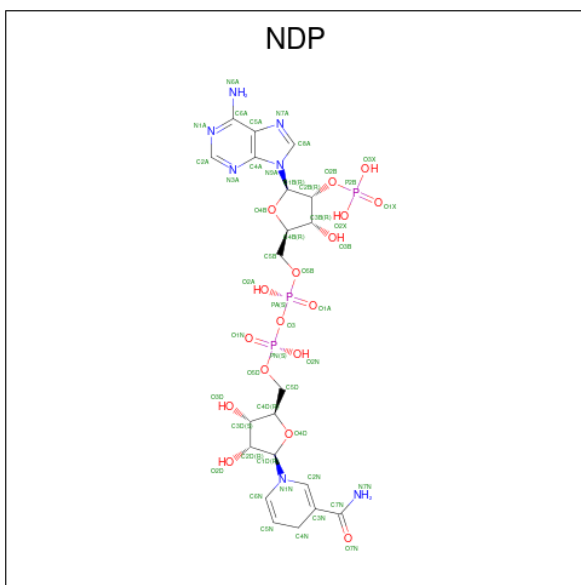
Chain	Residue	Modelled	Actual	Comment	Reference
O	?	-	ARG	deletion	UNP P19866
O	?	-	ASP	deletion	UNP P19866
A	?	-	ARG	deletion	UNP P19866
A	?	-	ASP	deletion	UNP P19866
B	?	-	ARG	deletion	UNP P19866
B	?	-	ASP	deletion	UNP P19866

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



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

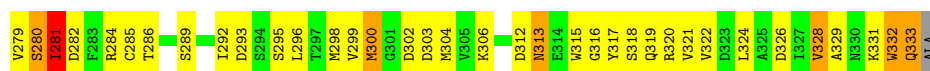
- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	O	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

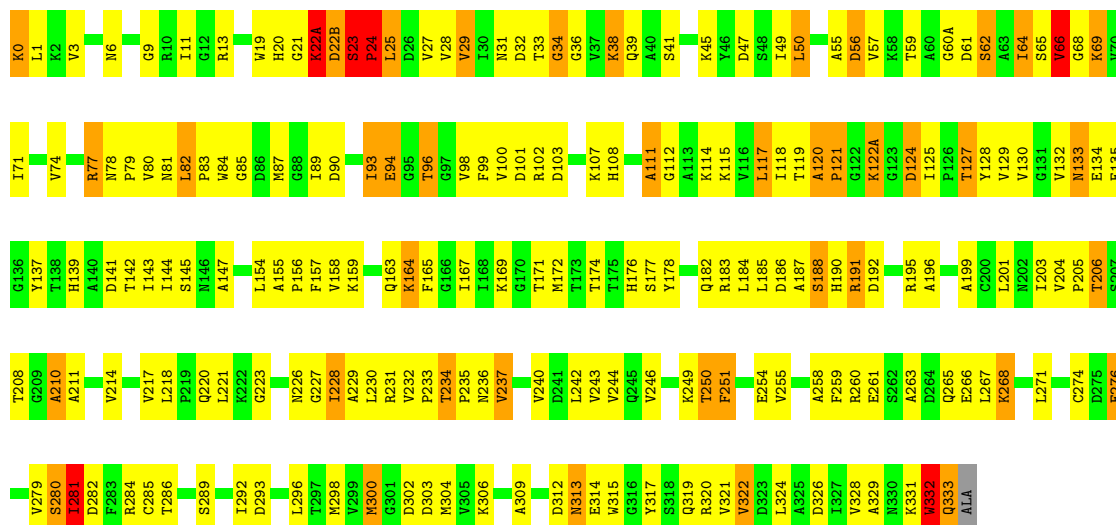
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	O	87	Total O 87 87	0	0
4	A	65	Total O 65 65	0	0
4	B	60	Total O 60 60	0	0



• Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE A

Chain B: 38% 48% 12%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	146.25Å 182.18Å 106.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.58 – 3.00	Depositor
% Data completeness (in resolution range)	93.0 (49.58-3.00)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.213 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7949	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NDP

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	0.74	4/2562 (0.2%)	1.14	21/3479 (0.6%)
1	B	0.65	3/2562 (0.1%)	1.13	26/3479 (0.7%)
1	O	0.77	5/2562 (0.2%)	1.20	28/3479 (0.8%)
All	All	0.72	12/7686 (0.2%)	1.15	75/10437 (0.7%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	333	GLN	CD-OE1	-8.78	1.06	1.23
1	O	332	TRP	CA-C	8.14	1.63	1.52
1	A	333	GLN	CD-OE1	-7.48	1.09	1.23
1	A	260	ARG	CA-C	7.02	1.62	1.52
1	B	333	GLN	CD-OE1	-6.57	1.11	1.23
1	O	19	TRP	CA-C	-6.54	1.44	1.52
1	O	266	GLU	CD-OE1	-6.23	1.13	1.25
1	B	331	LYS	C-O	-6.03	1.16	1.24
1	A	333	GLN	C-O	-6.00	1.11	1.23
1	O	19	TRP	CA-CB	-5.98	1.43	1.53
1	A	328	VAL	C-N	5.81	1.41	1.33
1	B	332	TRP	C-O	-5.37	1.17	1.24

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	19	TRP	CA-CB-CG	12.36	137.08	113.60
1	A	82	LEU	CA-C-N	8.83	130.88	119.84
1	A	82	LEU	C-N-CA	8.83	130.88	119.84
1	O	234	THR	CA-C-N	8.73	128.05	118.97
1	O	234	THR	C-N-CA	8.73	128.05	118.97
1	O	82	LEU	CA-C-N	8.64	130.63	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	82	LEU	C-N-CA	8.64	130.63	119.84
1	O	22(B)	ASP	N-CA-C	8.62	121.91	111.40
1	B	234	THR	CA-C-N	8.43	127.74	118.97
1	B	234	THR	C-N-CA	8.43	127.74	118.97
1	A	22(B)	ASP	N-CA-C	8.33	121.56	111.40
1	B	82	LEU	CA-C-N	8.32	130.24	119.84
1	B	82	LEU	C-N-CA	8.32	130.24	119.84
1	B	22(B)	ASP	N-CA-C	8.30	121.53	111.40
1	O	19	TRP	CB-CG-CD1	-8.30	114.45	126.90
1	B	69	LYS	N-CA-C	8.09	121.91	110.50
1	A	69	LYS	N-CA-C	7.75	121.44	110.50
1	O	19	TRP	CB-CG-CD2	7.75	137.65	126.80
1	A	234	THR	CA-C-N	7.69	126.97	118.97
1	A	234	THR	C-N-CA	7.69	126.97	118.97
1	B	23	SER	CA-C-N	7.66	129.42	119.84
1	B	23	SER	C-N-CA	7.66	129.42	119.84
1	O	23	SER	CA-C-N	7.54	129.26	119.84
1	O	23	SER	C-N-CA	7.54	129.26	119.84
1	B	203	ILE	N-CA-C	-7.44	96.42	107.51
1	A	23	SER	CA-C-N	7.15	128.77	119.84
1	A	23	SER	C-N-CA	7.15	128.77	119.84
1	B	332	TRP	N-CA-C	7.03	125.77	110.80
1	A	203	ILE	N-CA-C	-6.86	97.28	107.51
1	O	203	ILE	N-CA-C	-6.85	97.31	107.51
1	A	24	PRO	N-CA-C	6.84	126.57	112.47
1	O	24	PRO	N-CA-C	6.68	126.24	112.47
1	O	164	LYS	N-CA-C	6.55	120.53	112.54
1	O	265	GLN	N-CA-C	6.46	118.38	108.30
1	B	111	ALA	N-CA-C	-6.40	105.23	113.16
1	O	333	GLN	CB-CA-C	-6.39	97.96	110.10
1	O	276	GLU	CA-C-N	6.39	127.83	119.84
1	O	276	GLU	C-N-CA	6.39	127.83	119.84
1	B	121	PRO	CA-N-CD	-6.35	103.11	112.00
1	O	232	VAL	CA-C-N	6.32	127.74	119.84
1	O	232	VAL	C-N-CA	6.32	127.74	119.84
1	O	69	LYS	N-CA-C	6.29	119.78	110.48
1	A	164	LYS	N-CA-C	6.27	120.19	112.54
1	B	24	PRO	N-CA-C	6.26	125.38	112.47
1	A	232	VAL	CA-C-N	6.22	127.62	119.84
1	A	232	VAL	C-N-CA	6.22	127.62	119.84
1	O	19	TRP	N-CA-CB	-6.14	101.05	110.20
1	B	191	ARG	N-CA-C	-6.12	104.61	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	GLN	OE1-CD-NE2	6.07	128.67	122.60
1	A	276	GLU	CA-C-N	5.92	127.24	119.84
1	A	276	GLU	C-N-CA	5.92	127.24	119.84
1	O	111	ALA	N-CA-C	-5.85	105.91	113.16
1	B	333	GLN	CB-CA-C	5.80	121.12	110.10
1	B	276	GLU	CA-C-N	5.77	127.05	119.84
1	B	276	GLU	C-N-CA	5.77	127.05	119.84
1	A	111	ALA	N-CA-C	-5.73	106.05	113.16
1	B	164	LYS	N-CA-C	5.73	119.53	112.54
1	B	232	VAL	CA-C-N	5.62	126.87	119.84
1	B	232	VAL	C-N-CA	5.62	126.87	119.84
1	O	191	ARG	N-CA-C	-5.40	105.39	111.28
1	B	232	VAL	N-CA-C	5.40	113.83	107.84
1	A	191	ARG	N-CA-C	-5.37	105.43	111.28
1	B	154	LEU	N-CA-C	5.36	116.93	111.14
1	A	333	GLN	OE1-CD-NE2	5.31	127.91	122.60
1	O	184	LEU	N-CA-C	-5.29	105.59	111.36
1	O	333	GLN	OE1-CD-NE2	5.27	127.87	122.60
1	A	205	PRO	CB-CA-C	5.19	117.87	111.23
1	B	199	ALA	N-CA-C	5.18	116.61	111.07
1	O	154	LEU	N-CA-C	5.10	116.65	111.14
1	B	184	LEU	N-CA-C	-5.05	105.85	111.36
1	A	328	VAL	CA-C-O	5.05	126.30	121.05
1	O	332	TRP	CA-C-O	-5.05	113.29	120.51
1	B	322	VAL	N-CA-C	-5.05	105.79	110.53
1	O	302	ASP	CB-CA-C	-5.03	103.16	111.36
1	A	121	PRO	CA-N-CD	-5.02	104.98	112.00

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	2521	0	2558	264	0
1	B	2521	0	2561	238	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	2521	0	2562	254	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
2	O	10	0	0	0	0
3	A	48	0	26	5	0
3	B	48	0	26	5	0
3	O	48	0	26	7	0
4	A	65	0	0	8	0
4	B	60	0	0	9	0
4	O	87	0	0	11	0
All	All	7949	0	7759	746	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 48.

