



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2017 – 07:57 AM EDT

PDB ID : 1SEJ
Title : Crystal Structure of Dihydrofolate Reductase-Thymidylate Synthase from *Cryptosporidium hominis* Bound to 1843U89/NADPH/dUMP
Authors : Anderson, A.C.
Deposited on : unknown
Resolution : 2.87 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

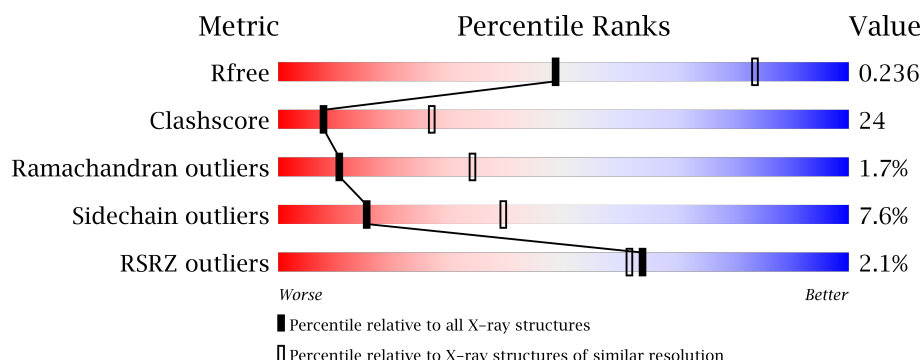
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2135 (2.90-2.86)
Clashscore	112137	2400 (2.90-2.86)
Ramachandran outliers	110173	2346 (2.90-2.86)
Sidechain outliers	110143	2349 (2.90-2.86)
RSRZ outliers	101464	2149 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	521	<div> <div>2%</div> <div>60% 33% 6%</div> </div>
1	B	521	<div> <div>2%</div> <div>60% 32% 7%</div> </div>
1	C	521	<div> <div>2%</div> <div>60% 32% 6%</div> </div>
1	D	521	<div> <div>2%</div> <div>61% 32% 6%</div> </div>
1	E	521	<div> <div>3%</div> <div>62% 31% 6%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UMP	A	603	-	-	-	X
2	UMP	B	607	-	-	-	X
2	UMP	C	611	-	-	-	X
3	F89	A	605	-	-	-	X
3	F89	B	609	-	-	-	X
3	F89	C	612	-	-	-	X
3	F89	C	613	-	-	-	X
3	F89	D	617	-	-	-	X
3	F89	E	621	-	-	-	X

2 Entry composition [i](#)

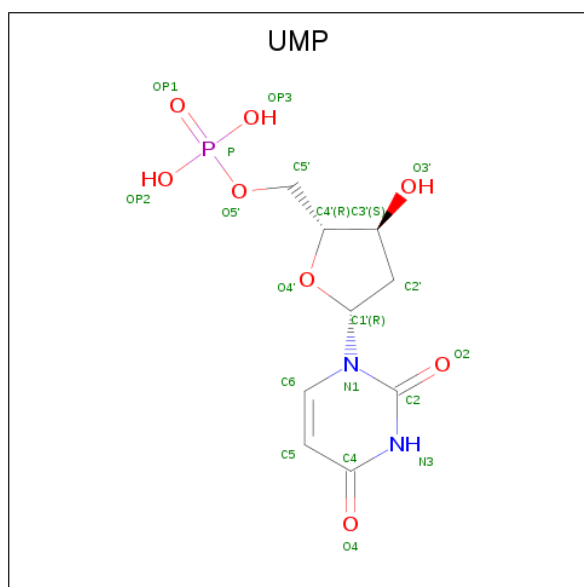
There are 5 unique types of molecules in this entry. The entry contains 22194 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			4223	2694	713	793	23			
1	B	519	Total	C	N	O	S	0	0	0
			4223	2694	713	793	23			
1	C	519	Total	C	N	O	S	0	0	0
			4223	2694	713	793	23			
1	D	519	Total	C	N	O	S	0	0	0
			4223	2694	713	793	23			
1	E	519	Total	C	N	O	S	0	0	0
			4223	2694	713	793	23			

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



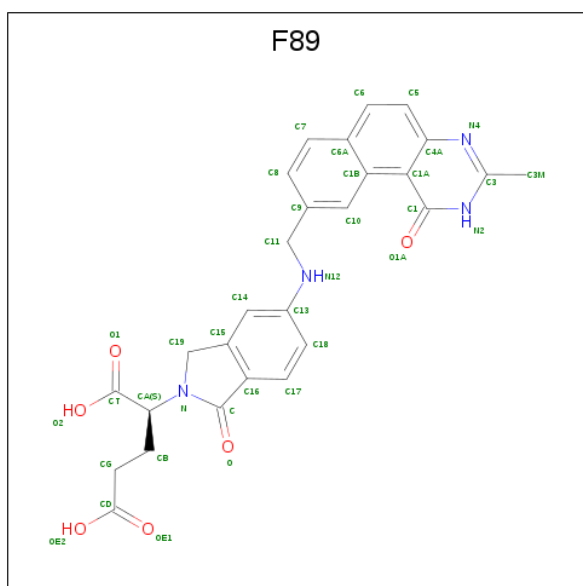
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is S)-2-(5(((1,2-DIHYDRO-3-METHYL-1-OXOBENZO(F)QUINAZOLIN-9-YL) METHYL)AMINO)1-OXO-2-ISOINDOLINYL)GLUTARIC ACID (three-letter code: F89) (formula: C₂₇H₂₄N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			37	27	4	6		
3	A	1	Total	C	N	O	0	0
			37	27	4	6		
3	B	1	Total	C	N	O	0	0
			37	27	4	6		
3	B	1	Total	C	N	O	0	0
			37	27	4	6		
3	C	1	Total	C	N	O	0	0
			37	27	4	6		
3	C	1	Total	C	N	O	0	0
			37	27	4	6		

Continued on next page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total 37	C 27	N 4	O 6	0	0
3	D	1	Total 37	C 27	N 4	O 6	0	0
3	E	1	Total 37	C 27	N 4	O 6	0	0
3	E	1	Total 37	C 27	N 4	O 6	0	0

- # NDP

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

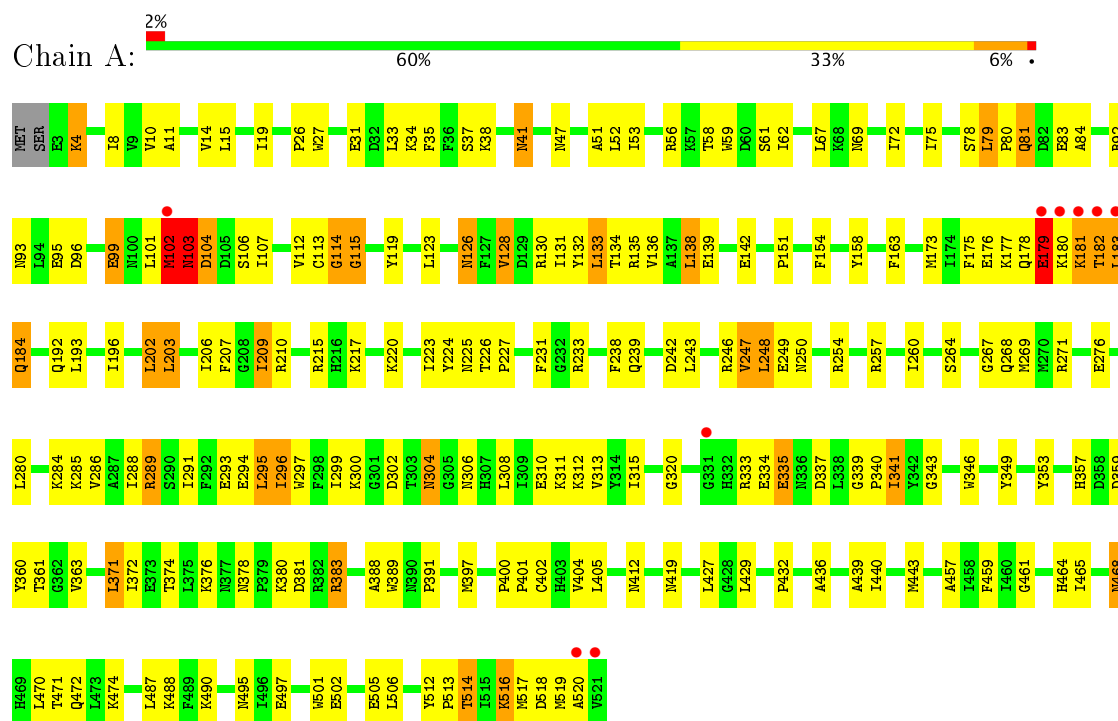
- 

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	93	Total 93	O 93	0	0
5	B	101	Total 101	O 101	0	0
5	C	77	Total 77	O 77	0	0
5	D	67	Total 67	O 67	0	0
5	E	31	Total 31	O 31	0	0