All (746) 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:O:56:ASP:H	1:O:66:VAL:CG1	1.21	1.50
1:A:56:ASP:H	1:A:66:VAL:CG1	1.25	1.47
1:B:56:ASP:N	1:B:66:VAL:HG12	1.45	1.31
1:B:56:ASP:H	1:B:66:VAL:CG1	1.46	1.28
1:O:56:ASP:N	1:O:66:VAL:CG1	2.04	1.19
1:A:56:ASP:N	1:A:66:VAL:CG1	2.09	1.15
1:A:0:LYS:HB3	4:A:1387:HOH:O	1.47	1.13
1:A:333:GLN:CD	1:A:333:GLN:O	1.92	1.13
1:A:333:GLN:O	1:A:333:GLN:NE2	1.82	1.12
1:A:183:ARG:HD2	1:A:187:ALA:HB3	1.26	1.11
1:A:56:ASP:H	1:A:66:VAL:HG12	1.01	1.10
1:O:56:ASP:H	1:O:66:VAL:HG12	0.92	1.09
1:A:332:TRP:CE3	1:A:333:GLN:CB	2.37	1.08
1:B:260:ARG:NH2	4:B:2365:HOH:O	1.89	1.05
1:A:19:TRP:HE1	1:A:27:VAL:HG21	1.17	1.05
1:A:38:LYS:H	1:A:38:LYS:HD3	1.17	1.05
1:B:38:LYS:H	1:B:38:LYS:HD3	1.19	1.05
1:O:38:LYS:H	1:O:38:LYS:HD3	1.20	1.04
1:O:56:ASP:N	1:O:66:VAL:HG12	1.68	1.03
1:A:332:TRP:CE3	1:A:333:GLN:HB2	1.93	1.01
1:B:24:PRO:HG3	4:B:2339:HOH:O	1.60	1.01
1:O:19:TRP:NE1	1:O:27:VAL:HG23	1.76	1.00
1:O:19:TRP:HE1	1:O:27:VAL:CG2	1.75	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:PRO:HB3	1:B:25:LEU:HD12	1.44	1.00
1:O:19:TRP:HE1	1:O:27:VAL:HG23	1.26	0.99
1:B:19:TRP:HE1	1:B:27:VAL:HG21	1.28	0.98
1:A:332:TRP:CE3	1:A:333:GLN:HB3	1.98	0.98
1:A:56:ASP:HB2	1:A:66:VAL:HG12	1.46	0.97
1:A:56:ASP:H	1:A:66:VAL:HG13	1.24	0.97
1:O:24:PRO:HB3	1:O:25:LEU:HD12	1.48	0.95
1:A:56:ASP:N	1:A:66:VAL:HG12	1.77	0.95
1:O:56:ASP:H	1:O:66:VAL:HG13	1.32	0.94
1:B:333:GLN:O	1:B:333:GLN:NE2	2.01	0.93
1:O:56:ASP:HB2	1:O:66:VAL:HG12	1.50	0.93
1:A:96:THR:OG1	1:A:98:VAL:HG22	1.69	0.93
1:A:19:TRP:HE1	1:A:27:VAL:CG2	1.82	0.93
1:B:183:ARG:HD2	1:B:187:ALA:HB3	1.48	0.92
1:O:83:PRO:HB2	1:O:87:MET:HE2	1.50	0.92
1:A:83:PRO:HB2	1:A:87:MET:HE2	1.49	0.92
1:A:24:PRO:HB3	1:A:25:LEU:HD12	1.52	0.92
1:A:332:TRP:CZ3	1:A:333:GLN:CB	2.53	0.91
1:B:129:VAL:H	1:B:133:ASN:HD21	1.18	0.91
1:A:124:ASP:HB3	4:A:1361:HOH:O	1.70	0.91
1:O:56:ASP:N	1:O:66:VAL:HG13	1.85	0.90
1:O:19:TRP:NE1	1:O:27:VAL:CG2	2.35	0.89
1:A:56:ASP:N	1:A:66:VAL:HG13	1.81	0.89
1:B:55:ALA:HB1	1:B:66:VAL:HG13	1.53	0.89
1:B:83:PRO:HB2	1:B:87:MET:HE2	1.54	0.88
2:A:1336:SO4:O2	4:A:1343:HOH:O	1.91	0.88
1:A:121:PRO:HD3	1:A:147:ALA:C	1.99	0.88
1:A:129:VAL:H	1:A:133:ASN:HD21	1.21	0.88
1:O:96:THR:OG1	1:O:98:VAL:HG22	1.74	0.87
1:A:25:LEU:HD12	1:A:25:LEU:H	1.39	0.87
1:O:79:PRO:HB2	1:O:107:LYS:HB3	1.56	0.87
1:B:96:THR:OG1	1:B:98:VAL:HG22	1.73	0.87
1:O:121:PRO:HD3	1:O:147:ALA:C	2.00	0.87
1:O:25:LEU:HD12	1:O:25:LEU:H	1.40	0.86
1:O:129:VAL:H	1:O:133:ASN:HD21	1.22	0.86
1:O:19:TRP:CE2	1:O:27:VAL:HG23	2.10	0.86
1:A:24:PRO:HG3	4:A:1388:HOH:O	1.75	0.86
1:B:29:VAL:HG11	1:B:87:MET:HE1	1.56	0.85
1:B:79:PRO:HB2	1:B:107:LYS:HB3	1.58	0.85
1:O:64:ILE:C	1:O:64:ILE:HD12	2.02	0.85
1:A:79:PRO:HB2	1:A:107:LYS:HB3	1.58	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:THR:O	1:A:119:THR:HG22	1.77	0.84
1:B:25:LEU:HD12	1:B:25:LEU:H	1.43	0.83
1:O:65:SER:O	1:O:68:GLY:N	2.10	0.83
1:O:56:ASP:CB	1:O:66:VAL:HG12	2.08	0.83
1:O:19:TRP:CZ2	1:O:27:VAL:HG23	2.14	0.82
1:A:22(A):LYS:HE3	1:A:322:VAL:HG11	1.58	0.82
1:A:142:THR:HG23	1:A:143:ILE:HG13	1.61	0.82
1:A:261:GLU:O	1:A:265:GLN:HG2	1.79	0.82
1:A:56:ASP:CB	1:A:66:VAL:HG12	2.10	0.81
1:A:65:SER:O	1:A:68:GLY:N	2.12	0.81
1:A:129:VAL:H	1:A:133:ASN:ND2	1.77	0.81
1:A:332:TRP:CZ3	1:A:333:GLN:HB2	2.14	0.81
1:O:25:LEU:HA	4:O:6340:HOH:O	1.80	0.81
1:O:172:MET:HE2	1:O:240:VAL:HG23	1.62	0.81
1:B:129:VAL:H	1:B:133:ASN:ND2	1.79	0.80
1:O:38:LYS:H	1:O:38:LYS:CD	1.95	0.80
1:B:56:ASP:H	1:B:66:VAL:HG12	0.67	0.80
1:O:119:THR:HG22	1:O:119:THR:O	1.80	0.80
1:A:90:ASP:HB3	1:A:333:GLN:OE1	1.81	0.80
1:A:19:TRP:NE1	1:A:27:VAL:CG2	2.45	0.80
1:B:90:ASP:HB3	1:B:333:GLN:HE22	1.46	0.80
1:B:167:ILE:HG12	1:B:244:VAL:HG21	1.62	0.80
1:O:236:ASN:OD1	1:O:313:ASN:ND2	2.14	0.80
1:A:19:TRP:NE1	1:A:27:VAL:HG21	1.96	0.80
1:O:228:ILE:HD13	1:O:228:ILE:H	1.46	0.79
1:B:77:ARG:H	1:B:77:ARG:HD3	1.47	0.79
1:A:332:TRP:HE3	1:A:333:GLN:HB3	1.44	0.79
1:O:183:ARG:NH1	1:O:190:HIS:HD2	1.81	0.79
1:B:228:ILE:HD13	1:B:228:ILE:H	1.45	0.79
1:O:129:VAL:H	1:O:133:ASN:ND2	1.80	0.79
1:A:167:ILE:HG12	1:A:244:VAL:HG21	1.63	0.79
1:O:29:VAL:HG11	1:O:87:MET:HE1	1.65	0.79
1:O:77:ARG:H	1:O:77:ARG:HD3	1.47	0.79
1:O:183:ARG:NH1	1:O:190:HIS:CD2	2.50	0.78
1:A:228:ILE:HD13	1:A:228:ILE:H	1.45	0.78
1:B:100:VAL:HG23	1:B:122(A):LYS:HG2	1.65	0.78
1:B:121:PRO:HD3	1:B:147:ALA:C	2.08	0.78
1:B:142:THR:HG23	1:B:143:ILE:HG13	1.64	0.78
1:B:19:TRP:HE1	1:B:27:VAL:CG2	1.96	0.77
1:B:101:ASP:HA	1:B:122(A):LYS:HB2	1.67	0.77
1:B:172:MET:HE2	1:B:240:VAL:HG23	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:SER:O	1:B:68:GLY:N	2.17	0.77
1:A:29:VAL:HG11	1:A:87:MET:HE1	1.65	0.77
1:B:56:ASP:N	1:B:66:VAL:CG1	2.22	0.76
1:O:22(A):LYS:HE3	1:O:322:VAL:HG11	1.65	0.76
1:O:62:SER:HB2	1:O:71:ILE:O	1.85	0.76
1:B:19:TRP:NE1	1:B:27:VAL:HG21	1.99	0.76
1:B:155:ALA:HB3	1:B:156:PRO:HD3	1.65	0.76
1:B:78:ASN:OD1	1:B:80:VAL:HG22	1.86	0.76
1:O:114:LYS:HD3	1:O:333:GLN:CD	2.10	0.76
1:B:22(A):LYS:HE3	1:B:322:VAL:HG11	1.66	0.76
1:O:167:ILE:HG12	1:O:244:VAL:HG21	1.67	0.76
1:A:38:LYS:H	1:A:38:LYS:CD	1.93	0.76
1:O:19:TRP:HZ2	1:O:27:VAL:H	1.34	0.76
1:A:100:VAL:HG23	1:A:122(A):LYS:HG2	1.67	0.76
1:O:142:THR:HG23	1:O:143:ILE:HG13	1.66	0.75
1:O:155:ALA:HB3	1:O:156:PRO:HD3	1.66	0.75
1:A:77:ARG:H	1:A:77:ARG:HD3	1.49	0.75
1:A:298:MET:HE3	1:A:306:LYS:HD2	1.69	0.75
1:B:66:VAL:HG23	1:B:66:VAL:O	1.86	0.75
1:A:172:MET:HE2	1:A:240:VAL:HG23	1.67	0.75
1:A:236:ASN:OD1	1:A:313:ASN:ND2	2.20	0.75
1:B:23:SER:N	1:B:24:PRO:HD3	2.02	0.75
1:B:298:MET:HE3	1:B:306:LYS:HD2	1.70	0.74
1:A:332:TRP:CZ3	1:A:333:GLN:HB3	2.21	0.73
1:O:124:ASP:OD2	4:O:6363:HOH:O	2.06	0.73
1:A:333:GLN:NE2	1:A:333:GLN:C	2.46	0.73
1:B:62:SER:HB2	1:B:71:ILE:O	1.88	0.73
1:A:332:TRP:HE3	1:A:333:GLN:CB	1.96	0.73
1:B:19:TRP:NE1	1:B:27:VAL:CG2	2.52	0.73
1:O:78:ASN:OD1	1:O:80:VAL:HG22	1.88	0.72
1:O:159:LYS:HG2	1:O:163:GLN:HE21	1.54	0.72
1:O:23:SER:N	1:O:24:PRO:HD3	2.04	0.72
1:A:23:SER:N	1:A:24:PRO:HD3	2.04	0.72
1:O:298:MET:HE3	1:O:306:LYS:HD2	1.71	0.72
1:O:19:TRP:HA	1:O:22(A):LYS:HB2	1.72	0.72
1:O:100:VAL:HG23	1:O:122(A):LYS:HG2	1.70	0.72
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.71	0.72
1:O:101:ASP:HA	1:O:122(A):LYS:HB2	1.72	0.72
1:A:159:LYS:HG2	1:A:163:GLN:HE21	1.55	0.71
1:A:300:MET:HE3	1:A:300:MET:HA	1.73	0.71
1:A:78:ASN:OD1	1:A:80:VAL:HG22	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:THR:HG23	1:B:251:PHE:N	2.06	0.70
1:B:236:ASN:OD1	1:B:313:ASN:ND2	2.24	0.70
1:A:28:VAL:HG23	1:A:29:VAL:HG23	1.72	0.70
1:B:119:THR:HG22	1:B:119:THR:O	1.90	0.70
1:O:28:VAL:HG23	1:O:29:VAL:HG23	1.73	0.70
1:A:101:ASP:HA	1:A:122(A):LYS:HB2	1.74	0.70
1:O:11:ILE:HD11	3:O:6335:NDP:C3N	2.22	0.70
1:B:100:VAL:HG23	1:B:122(A):LYS:CG	2.22	0.70
1:A:19:TRP:HA	1:A:22(A):LYS:HB2	1.74	0.69
1:A:207:SER:N	4:A:1399:HOH:O	2.25	0.69
1:A:62:SER:HB2	1:A:71:ILE:O	1.91	0.69
1:A:64:ILE:HG13	1:A:64:ILE:O	1.91	0.69
1:B:28:VAL:HG23	1:B:29:VAL:HG23	1.73	0.69
1:B:24:PRO:CB	1:B:25:LEU:HD12	2.23	0.68
1:B:165:PHE:HE2	1:B:250:THR:HG1	1.37	0.68
1:B:249:LYS:HA	1:B:302:ASP:O	1.94	0.68
1:A:100:VAL:HG23	1:A:122(A):LYS:CG	2.24	0.68
1:O:100:VAL:HG23	1:O:122(A):LYS:CG	2.24	0.68
1:O:191:ARG:HG2	1:O:191:ARG:HH11	1.58	0.68
1:A:33:THR:HG23	3:A:1335:NDP:C2A	2.24	0.67
1:B:159:LYS:HG2	1:B:163:GLN:HE21	1.60	0.67
1:B:19:TRP:O	1:B:20:HIS:C	2.37	0.67
1:A:139:HIS:HB2	1:A:331:LYS:O	1.93	0.67
1:A:11:ILE:HD11	3:A:1335:NDP:C3N	2.26	0.66
1:B:19:TRP:HA	1:B:22(A):LYS:HB2	1.78	0.66
1:A:19:TRP:O	1:A:20:HIS:C	2.37	0.66
1:A:22(A):LYS:HE3	1:A:322:VAL:CG1	2.26	0.65
1:B:24:PRO:HB3	1:B:25:LEU:CD1	2.21	0.65
1:O:56:ASP:CA	1:O:66:VAL:HG12	2.26	0.65
1:B:228:ILE:HD13	1:B:228:ILE:N	2.11	0.65
1:O:129:VAL:N	1:O:133:ASN:HD21	1.95	0.65
1:B:271:LEU:HD11	1:B:292:ILE:HG12	1.78	0.65
1:B:64:ILE:HG13	1:B:64:ILE:O	1.96	0.65
1:O:19:TRP:O	1:O:20:HIS:C	2.39	0.65
1:O:177:SER:HB3	1:O:234:THR:O	1.96	0.65
1:A:177:SER:HB3	1:A:234:THR:O	1.97	0.65
1:B:129:VAL:N	1:B:133:ASN:HD21	1.92	0.64
1:A:333:GLN:CD	1:A:333:GLN:C	2.65	0.64
1:A:191:ARG:HH11	1:A:191:ARG:HG2	1.62	0.64
1:O:228:ILE:HD13	1:O:228:ILE:N	2.13	0.64
1:O:24:PRO:HB3	1:O:25:LEU:CD1	2.25	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ASP:O	1:A:329:ALA:HB3	1.98	0.63
1:B:211:ALA:HB1	1:B:226:ASN:HA	1.80	0.63
1:O:183:ARG:HH12	1:O:190:HIS:CD2	2.16	0.63
1:A:228:ILE:HD13	1:A:228:ILE:N	2.13	0.63
1:B:59:THR:HG22	1:B:60(A):GLY:H	1.64	0.63
1:O:211:ALA:HB1	1:O:226:ASN:HA	1.81	0.62
1:O:284:ARG:HD2	4:O:6370:HOH:O	1.99	0.62
1:B:6:ASN:HD22	1:B:96:THR:HG21	1.63	0.62
1:O:6:ASN:ND2	1:O:96:THR:HG21	2.14	0.62
1:A:144:ILE:HG21	1:A:324:LEU:HD21	1.82	0.62
1:B:6:ASN:ND2	1:B:96:THR:HG21	2.13	0.62
1:B:64:ILE:HD12	1:B:65:SER:O	1.98	0.62
1:A:19:TRP:NE1	1:A:27:VAL:HG23	2.13	0.62
1:B:55:ALA:HA	1:B:66:VAL:HG11	1.81	0.62
1:A:59:THR:HG22	1:A:60(A):GLY:H	1.65	0.62
1:B:38:LYS:H	1:B:38:LYS:CD	1.95	0.62
1:O:55:ALA:HB1	1:O:66:VAL:HG13	1.81	0.61
1:A:24:PRO:CB	1:A:25:LEU:HD12	2.30	0.61
1:B:144:ILE:HG21	1:B:324:LEU:HD21	1.81	0.61
1:B:191:ARG:HG2	1:B:191:ARG:HH11	1.65	0.61
1:B:332:TRP:CE3	1:B:333:GLN:HB3	2.35	0.61
1:O:28:VAL:HG23	1:O:29:VAL:CG2	2.31	0.61
1:B:177:SER:HB3	1:B:234:THR:O	2.01	0.61
1:B:129:VAL:HG23	1:B:217:VAL:HG11	1.82	0.61
1:O:24:PRO:HA	4:O:6356:HOH:O	2.00	0.61
1:O:64:ILE:HD12	1:O:65:SER:O	2.01	0.61
1:A:137:TYR:CE1	1:A:144:ILE:HD11	2.36	0.61
1:A:129:VAL:N	1:A:133:ASN:HD21	1.94	0.61
1:B:66:VAL:O	1:B:66:VAL:CG2	2.48	0.61
1:O:24:PRO:HG3	4:O:6360:HOH:O	2.00	0.60
1:A:326:ASP:OD1	4:A:1388:HOH:O	2.16	0.60
1:O:33:THR:HG23	3:O:6335:NDP:C2A	2.31	0.60
1:B:300:MET:HA	1:B:300:MET:HE3	1.83	0.60
1:O:144:ILE:HG21	1:O:324:LEU:HD21	1.82	0.60
1:B:28:VAL:HG23	1:B:29:VAL:CG2	2.30	0.60
1:A:28:VAL:HG23	1:A:29:VAL:CG2	2.31	0.60
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.36	0.60
1:B:11:ILE:HG21	1:B:119:THR:HG21	1.83	0.60
1:A:172:MET:O	1:A:227:GLY:HA3	2.02	0.60
1:A:185:LEU:CD2	1:B:49:ILE:HD11	2.32	0.60
1:B:132:VAL:HG13	1:B:218:LEU:HD21	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLN:HG2	4:B:2338:HOH:O	2.00	0.60
1:A:324:LEU:O	1:A:328:VAL:HG23	2.02	0.60
1:O:271:LEU:HD11	1:O:292:ILE:HG12	1.84	0.59
1:A:6:ASN:HD22	1:A:96:THR:HG21	1.67	0.59
1:A:24:PRO:HB3	1:A:25:LEU:CD1	2.27	0.59
1:A:185:LEU:HD21	1:B:49:ILE:HD11	1.83	0.59
1:O:19:TRP:CZ2	1:O:27:VAL:CG2	2.85	0.59
1:O:249:LYS:HA	1:O:302:ASP:O	2.03	0.59
1:B:77:ARG:HH11	1:B:77:ARG:HG3	1.66	0.59
1:O:19:TRP:CE2	1:O:27:VAL:CG2	2.82	0.59
1:A:206:THR:HG22	1:A:229:ALA:HB3	1.85	0.59
1:O:6:ASN:HD22	1:O:96:THR:HG21	1.67	0.59
1:O:59:THR:HG22	1:O:60(A):GLY:H	1.68	0.59
1:A:271:LEU:HD11	1:A:292:ILE:HG12	1.84	0.59
1:O:129:VAL:HG23	1:O:217:VAL:HG11	1.85	0.59
1:A:19:TRP:CE2	1:A:27:VAL:HG23	2.38	0.59
1:B:49:ILE:HA	1:B:284:ARG:NH2	2.18	0.59
1:O:242:LEU:HD12	1:O:243:VAL:N	2.18	0.58
1:A:211:ALA:HB1	1:A:226:ASN:HA	1.84	0.58
1:O:181:ASP:O	1:O:183:ARG:NH1	2.35	0.58