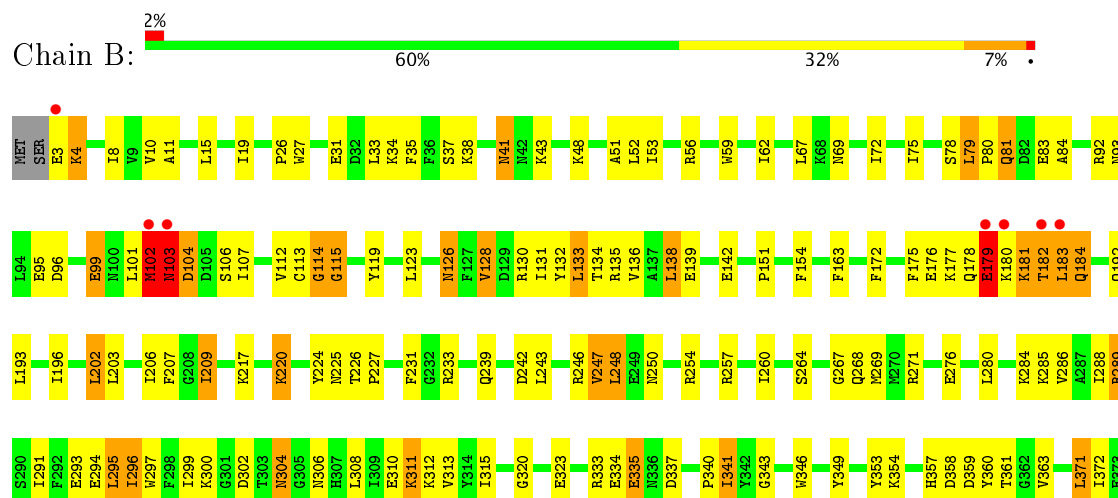
3 Residue-property plots

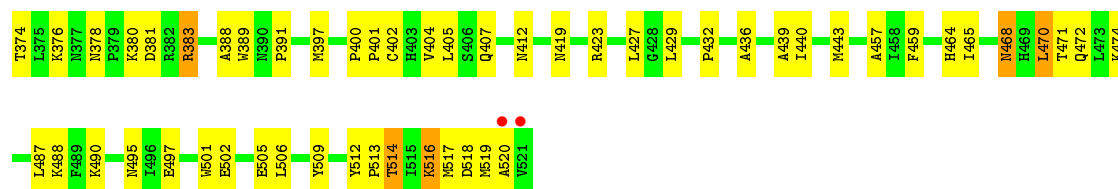
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: bifunctional dihydrofolate reductase-thymidylate synthase

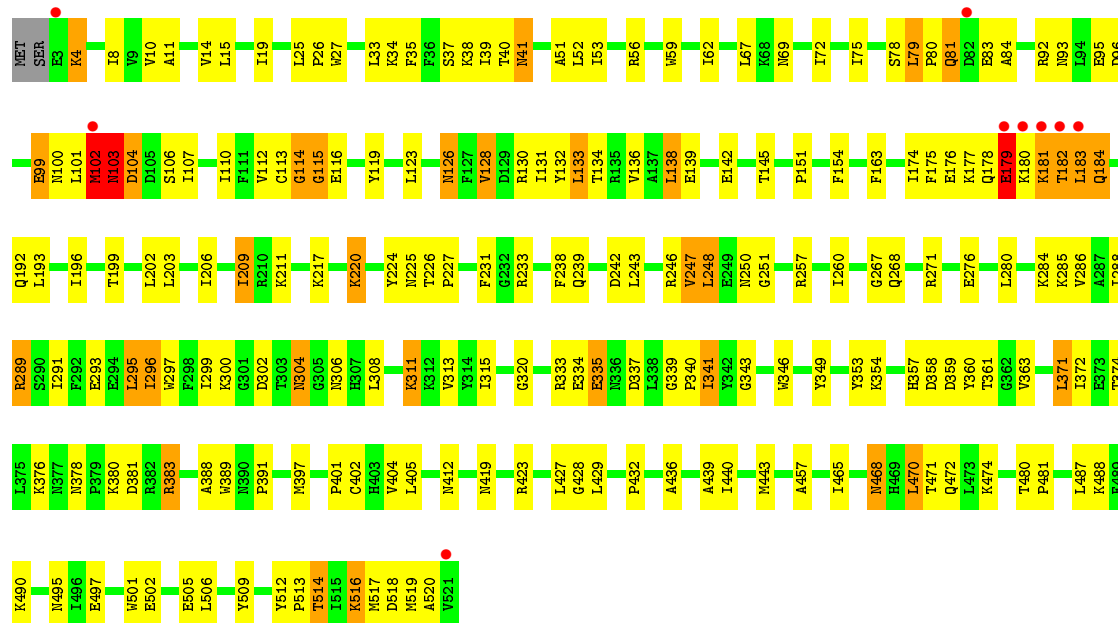


- Molecule 1: bifunctional dihydrofolate reductase-thymidylate synthase

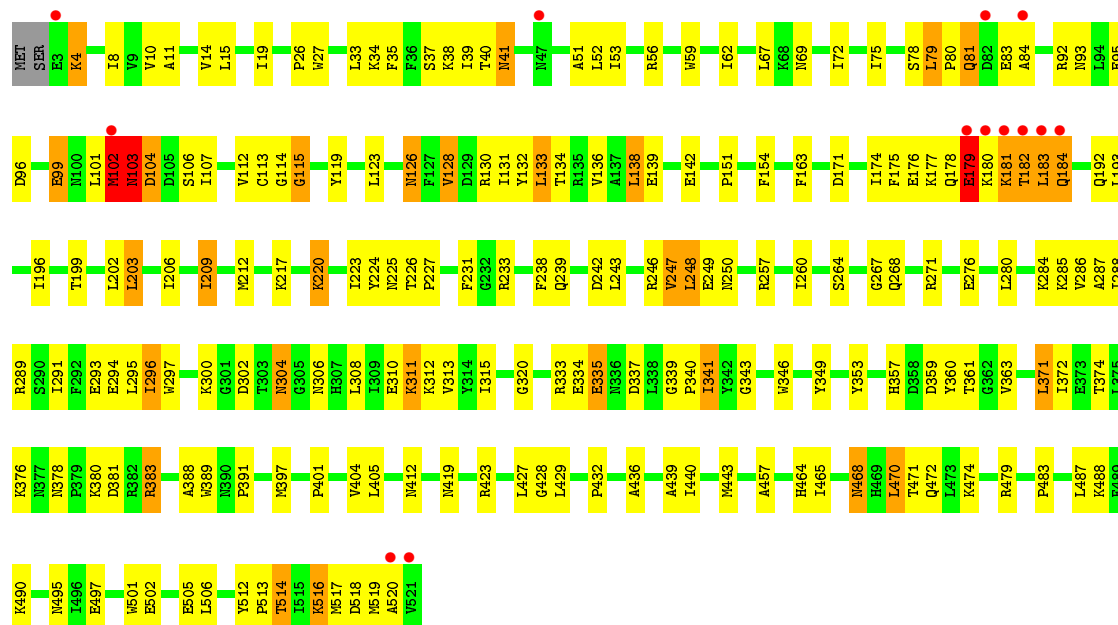




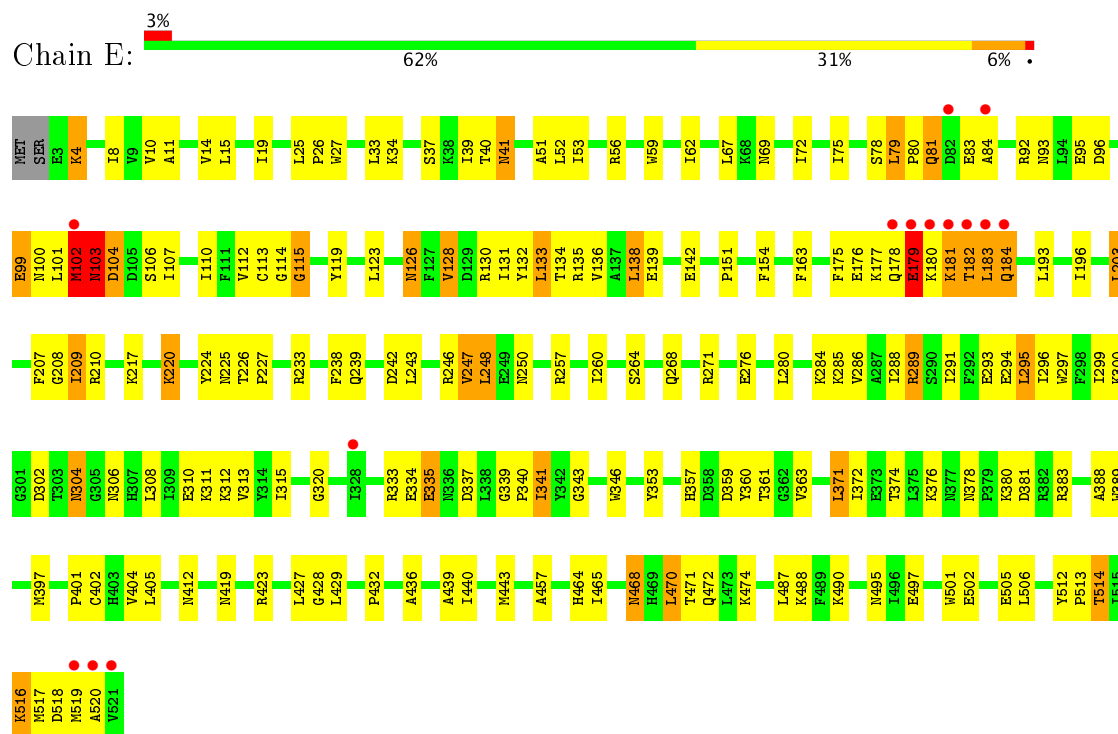
- Molecule 1: bifunctional dihydrofolate reductase-thymidylate synthase