1:A:249:LYS:HA	1:A:302:ASP:O	2.02	0.58
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.38	0.58
1:B:172:MET:O	1:B:227:GLY:HA3	2.04	0.58
1:O:22(A):LYS:HE3	1:O:322:VAL:CG1	2.33	0.58
1:O:64:ILE:HA	1:O:69:LYS:O	2.03	0.58
1:A:144:ILE:HG22	1:A:145:SER:N	2.18	0.58
1:O:121:PRO:HD3	1:O:147:ALA:O	2.02	0.58
1:A:192:ASP:HB3	1:A:195:ARG:HB2	1.86	0.58
1:B:90:ASP:CB	1:B:333:GLN:HE22	2.15	0.58
1:B:144:ILE:HG22	1:B:145:SER:N	2.18	0.58
1:O:24:PRO:CB	1:O:25:LEU:HD12	2.28	0.57
1:B:90:ASP:HB3	1:B:333:GLN:NE2	2.17	0.57
1:O:139:HIS:O	1:O:139:HIS:CG	2.58	0.57
1:O:144:ILE:HG22	1:O:145:SER:N	2.19	0.57
1:A:64:ILE:HA	1:A:69:LYS:O	2.05	0.57
1:O:132:VAL:HG13	1:O:218:LEU:HD21	1.87	0.57
1:A:64:ILE:HD12	1:A:65:SER:O	2.04	0.57
1:A:121:PRO:HD3	1:A:147:ALA:O	2.03	0.57
1:O:49:ILE:HA	1:O:284:ARG:NH2	2.20	0.57
1:O:115:LYS:HD3	1:O:141:ASP:O	2.04	0.57
1:O:300:MET:HE3	1:O:300:MET:HA	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HA	1:A:284:ARG:NH2	2.20	0.57
1:A:210:ALA:O	1:A:214:VAL:HG23	2.05	0.57
1:B:127:THR:HB	1:B:145:SER:HB3	1.87	0.57
1:O:324:LEU:O	1:O:328:VAL:HG23	2.04	0.56
1:B:22(A):LYS:HE3	1:B:322:VAL:CG1	2.34	0.56
1:B:31:ASN:HA	1:B:74:VAL:O	2.05	0.56
1:B:210:ALA:O	1:B:214:VAL:HG23	2.05	0.56
1:O:172:MET:O	1:O:227:GLY:HA3	2.06	0.56
1:B:11:ILE:HG21	1:B:119:THR:CG2	2.35	0.56
1:B:137:TYR:CE1	1:B:144:ILE:HD11	2.41	0.56
1:B:326:ASP:O	1:B:329:ALA:HB3	2.06	0.56
1:O:66:VAL:HG23	1:O:66:VAL:O	2.05	0.56
1:A:56:ASP:CA	1:A:66:VAL:HG12	2.36	0.56
1:A:129:VAL:HG23	1:A:217:VAL:HG11	1.86	0.56
1:A:223:GLY:N	4:A:1365:HOH:O	2.29	0.56
1:A:6:ASN:ND2	1:A:96:THR:HG21	2.19	0.56
1:A:77:ARG:HG3	1:A:77:ARG:HH11	1.70	0.56
1:O:45:LYS:HG2	1:O:57:VAL:HB	1.88	0.56
1:O:284:ARG:NH1	4:O:6370:HOH:O	2.38	0.56
1:A:38:LYS:HG2	1:A:39:GLN:H	1.70	0.56
1:O:38:LYS:HG2	1:O:39:GLN:H	1.71	0.56
1:O:210:ALA:O	1:O:214:VAL:HG23	2.05	0.56
1:A:139:HIS:CG	1:A:139:HIS:O	2.59	0.56
1:O:137:TYR:CE1	1:O:144:ILE:HD11	2.41	0.55
1:A:132:VAL:HG13	1:A:218:LEU:HD21	1.87	0.55
1:O:64:ILE:HD12	1:O:65:SER:N	2.21	0.55
1:A:31:ASN:HA	1:A:74:VAL:O	2.06	0.55
1:B:324:LEU:O	1:B:328:VAL:HG23	2.05	0.55
1:O:300:MET:HB3	4:O:6416:HOH:O	2.05	0.55
1:B:192:ASP:HB3	1:B:195:ARG:HB2	1.87	0.55
1:B:281:ILE:HD11	1:B:284:ARG:HH11	1.72	0.55
1:O:100:VAL:HA	1:O:118:ILE:HD13	1.89	0.55
1:A:96:THR:HG1	1:A:98:VAL:HG22	1.69	0.55
1:B:77:ARG:HD3	1:B:77:ARG:N	2.20	0.55
1:A:25:LEU:HD12	1:A:25:LEU:N	2.17	0.55
1:B:100:VAL:HA	1:B:118:ILE:HD13	1.89	0.55
1:B:102:ARG:HH12	1:B:142:THR:CG2	2.20	0.55
1:O:191:ARG:HG2	1:O:191:ARG:NH1	2.22	0.55
1:O:192:ASP:HB3	1:O:195:ARG:HB2	1.89	0.55
1:A:66:VAL:O	1:A:66:VAL:HG23	2.07	0.54
1:B:19:TRP:CE2	1:B:27:VAL:HG23	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LEU:HD13	1:B:84:TRP:CZ2	2.42	0.54
1:O:127:THR:HB	1:O:145:SER:HB3	1.89	0.54
1:A:119:THR:O	1:A:119:THR:CG2	2.50	0.54
1:O:77:ARG:HG3	1:O:77:ARG:HH11	1.71	0.54
1:B:23:SER:N	1:B:24:PRO:CD	2.70	0.54
1:O:79:PRO:HA	1:O:82:LEU:CD1	2.37	0.54
1:O:159:LYS:HB2	1:O:218:LEU:HD11	1.90	0.54
1:B:79:PRO:HA	1:B:82:LEU:CD1	2.37	0.54
1:B:176:HIS:O	1:B:231:ARG:HA	2.06	0.54
1:O:21:GLY:O	1:O:22(A):LYS:C	2.50	0.54
1:O:77:ARG:HD3	1:O:77:ARG:N	2.21	0.54
1:A:176:HIS:O	1:A:231:ARG:HA	2.07	0.54
1:B:55:ALA:CA	1:B:66:VAL:CG1	2.86	0.54
1:O:64:ILE:O	1:O:64:ILE:HG13	2.07	0.54
1:A:157:PHE:HB2	1:A:259:PHE:CE1	2.43	0.54
1:B:22(A):LYS:HE2	1:B:319:GLN:OE1	2.07	0.54
1:B:64:ILE:HA	1:B:69:LYS:O	2.08	0.54
1:A:33:THR:HG23	3:A:1335:NDP:N3A	2.23	0.54
1:B:6:ASN:HD22	1:B:96:THR:CG2	2.20	0.54
1:B:45:LYS:HG2	1:B:57:VAL:HB	1.90	0.54
1:O:31:ASN:HA	1:O:74:VAL:O	2.08	0.53
1:B:38:LYS:HG2	1:B:39:GLN:H	1.73	0.53
1:A:39:GLN:NE2	1:B:190:HIS:H	2.04	0.53
1:B:80:VAL:CG1	1:B:107:LYS:HG3	2.37	0.53
1:O:211:ALA:CB	1:O:226:ASN:HA	2.37	0.53
1:A:77:ARG:HD3	1:A:77:ARG:N	2.21	0.53
1:A:79:PRO:HA	1:A:82:LEU:CD1	2.39	0.53
1:A:251:PHE:CD1	1:A:251:PHE:N	2.76	0.53
1:B:157:PHE:HB2	1:B:259:PHE:CE1	2.44	0.53
1:B:211:ALA:CB	1:B:226:ASN:HA	2.37	0.53
1:A:332:TRP:HZ3	1:A:333:GLN:HG3	1.72	0.53
1:B:242:LEU:HD12	1:B:243:VAL:N	2.23	0.53
1:O:179:THR:HB	4:O:6341:HOH:O	2.08	0.53
1:A:21:GLY:O	1:A:22(A):LYS:C	2.51	0.53
1:A:242:LEU:HD12	1:A:243:VAL:N	2.24	0.53
1:B:33:THR:HG23	3:B:2335:NDP:C2A	2.38	0.53
1:A:159:LYS:HB2	1:A:218:LEU:HD11	1.91	0.53
1:O:1:LEU:HD22	1:O:329:ALA:HA	1.91	0.53
1:O:80:VAL:CG1	1:O:107:LYS:HG3	2.39	0.53
1:A:80:VAL:CG1	1:A:107:LYS:HG3	2.40	0.52
1:A:36:GLY:HA3	1:A:38:LYS:HE2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ALA:HB1	1:A:66:VAL:HG13	1.90	0.52
1:A:94:GLU:OE2	1:A:96:THR:HG23	2.09	0.52
1:A:319:GLN:HA	1:A:319:GLN:OE1	2.08	0.52
1:B:82:LEU:HD11	4:B:2380:HOH:O	2.09	0.52
1:B:159:LYS:HB2	1:B:218:LEU:HD11	1.92	0.52
1:O:55:ALA:HA	1:O:66:VAL:HG11	1.90	0.52
1:O:84:TRP:HA	1:O:89:ILE:HG12	1.91	0.52
1:A:11:ILE:HD11	3:A:1335:NDP:H42N	1.91	0.52
1:A:102:ARG:HH12	1:A:142:THR:CG2	2.22	0.52
1:B:115:LYS:HD3	1:B:141:ASP:O	2.10	0.52
1:O:183:ARG:CZ	1:O:190:HIS:CD2	2.92	0.52
1:A:38:LYS:HD3	1:A:38:LYS:N	2.03	0.52
1:A:128:TYR:HA	1:A:133:ASN:HD21	1.74	0.52
1:B:19:TRP:NE1	1:B:27:VAL:HG23	2.24	0.52
1:B:33:THR:HG23	3:B:2335:NDP:N3A	2.24	0.52
1:B:289:SER:OG	1:B:320:ARG:HD2	2.08	0.52
1:O:22(A):LYS:HE2	1:O:319:GLN:OE1	2.09	0.52
1:O:102:ARG:HH12	1:O:142:THR:CG2	2.23	0.52
1:O:206:THR:HG22	1:O:229:ALA:HB3	1.92	0.52
1:B:11:ILE:HD11	3:B:2335:NDP:C3N	2.40	0.52
1:B:21:GLY:O	1:B:22(A):LYS:C	2.50	0.52
1:B:293:ASP:OD2	1:B:296:LEU:HG	2.10	0.52
1:A:84:TRP:HA	1:A:89:ILE:HG12	1.92	0.52
1:O:176:HIS:O	1:O:231:ARG:HA	2.10	0.52
1:A:22(A):LYS:HE2	1:A:319:GLN:OE1	2.09	0.52
1:B:251:PHE:N	1:B:251:PHE:CD1	2.78	0.52
1:O:139:HIS:NE2	1:O:332:TRP:HE3	2.07	0.52
1:A:11:ILE:HG21	1:A:119:THR:HG21	1.92	0.52
1:O:62:SER:HA	1:O:73:VAL:HG23	1.92	0.51
1:A:23:SER:N	1:A:24:PRO:CD	2.73	0.51
1:A:65:SER:O	1:A:66:VAL:C	2.54	0.51
1:A:211:ALA:CB	1:A:226:ASN:HA	2.40	0.51
1:A:250:THR:HG23	1:A:251:PHE:N	2.25	0.51
1:A:266:GLU:HG2	1:A:267:LEU:HG	1.91	0.51
1:B:266:GLU:HG2	1:B:267:LEU:HG	1.92	0.51
1:O:167:ILE:HG23	1:O:244:VAL:CG2	2.41	0.51
1:O:23:SER:N	1:O:24:PRO:CD	2.73	0.51
1:O:157:PHE:HB2	1:O:259:PHE:CE1	2.45	0.51
1:B:139:HIS:CG	1:B:139:HIS:O	2.63	0.51
1:O:312:ASP:OD1	1:O:315:TRP:N	2.42	0.51
1:B:211:ALA:HB3	4:B:2357:HOH:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:25:LEU:HD12	1:O:25:LEU:N	2.18	0.51
1:O:260:ARG:HD3	4:O:6339:HOH:O	2.09	0.51
1:O:172:MET:C	1:O:172:MET:SD	2.94	0.51
1:O:251:PHE:N	1:O:251:PHE:CD1	2.79	0.51
1:B:85:GLY:CA	1:B:112:GLY:HA3	2.41	0.51
1:B:172:MET:SD	1:B:172:MET:C	2.94	0.51
1:O:11:ILE:HG21	1:O:119:THR:HG21	1.93	0.50
1:O:19:TRP:HZ2	1:O:27:VAL:HG23	1.73	0.50
1:A:1:LEU:HB3	1:A:25:LEU:HB3	1.92	0.50
1:B:96:THR:HG1	1:B:98:VAL:HG22	1.76	0.50
1:B:55:ALA:CB	1:B:66:VAL:HG13	2.33	0.50
1:B:34:GLY:HA3	1:B:39:GLN:OE1	2.11	0.50
1:B:36:GLY:HA3	1:B:38:LYS:HE2	1.94	0.50
1:B:55:ALA:HA	1:B:66:VAL:CG1	2.41	0.50
1:O:250:THR:HG23	1:O:251:PHE:N	2.25	0.50
1:A:261:GLU:O	1:A:265:GLN:CG	2.58	0.50
1:B:1:LEU:HB3	1:B:25:LEU:HB3	1.92	0.50
1:B:56:ASP:CA	1:B:66:VAL:HG12	2.35	0.50
1:B:121:PRO:HD3	1:B:147:ALA:O	2.10	0.50
1:B:165:PHE:HE2	1:B:250:THR:OG1	1.92	0.50
1:O:45:LYS:HE2	1:O:55:ALA:O	2.11	0.50
1:O:128:TYR:HA	1:O:133:ASN:HD21	1.77	0.50
1:O:208:THR:HG22	1:O:228:ILE:HA	1.94	0.50
1:A:85:GLY:CA	1:A:112:GLY:HA3	2.42	0.50
1:B:101:ASP:CA	1:B:122(A):LYS:HB2	2.38	0.50
1:O:84:TRP:CE3	1:O:89:ILE:HG13	2.47	0.50
1:B:45:LYS:HE2	1:B:55:ALA:O	2.12	0.50
1:B:84:TRP:CE3	1:B:89:ILE:HG13	2.47	0.50
1:O:281:ILE:HD11	1:O:284:ARG:HH11	1.77	0.49
1:A:34:GLY:HA3	1:A:39:GLN:OE1	2.12	0.49
1:A:100:VAL:HA	1:A:118:ILE:HD13	1.94	0.49
1:B:25:LEU:HD12	1:B:25:LEU:N	2.21	0.49
1:A:139:HIS:O	1:A:139:HIS:ND1	2.46	0.49
1:B:167:ILE:HG23	1:B:244:VAL:CG2	2.42	0.49
1:O:83:PRO:HB2	1:O:87:MET:CE	2.32	0.49
1:A:165:PHE:CE2	1:A:250:THR:OG1	2.65	0.49
1:A:191:ARG:HG2	1:A:191:ARG:NH1	2.24	0.49
1:O:6:ASN:HD22	1:O:96:THR:CG2	2.24	0.49
1:O:85:GLY:CA	1:O:112:GLY:HA3	2.43	0.49
1:A:61:ASP:O	1:A:62:SER:HB3	2.13	0.49
1:O:319:GLN:OE1	1:O:319:GLN:HA	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TRP:CE3	1:A:89:ILE:HG13	2.48	0.49
1:A:167:ILE:HG23	1:A:244:VAL:CG2	2.42	0.49
1:A:6:ASN:HD22	1:A:96:THR:CG2	2.24	0.49
1:A:172:MET:SD	1:A:172:MET:C	2.96	0.49
1:A:80:VAL:HG23	1:A:81:ASN:ND2	2.27	0.49
1:A:332:TRP:CZ3	1:A:333:GLN:HG3	2.47	0.49
1:B:129:VAL:CG2	1:B:217:VAL:HG11	2.42	0.49
1:O:119:THR:O	1:O:119:THR:CG2	2.53	0.49
1:A:235:PRO:CG	1:B:201:LEU:HD21	2.42	0.49
1:O:293:ASP:OD2	1:O:296:LEU:HG	2.12	0.49
1:B:79:PRO:HB2	1:B:107:LYS:CB	2.37	0.49
1:A:300:MET:O	1:A:304:MET:HB3	2.13	0.48
1:O:172:MET:HE2	1:O:240:VAL:CG2	2.39	0.48
1:A:11:ILE:HG21	1:A:119:THR:CG2	2.44	0.48
1:A:32:ASP:O	1:A:33:THR:C	2.55	0.48
1:A:165:PHE:HE2	1:A:250:THR:OG1	1.96	0.48
1:B:80:VAL:HG23	1:B:81:ASN:ND2	2.28	0.48
1:O:119:THR:HG23	1:O:317:TYR:HE2	1.78	0.48
1:O:139:HIS:NE2	1:O:332:TRP:CE3	2.81	0.48
1:A:77:ARG:O	1:A:79:PRO:HD3	2.13	0.48
1:A:263:ALA:O	1:A:268:LYS:HA	2.13	0.48
1:B:84:TRP:HA	1:B:89:ILE:HG12	1.95	0.48
1:B:319:GLN:OE1	1:B:319:GLN:HA	2.12	0.48
1:O:101:ASP:CA	1:O:122(A):LYS:HB2	2.42	0.48
1:B:171:THR:HA	1:B:226:ASN:O	2.12	0.48
1:O:84:TRP:HA	1:O:89:ILE:CG1	2.43	0.48
1:A:115:LYS:HD3	1:A:141:ASP:O	2.13	0.48
1:A:174:THR:HG23	1:A:174:THR:O	2.12	0.48
1:B:47:ASP:OD2	4:B:2378:HOH:O	2.20	0.48
1:B:133:ASN:H	1:B:133:ASN:HD22	1.60	0.48
1:A:281:ILE:HD11	1:A:284:ARG:HH11	1.78	0.48
1:A:289:SER:OG	1:A:320:ARG:HD2	2.12	0.48
1:B:98:VAL:HG23	1:B:99:PHE:CD2	2.48	0.48
1:O:33:THR:HG23	3:O:6335:NDP:N3A	2.28	0.48
1:O:94:GLU:OE2	1:O:96:THR:HG23	2.13	0.48
1:O:98:VAL:HG23	1:O:99:PHE:CD2	2.49	0.48
1:B:191:ARG:HG2	1:B:191:ARG:NH1	2.28	0.48
1:A:19:TRP:CZ2	1:A:27:VAL:HG23	2.49	0.48
1:A:83:PRO:HB2	1:A:87:MET:CE	2.33	0.48
1:A:332:TRP:CZ3	1:A:333:GLN:CG	2.97	0.48
1:B:90:ASP:O	1:B:114:LYS:HB2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LYS:HG2	1:A:57:VAL:HB	1.96	0.47
1:O:36:GLY:HA3	1:O:38:LYS:HE2	1.95	0.47
1:O:80:VAL:HG23	1:O:81:ASN:ND2	2.29	0.47
1:O:82:LEU:HA	1:O:83:PRO:HD3	1.63	0.47
1:A:208:THR:HG22	1:A:228:ILE:HA	1.96	0.47
1:B:263:ALA:O	1:B:268:LYS:HA	2.14	0.47
1:A:94:GLU:CD	1:A:96:THR:HG23	2.39	0.47
1:A:127:THR:HB	1:A:145:SER:HB3	1.97	0.47
1:B:261:GLU:O	1:B:265:GLN:HG2	2.15	0.47
1:O:19:TRP:NE1	1:O:27:VAL:HG21	2.23	0.47
1:O:90:ASP:O	1:O:114:LYS:HB2	2.15	0.47
1:O:128:TYR:CE2	1:O:137:TYR:HA	2.50	0.47
1:O:326:ASP:O	1:O:329:ALA:HB3	2.15	0.47
1:A:9:GLY:O	1:A:13:ARG:HG3	2.15	0.47
1:A:49:ILE:HD11	1:B:185:LEU:HD21	1.97	0.47
1:A:55:ALA:HA	1:A:66:VAL:HG11	1.96	0.47
1:B:312:ASP:OD1	1:B:315:TRP:N	2.46	0.47
1:O:64:ILE:O	1:O:64:ILE:CG1	2.62	0.47
1:A:281:ILE:HG22	1:A:282:ASP:N	2.30	0.47
1:O:1:LEU:HB3	1:O:25:LEU:HB3	1.97	0.47
1:O:11:ILE:HG21	1:O:119:THR:CG2	2.45	0.47
1:A:22(A):LYS:HB3	1:A:24:PRO:HG2	1.97	0.47
1:A:119:THR:HG23	1:A:317:TYR:HE2	1.80	0.47
1:A:171:THR:HA	1:A:226:ASN:O	2.14	0.47
1:O:137:TYR:OH	1:O:328:VAL:HG13	2.14	0.47
1:B:1:LEU:HD22	1:B:329:ALA:HA	1.97	0.47