- Molecule 1: bifunctional dihydrofolate reductase-thymidylate synthase



- Molecule 1: bifunctional dihydrofolate reductase-thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.90 Å 116.30 Å 219.70 Å 90.00° 95.23° 90.00°	Depositor
Resolution (Å)	45.15 – 2.87 45.15 – 2.87	Depositor EDS
% Data completeness (in resolution range)	90.4 (45.15-2.87) 90.5 (45.15-2.87)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.86 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.237 0.219 , 0.236	Depositor DCC
R_{free} test set	11178 reflections (9.99%)	DCC
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	22194	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: NDP, F89, UMP

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	0.40	0/4320	0.70	5/5838 (0.1%)
1	B	0.41	0/4320	0.73	6/5838 (0.1%)
1	C	0.40	0/4320	0.70	5/5838 (0.1%)
1	D	0.40	0/4320	0.70	4/5838 (0.1%)
1	E	0.42	0/4320	0.73	5/5838 (0.1%)
All	All	0.41	0/21600	0.71	25/29190 (0.1%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	257	ARG	NE-CZ-NH2	-14.20	113.20	120.30
1	E	257	ARG	NE-CZ-NH1	13.77	127.18	120.30
1	B	257	ARG	NE-CZ-NH2	-13.71	113.44	120.30
1	B	257	ARG	NE-CZ-NH1	13.56	127.08	120.30
1	A	257	ARG	NE-CZ-NH1	-9.18	115.71	120.30
1	D	257	ARG	NE-CZ-NH1	-9.02	115.79	120.30
1	A	257	ARG	NE-CZ-NH2	8.32	124.46	120.30
1	C	257	ARG	NE-CZ-NH1	-8.20	116.20	120.30
1	D	257	ARG	NE-CZ-NH2	8.14	124.37	120.30
1	C	257	ARG	NE-CZ-NH2	7.90	124.25	120.30
1	E	257	ARG	CD-NE-CZ	6.67	132.94	123.60
1	B	257	ARG	CD-NE-CZ	6.47	132.66	123.60
1	A	115	GLY	N-CA-C	-5.40	99.61	113.10
1	E	115	GLY	N-CA-C	-5.37	99.67	113.10
1	C	115	GLY	N-CA-C	-5.30	99.86	113.10
1	D	115	GLY	N-CA-C	-5.26	99.96	113.10
1	B	115	GLY	N-CA-C	-5.24	100.00	113.10
1	A	114	GLY	N-CA-C	5.21	126.11	113.10
1	B	114	GLY	N-CA-C	5.17	126.02	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	LYS	N-CA-C	-5.12	97.17	111.00
1	E	180	LYS	N-CA-C	-5.11	97.22	111.00
1	C	114	GLY	N-CA-C	5.08	125.81	113.10
1	A	180	LYS	N-CA-C	-5.06	97.33	111.00
1	B	180	LYS	N-CA-C	-5.05	97.37	111.00
1	D	180	LYS	N-CA-C	-5.02	97.44	111.00

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	4223	0	4159	218	0
1	B	4223	0	4159	211	0
1	C	4223	0	4159	207	0
1	D	4223	0	4159	206	0
1	E	4223	0	4159	197	0
2	A	20	0	11	2	0
2	B	20	0	11	3	0
2	C	20	0	11	3	0
2	D	20	0	11	2	0
2	E	20	0	11	2	0
3	A	74	0	44	16	0
3	B	74	0	44	13	0
3	C	74	0	44	15	0
3	D	74	0	44	17	0
3	E	74	0	44	17	0
4	A	48	0	26	10	0
4	B	48	0	26	8	0
4	C	48	0	26	8	0
4	D	48	0	26	8	0
4	E	48	0	26	8	0
5	A	93	0	0	2	0
5	B	101	0	0	3	0
5	C	77	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	67	0	0	4	0
5	E	31	0	0	1	0
All	All	22194	0	21200	1028	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 24.

All (1028) 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:E:341:ILE:HA	1:E:397:MET:HE3	1.32	1.10
1:C:341:ILE:HA	1:C:397:MET:HE3	1.35	1.09
1:A:341:ILE:HA	1:A:397:MET:HE3	1.34	1.07
1:D:341:ILE:HA	1:D:397:MET:HE3	1.34	1.06
1:B:341:ILE:HA	1:B:397:MET:HE3	1.34	1.04
1:D:209:ILE:H	1:D:209:ILE:HD12	1.25	1.02
1:B:209:ILE:HD12	1:B:209:ILE:H	1.24	1.01
1:A:209:ILE:H	1:A:209:ILE:HD12	1.23	1.00
1:E:209:ILE:HD12	1:E:209:ILE:H	1.23	1.00
1:C:209:ILE:H	1:C:209:ILE:HD12	1.24	0.99
1:B:178:GLN:O	1:B:179:GLU:HB2	1.70	0.91
1:D:178:GLN:O	1:D:179:GLU:HB2	1.70	0.91
1:E:178:GLN:O	1:E:179:GLU:HB2	1.70	0.91
1:C:178:GLN:O	1:C:179:GLU:HB2	1.70	0.91
1:D:33:LEU:HB3	3:D:617:F89:HG1	1.55	0.89
1:A:178:GLN:O	1:A:179:GLU:HB2	1.71	0.88
1:E:360:TYR:O	1:E:363:VAL:HG12	1.81	0.81
1:C:26:PRO:HG2	1:C:27:TRP:CE3	2.16	0.80
3:A:605:F89:H10	3:A:605:F89:O1A	1.81	0.80
1:E:209:ILE:CD1	1:E:209:ILE:H	1.95	0.80
1:A:209:ILE:H	1:A:209:ILE:CD1	1.94	0.80
1:A:289:ARG:HH11	1:A:289:ARG:HB3	1.47	0.79
3:D:617:F89:H10	3:D:617:F89:O1A	1.81	0.79
1:C:231:PHE:CD2	1:D:192:GLN:HG3	2.16	0.79
1:D:360:TYR:O	1:D:363:VAL:HG12	1.83	0.79
3:B:609:F89:H10	3:B:609:F89:O1A	1.81	0.79
3:A:604:F89:O1A	3:A:604:F89:H10	1.83	0.78
1:A:304:ASN:ND2	1:A:306:ASN:H	1.82	0.78
1:B:26:PRO:HG2	1:B:27:TRP:CE3	2.17	0.78
1:E:304:ASN:ND2	1:E:306:ASN:H	1.81	0.78
1:C:4:LYS:CB	1:C:101:LEU:HD23	2.13	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:613:F89:O1A	3:C:613:F89:H10	1.82	0.78
1:C:209:ILE:CD1	1:C:209:ILE:H	1.94	0.78
1:E:26:PRO:HG2	1:E:27:TRP:CE3	2.18	0.78
1:A:360:TYR:O	1:A:363:VAL:HG12	1.82	0.78
1:B:209:ILE:H	1:B:209:ILE:CD1	1.95	0.78
1:C:304:ASN:ND2	1:C:306:ASN:H	1.82	0.77
3:B:608:F89:O1A	3:B:608:F89:H10	1.83	0.77
1:E:4:LYS:CB	1:E:101:LEU:HD23	2.14	0.77
1:E:289:ARG:HH11	1:E:289:ARG:HB3	1.50	0.77
1:D:26:PRO:HG2	1:D:27:TRP:CE3	2.19	0.77
3:E:620:F89:H10	3:E:620:F89:O1A	1.84	0.77
1:A:192:GLN:HG3	1:B:231:PHE:CD2	2.20	0.77
1:C:193:LEU:HD21	1:C:196:ILE:HD12	1.66	0.77
1:C:289:ARG:HH11	1:C:289:ARG:HB3	1.50	0.77
3:C:612:F89:H10	3:C:612:F89:O1A	1.82	0.77
1:E:26:PRO:HG2	1:E:27:TRP:CZ3	2.19	0.77
1:D:209:ILE:H	1:D:209:ILE:CD1	1.96	0.76
1:C:304:ASN:HD22	1:C:304:ASN:C	1.88	0.76
1:B:289:ARG:HB3	1:B:289:ARG:HH11	1.50	0.76
1:C:192:GLN:HG3	1:D:231:PHE:CD2	2.21	0.76
3:E:621:F89:H10	3:E:621:F89:O1A	1.82	0.76
3:D:616:F89:O1A	3:D:616:F89:H10	1.83	0.76