1:B:128:TYR:CE2	1:B:137:TYR:HA	2.49	0.47
1:O:118:ILE:HG22	1:O:120:ALA:H	1.79	0.46
1:A:262:SER:HA	1:A:266:GLU:OE1	2.16	0.46
1:O:32:ASP:O	1:O:33:THR:C	2.58	0.46
1:O:79:PRO:HA	1:O:82:LEU:HD12	1.96	0.46
1:O:263:ALA:O	1:O:268:LYS:HA	2.16	0.46
1:O:157:PHE:CE2	1:O:242:LEU:HD23	2.51	0.46
1:O:332:TRP:CZ3	1:O:333:GLN:HB3	2.51	0.46
1:A:124:ASP:OD1	1:A:124:ASP:N	2.45	0.46
1:A:137:TYR:OH	1:A:328:VAL:HG13	2.16	0.46
1:A:293:ASP:OD2	1:A:296:LEU:HG	2.14	0.46
1:B:144:ILE:CG2	1:B:145:SER:N	2.78	0.46
1:O:11:ILE:HD11	3:O:6335:NDP:H42N	1.96	0.46
1:O:144:ILE:CG2	1:O:145:SER:N	2.79	0.46
1:A:45:LYS:HE2	1:A:55:ALA:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:GLU:OE2	1:B:96:THR:HG23	2.15	0.46
1:O:171:THR:HA	1:O:226:ASN:O	2.15	0.46
1:A:195:ARG:HH22	1:A:231:ARG:NH2	2.13	0.46
1:A:235:PRO:HG2	1:B:201:LEU:HD21	1.98	0.46
1:B:77:ARG:HG3	1:B:77:ARG:NH1	2.30	0.46
1:O:165:PHE:O	1:O:247:SER:HB3	2.16	0.46
1:O:250:THR:OG1	1:O:254:GLU:OE1	2.31	0.46
1:O:129:VAL:CG2	1:O:217:VAL:HG11	2.47	0.45
1:O:139:HIS:O	1:O:139:HIS:ND1	2.49	0.45
1:B:82:LEU:HA	1:B:83:PRO:HD3	1.63	0.45
1:B:274:CYS:SG	1:B:276:GLU:HB2	2.56	0.45
1:O:120:ALA:O	1:O:145:SER:OG	2.27	0.45
1:O:174:THR:HG23	1:O:174:THR:O	2.16	0.45
1:A:22(A):LYS:HB3	1:A:24:PRO:CG	2.47	0.45
1:A:139:HIS:CD2	1:A:332:TRP:HB3	2.51	0.45
1:B:137:TYR:OH	1:B:328:VAL:HG13	2.16	0.45
1:O:64:ILE:C	1:O:64:ILE:CD1	2.70	0.45
1:O:281:ILE:HG22	1:O:282:ASP:N	2.31	0.45
1:B:133:ASN:HD22	1:B:133:ASN:N	2.13	0.45
1:B:139:HIS:NE2	1:B:332:TRP:HE3	2.14	0.45
1:B:246:VAL:HG22	1:B:303:ASP:O	2.17	0.45
1:A:228:ILE:N	1:A:228:ILE:CD1	2.80	0.45
1:B:228:ILE:N	1:B:228:ILE:CD1	2.78	0.45
1:O:19:TRP:O	1:O:22(A):LYS:N	2.50	0.45
1:O:34:GLY:HA3	1:O:39:GLN:OE1	2.16	0.45
1:A:11:ILE:HD11	3:A:1335:NDP:C4N	2.46	0.45
1:A:118:ILE:HG22	1:A:120:ALA:H	1.81	0.45
1:B:218:LEU:HB2	1:B:221:LEU:HD12	1.98	0.45
1:O:38:LYS:HD3	1:O:38:LYS:N	2.05	0.45
1:O:292:ILE:HD13	1:O:309:ALA:HB2	1.98	0.45
1:O:9:GLY:O	1:O:13:ARG:HG3	2.16	0.45
1:O:55:ALA:CA	1:O:66:VAL:HG13	2.47	0.45
1:O:55:ALA:CA	1:O:66:VAL:CG1	2.95	0.45
1:O:125:ILE:O	1:O:127:THR:HG22	2.17	0.45
1:A:129:VAL:CG2	1:A:217:VAL:HG11	2.46	0.45
1:A:144:ILE:CG2	1:A:145:SER:N	2.78	0.45
1:A:84:TRP:HA	1:A:89:ILE:CG1	2.46	0.45
1:A:90:ASP:O	1:A:114:LYS:HB2	2.16	0.45
1:A:94:GLU:HG2	1:A:108:HIS:CD2	2.52	0.45
1:A:279:VAL:O	1:A:280:SER:C	2.60	0.45
1:B:279:VAL:O	1:B:280:SER:C	2.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:32:ASP:C	1:O:34:GLY:N	2.73	0.45
1:A:167:ILE:HG23	1:A:244:VAL:HG23	1.99	0.45
1:B:101:ASP:OD2	1:B:103:ASP:HB2	2.17	0.45
1:B:139:HIS:O	1:B:139:HIS:ND1	2.50	0.45
1:B:178:TYR:HA	1:B:182:GLN:OE1	2.17	0.45
1:B:206:THR:HG22	1:B:229:ALA:HB3	1.99	0.45
1:O:96:THR:HG1	1:O:98:VAL:HG22	1.78	0.45
1:A:82:LEU:HA	1:A:83:PRO:HD3	1.64	0.45
1:B:100:VAL:HG23	1:B:122(A):LYS:HG3	1.99	0.45
1:O:114:LYS:HE2	1:O:333:GLN:NE2	2.32	0.44
1:O:115:LYS:HZ2	1:O:137:TYR:HH	1.55	0.44
1:O:178:TYR:HA	1:O:182:GLN:OE1	2.16	0.44
1:A:101:ASP:CA	1:A:122(A):LYS:HB2	2.43	0.44
1:B:164:LYS:HD2	1:B:258:ALA:HB1	1.98	0.44
1:O:79:PRO:HB2	1:O:107:LYS:CB	2.37	0.44
1:A:32:ASP:C	1:A:34:GLY:N	2.72	0.44
1:A:114:LYS:HD2	1:A:333:GLN:OE1	2.18	0.44
1:A:133:ASN:HD22	1:A:133:ASN:H	1.66	0.44
1:B:208:THR:HG22	1:B:228:ILE:HA	1.99	0.44
1:B:32:ASP:O	1:B:33:THR:C	2.58	0.44
1:B:135:GLU:H	1:B:135:GLU:CD	2.26	0.44
1:O:83:PRO:O	1:O:84:TRP:C	2.59	0.44
1:B:167:ILE:HG23	1:B:244:VAL:HG23	1.99	0.44
1:B:3:VAL:HG13	1:B:93:ILE:HD13	2.00	0.44
1:B:119:THR:O	1:B:119:THR:CG2	2.62	0.44
1:O:55:ALA:HA	1:O:66:VAL:CG1	2.48	0.44
1:O:100:VAL:HG23	1:O:122(A):LYS:HG3	1.99	0.44
1:O:261:GLU:O	1:O:265:GLN:HG2	2.16	0.44
1:B:83:PRO:HB2	1:B:87:MET:CE	2.37	0.44
1:B:167:ILE:CG1	1:B:244:VAL:HG21	2.42	0.44
1:O:289:SER:OG	1:O:320:ARG:HD2	2.18	0.44
1:A:50:LEU:HD12	1:A:50:LEU:HA	1.83	0.44
1:A:101:ASP:OD2	1:A:103:ASP:HB2	2.18	0.44
1:A:167:ILE:CG1	1:A:244:VAL:HG21	2.43	0.44
1:A:274:CYS:SG	1:A:276:GLU:HB2	2.58	0.44
1:O:21:GLY:C	1:O:22(A):LYS:O	2.61	0.44
1:O:164:LYS:HD2	1:O:258:ALA:HB1	2.00	0.43
1:O:266:GLU:H	1:O:266:GLU:HG3	1.12	0.43
1:A:26:ASP:O	1:A:28:VAL:HG13	2.17	0.43
1:O:77:ARG:O	1:O:79:PRO:HD3	2.18	0.43
1:A:194:ARG:NH1	1:A:205:PRO:HB2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:TRP:HZ3	1:A:333:GLN:CB	2.25	0.43
1:B:9:GLY:O	1:B:13:ARG:HG3	2.18	0.43
1:O:133:ASN:HD22	1:O:133:ASN:H	1.65	0.43
1:B:21:GLY:C	1:B:22(A):LYS:O	2.61	0.43
1:O:94:GLU:HG2	1:O:108:HIS:CD2	2.54	0.43
1:B:118:ILE:HG22	1:B:120:ALA:H	1.83	0.43
1:O:228:ILE:N	1:O:228:ILE:CD1	2.79	0.43
1:O:236:ASN:O	1:O:237:VAL:HB	2.18	0.43
1:B:77:ARG:O	1:B:79:PRO:HD3	2.19	0.43
1:O:11:ILE:HD11	3:O:6335:NDP:C4N	2.48	0.43
1:O:117:LEU:C	1:O:117:LEU:HD12	2.43	0.43
1:B:128:TYR:CZ	1:B:137:TYR:HA	2.54	0.43
1:A:77:ARG:HG3	1:A:77:ARG:NH1	2.34	0.43
1:A:164:LYS:HD2	1:A:258:ALA:HB1	2.00	0.43
1:B:172:MET:HE2	1:B:240:VAL:CG2	2.45	0.43
1:O:25:LEU:CD1	1:O:25:LEU:N	2.81	0.43
1:O:65:SER:O	1:O:66:VAL:C	2.59	0.43
1:A:1:LEU:HD22	1:A:329:ALA:HA	2.00	0.43
1:A:98:VAL:HG23	1:A:99:PHE:CD2	2.53	0.43
1:B:83:PRO:O	1:B:84:TRP:C	2.62	0.43
1:B:84:TRP:HA	1:B:89:ILE:CG1	2.48	0.43
1:B:250:THR:OG1	1:B:254:GLU:OE1	2.37	0.43
1:O:0:LYS:HD2	4:O:6411:HOH:O	2.19	0.43
1:O:55:ALA:CB	1:O:66:VAL:HG13	2.48	0.43
1:O:77:ARG:H	1:O:77:ARG:CD	2.25	0.43
1:A:14:ASN:HB3	1:A:318:SER:OG	2.19	0.43
1:A:62:SER:HA	1:A:73:VAL:HG23	1.99	0.43
1:B:50:LEU:HD13	4:B:2346:HOH:O	2.19	0.43
1:B:61:ASP:O	1:B:62:SER:HB3	2.19	0.43
1:O:101:ASP:OD2	1:O:103:ASP:HB2	2.18	0.42
1:O:205:PRO:HA	1:O:230:LEU:HD23	2.01	0.42
1:B:11:ILE:HD11	3:B:2335:NDP:H42N	2.00	0.42
1:B:19:TRP:CZ2	1:B:27:VAL:HG23	2.53	0.42
1:B:82:LEU:O	1:B:111:ALA:HB1	2.19	0.42
1:O:62:SER:HA	1:O:73:VAL:CG2	2.48	0.42
1:A:55:ALA:CA	1:A:66:VAL:HG13	2.49	0.42
1:A:125:ILE:O	1:A:127:THR:HG22	2.19	0.42
1:A:172:MET:HE2	1:A:240:VAL:CG2	2.45	0.42
1:A:201:LEU:HD21	1:B:235:PRO:CG	2.48	0.42
1:B:22(A):LYS:HB3	1:B:24:PRO:CG	2.49	0.42
1:B:223:GLY:HA2	4:B:2384:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:248:LYS:NZ	1:O:248:LYS:HB3	2.28	0.42
1:A:0:LYS:HB2	1:A:0:LYS:HE3	1.28	0.42
1:A:178:TYR:HA	1:A:182:GLN:OE1	2.19	0.42
1:B:38:LYS:HD3	1:B:38:LYS:N	2.05	0.42
1:O:3:VAL:HG13	1:O:93:ILE:HD13	2.01	0.42
1:O:55:ALA:C	1:O:66:VAL:HG13	2.42	0.42
1:B:205:PRO:HA	1:B:230:LEU:HD23	2.02	0.42
1:O:64:ILE:CD1	1:O:65:SER:O	2.65	0.42
1:O:74:VAL:HG12	1:O:75:SER:N	2.35	0.42
1:O:281:ILE:CG2	1:O:282:ASP:N	2.82	0.42
1:A:3:VAL:HG13	1:A:93:ILE:HD13	2.02	0.42
1:B:90:ASP:CG	1:B:333:GLN:HE22	2.27	0.42
1:B:128:TYR:HA	1:B:133:ASN:HD21	1.83	0.42
1:A:82:LEU:O	1:A:111:ALA:HB1	2.19	0.42
1:B:139:HIS:NE2	1:B:332:TRP:CE3	2.88	0.42
1:B:174:THR:HG23	1:B:174:THR:O	2.18	0.42
1:B:281:ILE:HG22	1:B:282:ASP:N	2.34	0.42
1:O:14:ASN:HB3	1:O:318:SER:OG	2.20	0.42
1:O:234:THR:HA	1:O:235:PRO:HD3	1.85	0.42
1:O:279:VAL:O	1:O:280:SER:C	2.62	0.42
1:A:121:PRO:HD3	1:A:148:SER:N	2.34	0.42
1:O:203:ILE:O	1:O:205:PRO:HD3	2.20	0.42
1:A:22(A):LYS:CE	1:A:322:VAL:HG11	2.41	0.42
1:A:255:VAL:HG12	1:A:259:PHE:CE2	2.54	0.42
1:B:94:GLU:HG2	1:B:108:HIS:CD2	2.55	0.42
1:B:183:ARG:CD	1:B:187:ALA:HB3	2.34	0.42
1:O:22(A):LYS:HB3	1:O:24:PRO:CG	2.49	0.42
1:A:32:ASP:O	1:A:34:GLY:N	2.53	0.42
1:A:316:GLY:O	1:A:319:GLN:HB2	2.20	0.42
1:B:79:PRO:HA	1:B:82:LEU:HD12	2.00	0.42
1:A:128:TYR:CE2	1:A:137:TYR:HA	2.54	0.42
1:B:55:ALA:HB1	1:B:66:VAL:CG1	2.37	0.42
1:B:317:TYR:O	1:B:321:VAL:HG23	2.19	0.42
1:O:82:LEU:O	1:O:111:ALA:HB1	2.19	0.41
1:A:128:TYR:CA	1:A:133:ASN:HD21	2.31	0.41
1:B:300:MET:O	1:B:304:MET:HB3	2.20	0.41
1:A:280:SER:O	1:A:281:ILE:C	2.63	0.41
1:A:317:TYR:O	1:A:321:VAL:HG23	2.19	0.41
1:O:77:ARG:HG3	1:O:77:ARG:NH1	2.34	0.41
1:O:154:LEU:HA	1:O:157:PHE:CE1	2.55	0.41
1:O:167:ILE:CG1	1:O:244:VAL:HG21	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ALA:C	1:A:66:VAL:HG13	2.41	0.41
1:A:63:ALA:C	1:A:64:ILE:HG22	2.45	0.41
1:A:154:LEU:HA	1:A:157:PHE:CE1	2.55	0.41
1:A:158:VAL:HG11	1:A:221:LEU:HD13	2.02	0.41
1:A:251:PHE:CZ	1:A:254:GLU:HB2	2.56	0.41
1:O:130:VAL:HA	1:O:134:GLU:HB3	2.02	0.41
1:A:50:LEU:HD13	4:A:1340:HOH:O	2.20	0.41
1:A:94:GLU:OE1	1:A:96:THR:HG23	2.20	0.41
1:O:128:TYR:CA	1:O:133:ASN:HD21	2.33	0.41
1:O:133:ASN:ND2	1:O:133:ASN:C	2.78	0.41
1:A:100:VAL:HG23	1:A:122(A):LYS:HG3	2.01	0.41
1:A:117:LEU:HD12	1:A:117:LEU:C	2.46	0.41
1:A:194:ARG:HH11	1:A:205:PRO:HB2	1.86	0.41
1:A:281:ILE:CG2	1:A:282:ASP:N	2.81	0.41
1:A:312:ASP:OD1	1:A:315:TRP:N	2.46	0.41
1:B:124:ASP:HA	4:B:2386:HOH:O	2.19	0.41
1:B:236:ASN:O	1:B:237:VAL:HB	2.20	0.41
1:O:61:ASP:O	1:O:62:SER:HB3	2.20	0.41
1:B:32:ASP:C	1:B:34:GLY:N	2.76	0.41
1:O:11:ILE:HD11	3:O:6335:NDP:C7N	2.51	0.41
1:O:255:VAL:HG12	1:O:259:PHE:CE2	2.56	0.41
1:O:276:GLU:HA	1:O:277:PRO:HD3	1.72	0.41
1:A:137:TYR:HE1	1:A:144:ILE:HD11	1.83	0.41
1:B:117:LEU:C	1:B:117:LEU:HD12	2.46	0.41
1:B:204:VAL:HB	1:B:231:ARG:HB2	2.02	0.41
1:B:211:ALA:HB1	1:B:226:ASN:CA	2.48	0.41
1:O:135:GLU:H	1:O:135:GLU:CD	2.23	0.41
1:A:21:GLY:C	1:A:22(A):LYS:O	2.62	0.41
1:A:135:GLU:H	1:A:135:GLU:CD	2.24	0.41
1:B:31:ASN:ND2	3:B:2335:NDP:H2A	2.35	0.41
1:O:167:ILE:HG23	1:O:244:VAL:HG23	2.02	0.41
1:O:185:LEU:O	1:O:186:ASP:C	2.63	0.41
1:O:300:MET:O	1:O:304:MET:HB3	2.20	0.41
1:A:190:HIS:H	1:B:39:GLN:NE2	2.17	0.41
1:B:255:VAL:HG12	1:B:259:PHE:CE2	2.56	0.41
1:O:194:ARG:NH1	1:O:205:PRO:HG2	2.36	0.41
1:A:55:ALA:HA	1:A:66:VAL:CG1	2.51	0.41
1:B:23:SER:H	1:B:24:PRO:HD3	1.81	0.41
1:B:65:SER:O	1:B:66:VAL:C	2.64	0.41
1:O:22(A):LYS:HG3	4:O:6360:HOH:O	2.21	0.40
1:O:118:ILE:C	1:O:120:ALA:H	2.29	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:137:TYR:CD2	1:O:331:LYS:HG3	2.56	0.40
1:O:204:VAL:HB	1:O:231:ARG:HB2	2.02	0.40
1:A:176:HIS:HB3	1:A:231:ARG:HD3	2.03	0.40
1:A:236:ASN:O	1:A:237:VAL:HB	2.22	0.40
1:B:190:HIS:HB3	1:B:196:ALA:HB2	2.02	0.40
1:B:281:ILE:HD12	1:B:284:ARG:HD2	2.03	0.40
1:B:292:ILE:HD13	1:B:309:ALA:HB2	2.04	0.40
1:A:235:PRO:HG3	1:B:201:LEU:HD21	2.03	0.40
1:A:246:VAL:HG22	1:A:303:ASP:O	2.22	0.40
1:B:130:VAL:HA	1:B:134:GLU:HB3	2.03	0.40
1:B:195:ARG:HH22	1:B:231:ARG:NH2	2.19	0.40
1:O:50:LEU:HD12	1:O:50:LEU:HA	1.87	0.40
1:A:19:TRP:O	1:A:22(A):LYS:N	2.55	0.40
1:B:0:LYS:HB2	1:B:0:LYS:HE3	1.22	0.40
1:O:165:PHE:CE2	1:O:250:THR:OG1	2.75	0.40
1:A:39:GLN:OE1	1:B:188:SER:HB3	2.21	0.40
1:A:83:PRO:O	1:A:84:TRP:C	2.64	0.40
1:A:115:LYS:NZ	1:A:328:VAL:HG13	2.36	0.40
1:A:250:THR:O	1:A:299:VAL:HG11	2.22	0.40
1:B:236:ASN:OD1	1:B:314:GLU:HG3	2.22	0.40
1:O:317:TYR:CG	3:O:6335:NDP:H5N	2.57	0.40
1:A:49:ILE:HD11	1:B:185:LEU:CD2	2.52	0.40
1:A:260:ARG:O	1:A:264:ASP:OD2	2.40	0.40
1:A:276:GLU:HA	1:A:277:PRO:HD3	1.74	0.40
1:B:119:THR:HG23	1:B:317:TYR:HE2	1.86	0.40
1:B:158:VAL:HG11	1:B:221:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/335 (99%)	284 (86%)	36 (11%)	12 (4%)	2	16
1	B	332/335 (99%)	281 (85%)	38 (11%)	13 (4%)	2	14
1	O	332/335 (99%)	281 (85%)	38 (11%)	13 (4%)	2	14
All	All	996/1005 (99%)	846 (85%)	112 (11%)	38 (4%)	2	15

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	24	PRO
1	O	66	VAL
1	A	24	PRO
1	A	66	VAL
1	A	332	TRP
1	B	24	PRO
1	B	66	VAL
1	B	280	SER
1	O	34	GLY
1	O	124	ASP
1	O	280	SER
1	A	34	GLY
1	A	280	SER
1	B	34	GLY
1	O	233	PRO
1	A	124	ASP
1	A	210	ALA
1	A	233	PRO
1	B	124	ASP
1	O	22(A)	LYS
1	O	62	SER
1	O	210	ALA
1	O	237	VAL
1	O	332	TRP
1	A	62	SER
1	A	237	VAL
1	B	22(A)	LYS
1	B	62	SER
1	B	210	ALA
1	B	233	PRO
1	B	237	VAL
1	O	186	ASP
1	A	22(A)	LYS
1	A	281	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	186	ASP
1	O	281	ILE
1	B	281	ILE
1	B	120	ALA

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	277/277 (100%)	241 (87%)	36 (13%)	4	19
1	B	277/277 (100%)	241 (87%)	36 (13%)	4	19
1	O	277/277 (100%)	239 (86%)	38 (14%)	3	17
All	All	831/831 (100%)	721 (87%)	110 (13%)	4	18

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	0	LYS
1	O	19	TRP
1	O	22(A)	LYS
1	O	22(B)	ASP
1	O	23	SER
1	O	24	PRO
1	O	25	LEU
1	O	29	VAL
1	O	38	LYS
1	O	41	SER
1	O	50	LEU
1	O	56	ASP
1	O	64	ILE
1	O	77	ARG
1	O	93	ILE
1	O	94	GLU
1	O	96	THR
1	O	117	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	122(A)	LYS
1	O	125	ILE
1	O	127	THR
1	O	133	ASN
1	O	169	LYS
1	O	188	SER
1	O	206	THR
1	O	220	GLN
1	O	228	ILE
1	O	248	LYS
1	O	250	THR
1	O	251	PHE
1	O	266	GLU
1	O	268	LYS
1	O	281	ILE
1	O	285	CYS
1	O	286	THR
1	O	300	MET
1	O	313	ASN
1	O	333	GLN
1	A	0	LYS
1	A	22(A)	LYS
1	A	22(B)	ASP
1	A	23	SER
1	A	24	PRO
1	A	25	LEU
1	A	29	VAL
1	A	38	LYS
1	A	41	SER
1	A	50	LEU
1	A	56	ASP
1	A	64	ILE
1	A	77	ARG
1	A	93	ILE
1	A	94	GLU
1	A	96	THR
1	A	121	PRO
1	A	122(A)	LYS
1	A	125	ILE
1	A	127	THR
1	A	133	ASN
1	A	169	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	188	SER
1	A	205	PRO
1	A	206	THR
1	A	220	GLN
1	A	228	ILE
1	A	250	THR
1	A	251	PHE
1	A	268	LYS
1	A	281	ILE
1	A	285	CYS
1	A	286	THR
1	A	295	SER
1	A	300	MET
1	A	313	ASN
1	B	0	LYS
1	B	22(A)	LYS
1	B	22(B)	ASP
1	B	23	SER
1	B	24	PRO
1	B	25	LEU
1	B	29	VAL
1	B	38	LYS
1	B	41	SER
1	B	50	LEU
1	B	56	ASP
1	B	64	ILE
1	B	66	VAL
1	B	77	ARG
1	B	93	ILE
1	B	94	GLU
1	B	96	THR
1	B	117	LEU
1	B	122(A)	LYS
1	B	125	ILE
1	B	127	THR
1	B	133	ASN
1	B	169	LYS
1	B	188	SER
1	B	206	THR
1	B	220	GLN
1	B	228	ILE
1	B	250	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	251	PHE
1	B	268	LYS
1	B	281	ILE
1	B	285	CYS
1	B	286	THR
1	B	300	MET
1	B	313	ASN
1	B	332	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	42	HIS
1	O	81	ASN
1	O	133	ASN
1	O	152	ASN
1	O	163	GLN
1	O	202	ASN
1	O	256	ASN
1	O	333	GLN
1	A	42	HIS
1	A	81	ASN
1	A	133	ASN
1	A	152	ASN
1	A	163	GLN
1	A	202	ASN
1	A	220	GLN
1	A	256	ASN
1	B	42	HIS
1	B	81	ASN
1	B	133	ASN
1	B	152	ASN
1	B	163	GLN
1	B	202	ASN
1	B	220	GLN
1	B	256	ASN
1	B	333	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	O	6336	-	4,4,4	0.42	0	6,6,6	0.11	0
3	NDP	A	1335	2	51,52,52	1.56	8 (15%)	71,80,80	2.18	21 (29%)
3	NDP	O	6335	-	51,52,52	1.56	8 (15%)	71,80,80	2.18	21 (29%)
2	SO4	A	1336	3	4,4,4	0.33	0	6,6,6	0.10	0
3	NDP	B	2335	-	51,52,52	1.56	8 (15%)	71,80,80	2.18	21 (29%)
2	SO4	B	2337	-	4,4,4	0.35	0	6,6,6	0.19	0
2	SO4	B	2336	-	4,4,4	0.36	0	6,6,6	0.10	0
2	SO4	A	1337	-	4,4,4	0.20	0	6,6,6	0.13	0
2	SO4	O	6337	-	4,4,4	0.25	0	6,6,6	0.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	B	2335	-	-	8/34/77/77	0/5/5/5
3	NDP	A	1335	2	-	8/34/77/77	0/5/5/5
3	NDP	O	6335	-	-	8/34/77/77	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2335	NDP	C4N-C3N	-5.71	1.39	1.50
3	A	1335	NDP	C4N-C3N	-5.71	1.39	1.50
3	O	6335	NDP	C4N-C3N	-5.69	1.39	1.50
3	A	1335	NDP	P2B-O1X	4.12	1.63	1.50
3	B	2335	NDP	P2B-O1X	4.11	1.63	1.50
3	O	6335	NDP	P2B-O1X	4.11	1.63	1.50
3	A	1335	NDP	C4N-C5N	-3.62	1.39	1.49
3	O	6335	NDP	C4N-C5N	-3.62	1.39	1.49
3	B	2335	NDP	C4N-C5N	-3.58	1.39	1.49
3	B	2335	NDP	C5A-N7A	-3.11	1.33	1.39
3	A	1335	NDP	C5A-N7A	-3.08	1.33	1.39
3	O	6335	NDP	C5A-N7A	-3.04	1.33	1.39
3	A	1335	NDP	C7N-C3N	2.99	1.55	1.48
3	B	2335	NDP	C7N-C3N	2.98	1.55	1.48
3	O	6335	NDP	C7N-C3N	2.97	1.55	1.48
3	B	2335	NDP	C4A-N9A	-2.41	1.32	1.37
3	A	1335	NDP	C4A-N9A	-2.40	1.32	1.37
3	O	6335	NDP	C4A-N9A	-2.40	1.32	1.37
3	B	2335	NDP	C6N-C5N	2.33	1.40	1.33
3	A	1335	NDP	C6N-C5N	2.31	1.40	1.33
3	O	6335	NDP	C6N-C5N	2.31	1.40	1.33
3	A	1335	NDP	C2N-C3N	2.27	1.41	1.35
3	O	6335	NDP	C2N-C3N	2.25	1.41	1.35
3	B	2335	NDP	C2N-C3N	2.24	1.41	1.35