1:B:304:ASN:ND2	1:B:306:ASN:H	1.81	0.76
1:B:360:TYR:O	1:B:363:VAL:HG12	1.86	0.76
1:B:4:LYS:CB	1:B:101:LEU:HD23	2.15	0.75
3:C:613:F89:C6	4:C:614:NDP:H42N	2.16	0.75
1:D:304:ASN:ND2	1:D:306:ASN:H	1.84	0.75
1:A:193:LEU:HD21	1:A:196:ILE:HD12	1.69	0.75
1:A:304:ASN:HD22	1:A:304:ASN:C	1.90	0.75
1:D:4:LYS:CB	1:D:101:LEU:HD23	2.15	0.75
1:A:4:LYS:CB	1:A:101:LEU:HD23	2.15	0.75
1:B:209:ILE:HD12	1:B:209:ILE:N	2.01	0.75
1:C:26:PRO:HG2	1:C:27:TRP:CZ3	2.21	0.75
1:D:26:PRO:HG2	1:D:27:TRP:CZ3	2.21	0.75
1:C:360:TYR:O	1:C:363:VAL:HG12	1.86	0.75
1:A:26:PRO:HG2	1:A:27:TRP:CE3	2.20	0.75
1:D:289:ARG:HH11	1:D:289:ARG:HB3	1.51	0.74
1:D:304:ASN:C	1:D:304:ASN:HD22	1.90	0.74
1:C:209:ILE:N	1:C:209:ILE:HD12	2.02	0.74
1:D:193:LEU:HD21	1:D:196:ILE:HD12	1.68	0.74
1:E:246:ARG:HH11	1:E:268:GLN:HE21	1.35	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ARG:HH11	1:B:268:GLN:HE21	1.35	0.74
1:E:209:ILE:HD12	1:E:209:ILE:N	2.01	0.74
1:E:217:LYS:H	1:E:250:ASN:HD21	1.35	0.74
1:A:26:PRO:HG2	1:A:27:TRP:CZ3	2.22	0.74
1:C:56:ARG:HD3	4:C:614:NDP:O1X	1.87	0.74
1:B:304:ASN:HD22	1:B:304:ASN:C	1.91	0.74
1:A:209:ILE:N	1:A:209:ILE:HD12	2.01	0.73
1:B:26:PRO:HG2	1:B:27:TRP:CZ3	2.23	0.73
1:C:33:LEU:HB3	3:C:613:F89:HG1	1.70	0.73
1:C:246:ARG:HH11	1:C:268:GLN:HE21	1.34	0.73
1:A:359:ASP:OD2	1:A:361:THR:HG22	1.89	0.73
1:E:193:LEU:HD21	1:E:196:ILE:HD12	1.70	0.73
1:E:246:ARG:HH11	1:E:268:GLN:NE2	1.87	0.73
1:E:304:ASN:C	1:E:304:ASN:HD22	1.92	0.73
1:D:217:LYS:H	1:D:250:ASN:HD21	1.36	0.73
1:E:516:LYS:HE3	1:E:518:ASP:OD1	1.88	0.73
1:A:231:PHE:CD2	1:B:192:GLN:HG3	2.24	0.72
1:B:193:LEU:HD21	1:B:196:ILE:HD12	1.70	0.72
1:E:304:ASN:HD22	1:E:306:ASN:H	1.36	0.72
1:E:359:ASP:OD2	1:E:361:THR:HG22	1.89	0.72
1:E:151:PRO:HG2	1:E:154:PHE:HD2	1.54	0.72
1:A:38:LYS:HB3	1:B:202:LEU:HG	1.72	0.72
1:D:516:LYS:HE3	1:D:518:ASP:OD1	1.89	0.72
1:E:33:LEU:HB3	3:E:621:F89:HG1	1.70	0.72
1:B:217:LYS:H	1:B:250:ASN:HD21	1.38	0.71
1:A:271:ARG:NH2	1:B:267:GLY:O	2.23	0.71
1:C:246:ARG:HH11	1:C:268:GLN:NE2	1.87	0.71
1:D:209:ILE:N	1:D:209:ILE:HD12	2.02	0.71
1:D:246:ARG:HH11	1:D:268:GLN:HE21	1.37	0.71
1:C:217:LYS:H	1:C:250:ASN:HD21	1.38	0.71
1:D:34:LYS:HD3	5:D:678:HOH:O	1.90	0.71
1:A:217:LYS:H	1:A:250:ASN:HD21	1.38	0.71
1:C:304:ASN:HD22	1:C:306:ASN:H	1.39	0.70
1:A:516:LYS:HE3	1:A:518:ASP:OD1	1.91	0.70
1:D:151:PRO:HG2	1:D:154:PHE:HD2	1.56	0.70