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	6335	NDP	N3A-C4A-N9A	7.38	139.72	127.17
3	A	1335	NDP	N3A-C4A-N9A	7.35	139.67	127.17
3	B	2335	NDP	N3A-C4A-N9A	7.33	139.64	127.17
3	O	6335	NDP	C5A-C4A-N3A	-6.04	118.40	126.72
3	A	1335	NDP	C5A-C4A-N3A	-5.98	118.48	126.72
3	B	2335	NDP	C5A-C4A-N3A	-5.97	118.49	126.72
3	A	1335	NDP	C4A-N9A-C8A	5.04	111.03	105.74
3	O	6335	NDP	C4A-N9A-C8A	5.01	111.00	105.74
3	B	2335	NDP	C4A-N9A-C8A	5.00	110.99	105.74
3	A	1335	NDP	N3A-C2A-N1A	-4.24	122.17	128.58
3	O	6335	NDP	N3A-C2A-N1A	-4.22	122.19	128.58
3	B	2335	NDP	N3A-C2A-N1A	-4.22	122.19	128.58
3	A	1335	NDP	C4B-O4B-C1B	-4.19	100.22	109.47
3	B	2335	NDP	C4B-O4B-C1B	-4.17	100.27	109.47
3	O	6335	NDP	C4B-O4B-C1B	-4.16	100.29	109.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	6335	NDP	C6A-C5A-N7A	-3.99	124.40	132.09
3	A	1335	NDP	C6A-C5A-N7A	-3.98	124.42	132.09
3	B	2335	NDP	C6A-C5A-N7A	-3.95	124.48	132.09
3	A	1335	NDP	O3X-P2B-O2X	3.75	121.85	107.80
3	O	6335	NDP	O3X-P2B-O2X	3.74	121.83	107.80
3	B	2335	NDP	O3X-P2B-O2X	3.73	121.81	107.80
3	A	1335	NDP	C5A-C4A-N9A	-3.63	101.85	105.81
3	B	2335	NDP	C5A-C4A-N9A	-3.62	101.87	105.81
3	O	6335	NDP	C5A-C4A-N9A	-3.60	101.88	105.81
3	O	6335	NDP	C2B-C1B-N9A	-3.36	108.22	113.75
3	A	1335	NDP	C2B-C1B-N9A	-3.33	108.28	113.75
3	O	6335	NDP	C6A-C5A-C4A	3.30	121.69	117.18
3	B	2335	NDP	C2B-C1B-N9A	-3.30	108.33	113.75
3	A	1335	NDP	C6A-C5A-C4A	3.27	121.64	117.18
3	O	6335	NDP	C2A-N3A-C4A	3.27	119.81	111.83
3	B	2335	NDP	C2A-N3A-C4A	3.25	119.76	111.83
3	A	1335	NDP	C2A-N3A-C4A	3.25	119.76	111.83
3	B	2335	NDP	C6A-C5A-C4A	3.24	121.60	117.18
3	A	1335	NDP	N9A-C8A-N7A	-3.05	109.61	113.94
3	B	2335	NDP	N9A-C8A-N7A	-3.02	109.65	113.94
3	O	6335	NDP	N9A-C8A-N7A	-3.00	109.68	113.94
3	A	1335	NDP	C4A-C5A-N7A	2.94	113.94	110.58
3	B	2335	NDP	C4A-C5A-N7A	2.92	113.92	110.58
3	O	6335	NDP	C4A-C5A-N7A	2.91	113.91	110.58
3	O	6335	NDP	O3D-C3D-C4D	-2.91	102.72	111.08
3	B	2335	NDP	O3D-C3D-C4D	-2.90	102.74	111.08
3	A	1335	NDP	O3D-C3D-C4D	-2.89	102.77	111.08
3	A	1335	NDP	P2B-O2B-C2B	-2.56	116.60	123.43
3	B	2335	NDP	P2B-O2B-C2B	-2.56	116.60	123.43
3	O	6335	NDP	P2B-O2B-C2B	-2.55	116.61	123.43
3	B	2335	NDP	C1D-N1N-C6N	-2.35	115.81	120.77
3	O	6335	NDP	C1D-N1N-C6N	-2.34	115.81	120.77
3	A	1335	NDP	C1D-N1N-C6N	-2.34	115.83	120.77
3	B	2335	NDP	O5D-PN-O1N	-2.24	100.04	108.94
3	O	6335	NDP	O5D-PN-O1N	-2.23	100.08	108.94
3	B	2335	NDP	N6A-C6A-N1A	2.23	123.33	118.38
3	A	1335	NDP	O5D-PN-O1N	-2.22	100.12	108.94
3	A	1335	NDP	O2X-P2B-O1X	-2.22	102.20	110.83
3	O	6335	NDP	O2X-P2B-O1X	-2.21	102.23	110.83
3	B	2335	NDP	O2X-P2B-O1X	-2.21	102.23	110.83
3	A	1335	NDP	N6A-C6A-N1A	2.20	123.28	118.38
3	O	6335	NDP	N6A-C6A-N1A	2.19	123.26	118.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1335	NDP	C3N-C2N-N1N	-2.16	120.04	123.20
3	B	2335	NDP	C3N-C2N-N1N	-2.11	120.10	123.20
3	O	6335	NDP	C3N-C2N-N1N	-2.09	120.13	123.20
3	B	2335	NDP	O4B-C1B-C2B	-2.07	103.02	106.59
3	A	1335	NDP	O4B-C1B-C2B	-2.07	103.03	106.59
3	O	6335	NDP	O4B-C1B-C2B	-2.06	103.04	106.59

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	6335	NDP	C5B-O5B-PA-O1A
3	O	6335	NDP	PN-O3-PA-O5B
3	A	1335	NDP	C5B-O5B-PA-O1A
3	A	1335	NDP	PN-O3-PA-O5B
3	B	2335	NDP	C5B-O5B-PA-O1A
3	B	2335	NDP	PN-O3-PA-O5B
3	O	6335	NDP	PA-O3-PN-O2N
3	A	1335	NDP	PA-O3-PN-O2N
3	B	2335	NDP	PA-O3-PN-O2N
3	O	6335	NDP	C5B-O5B-PA-O3
3	A	1335	NDP	C5B-O5B-PA-O3
3	B	2335	NDP	C5B-O5B-PA-O3
3	O	6335	NDP	O4D-C1D-N1N-C6N
3	A	1335	NDP	O4D-C1D-N1N-C6N
3	B	2335	NDP	O4D-C1D-N1N-C6N
3	O	6335	NDP	C2D-C1D-N1N-C6N
3	A	1335	NDP	C2D-C1D-N1N-C6N
3	B	2335	NDP	C2D-C1D-N1N-C6N
3	B	2335	NDP	O4B-C4B-C5B-O5B
3	O	6335	NDP	PA-O3-PN-O1N
3	A	1335	NDP	PA-O3-PN-O1N
3	B	2335	NDP	PA-O3-PN-O1N
3	O	6335	NDP	O4B-C4B-C5B-O5B
3	A	1335	NDP	O4B-C4B-C5B-O5B

There are no ring outliers.

4 monomers are involved in 18 short contacts:

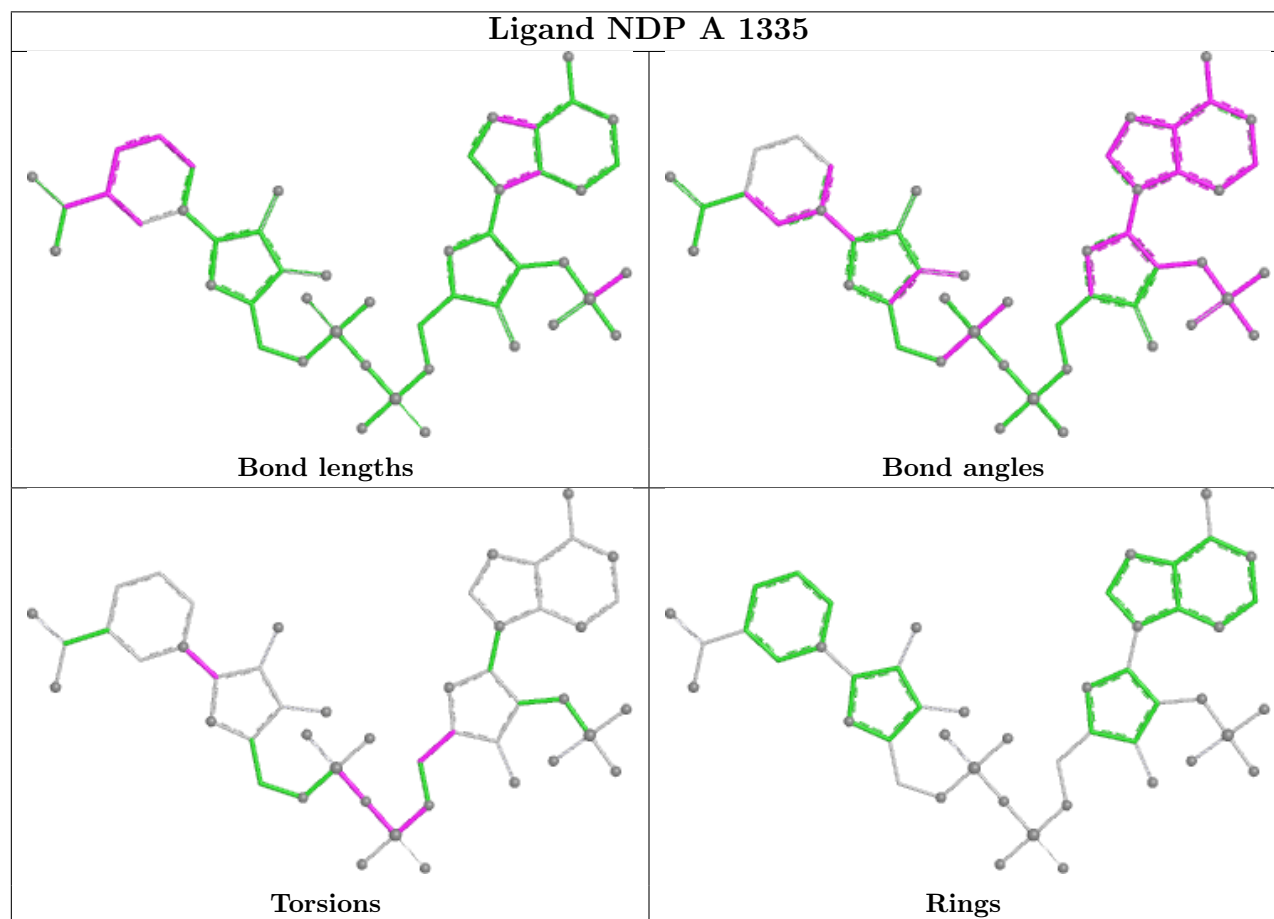
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1335	NDP	5	0

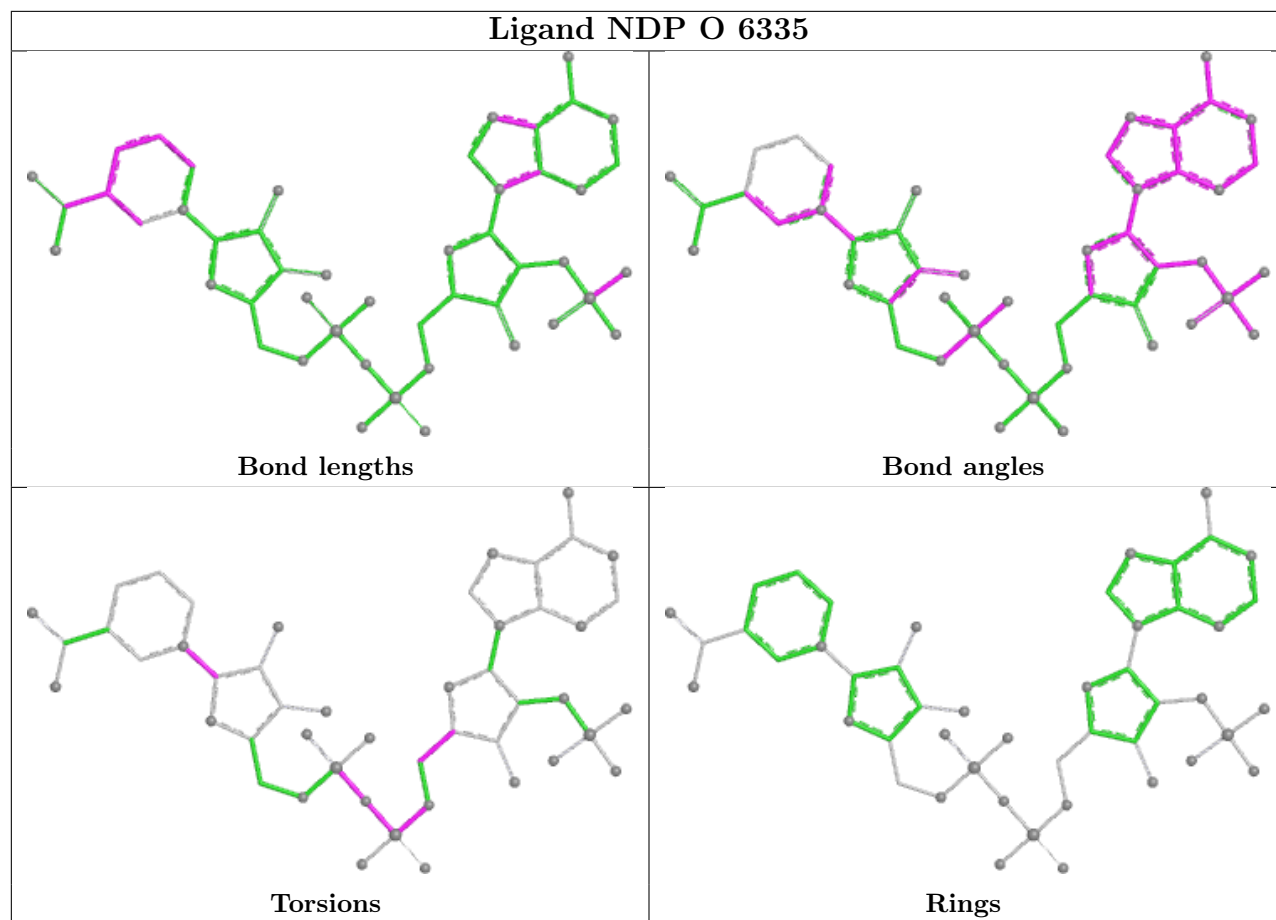
Continued on next page...

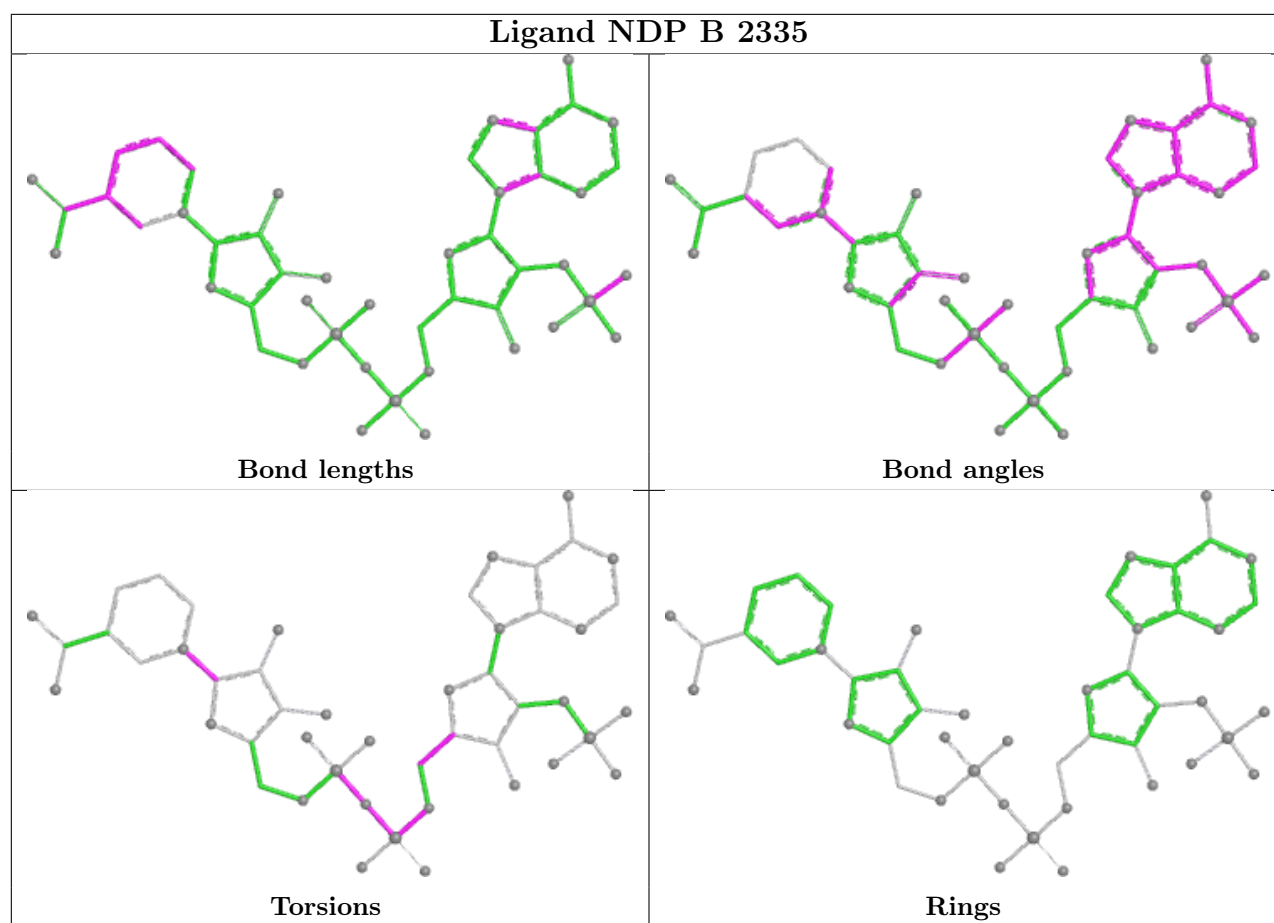
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	6335	NDP	7	0
2	A	1336	SO4	1	0
3	B	2335	NDP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.