1:C:349:TYR:CE2	1:D:391:PRO:HD2	2.27	0.70
1:C:4:LYS:HB2	1:C:101:LEU:HD23	1.72	0.70
1:D:359:ASP:OD2	1:D:361:THR:HG22	1.91	0.70
1:E:4:LYS:HB2	1:E:101:LEU:HD23	1.73	0.70
1:A:246:ARG:HH11	1:A:268:GLN:HE21	1.37	0.70
1:A:4:LYS:HB2	1:A:101:LEU:HD23	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ASN:HD22	1:B:306:ASN:H	1.37	0.70
1:D:296:ILE:O	1:D:300:LYS:HG2	1.92	0.70
1:C:516:LYS:HE3	1:C:518:ASP:OD1	1.92	0.69
1:B:246:ARG:HH11	1:B:268:GLN:NE2	1.90	0.69
1:E:289:ARG:HG3	1:E:501:TRP:CE2	2.28	0.69
1:A:202:LEU:HG	1:B:38:LYS:HB3	1.74	0.69
1:D:56:ARG:HD3	4:D:618:NDP:O1X	1.93	0.69
1:A:246:ARG:HH11	1:A:268:GLN:NE2	1.91	0.69
1:A:304:ASN:HD22	1:A:306:ASN:H	1.37	0.69
1:A:315:ILE:HD13	3:A:604:F89:C18	2.21	0.69
1:B:516:LYS:HE3	1:B:518:ASP:OD1	1.92	0.69
1:C:333:ARG:HG3	1:C:337:ASP:HB3	1.75	0.69
1:D:315:ILE:HD12	3:D:616:F89:C8	2.22	0.69
1:B:4:LYS:HE2	1:B:101:LEU:HA	1.75	0.69
1:C:419:ASN:ND2	1:C:457:ALA:HB3	2.08	0.69
1:D:289:ARG:HG3	1:D:501:TRP:CE2	2.28	0.69
1:C:151:PRO:HG2	1:C:154:PHE:HD2	1.57	0.68
1:C:296:ILE:HD12	1:C:297:TRP:H	1.58	0.68
1:B:4:LYS:HB2	1:B:101:LEU:HD23	1.75	0.68
1:D:246:ARG:HH11	1:D:268:GLN:NE2	1.92	0.68
1:A:4:LYS:HE2	1:A:101:LEU:HA	1.75	0.68
1:B:333:ARG:HG3	1:B:337:ASP:HB3	1.76	0.68
1:E:56:ARG:HD3	4:E:622:NDP:O1X	1.94	0.68
1:C:4:LYS:HE2	1:C:101:LEU:HA	1.75	0.68
1:C:206:ILE:HD11	1:D:35:PHE:HA	1.76	0.68
1:D:4:LYS:HB2	1:D:101:LEU:HD23	1.74	0.68
1:A:33:LEU:HB3	3:A:605:F89:HG1	1.76	0.67
1:B:151:PRO:HG2	1:B:154:PHE:HD2	1.59	0.67
1:C:296:ILE:HD12	1:C:297:TRP:N	2.10	0.67
1:A:391:PRO:HD2	1:B:349:TYR:CE2	2.30	0.67
1:E:333:ARG:HG3	1:E:337:ASP:HB3	1.75	0.67
1:C:81:GLN:HE22	1:C:92:ARG:NE	1.93	0.67
1:D:304:ASN:HD22	1:D:306:ASN:H	1.40	0.67
1:E:4:LYS:HE2	1:E:101:LEU:HA	1.76	0.67
1:C:391:PRO:HD2	1:D:349:TYR:CE2	2.29	0.67
1:B:99:GLU:C	1:B:99:GLU:OE2	2.34	0.67
1:C:104:ASP:C	1:C:106:SER:H	1.98	0.67
1:A:333:ARG:HG3	1:A:337:ASP:HB3	1.76	0.67
1:A:34:LYS:HG2	1:B:206:ILE:HG12	1.77	0.67
1:D:104:ASP:C	1:D:106:SER:H	1.99	0.66
1:B:359:ASP:OD2	1:B:361:THR:HG22	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:ARG:HG3	1:D:337:ASP:HB3	1.77	0.66
1:A:151:PRO:HG2	1:A:154:PHE:HD2	1.60	0.66
1:E:419:ASN:ND2	1:E:457:ALA:HB3	2.10	0.66
1:A:296:ILE:O	1:A:300:LYS:HG2	1.96	0.66
1:B:81:GLN:HE22	1:B:92:ARG:NE	1.93	0.66
1:C:315:ILE:HD13	3:C:612:F89:C18	2.25	0.66
1:B:296:ILE:O	1:B:300:LYS:HG2	1.95	0.66
1:E:217:LYS:N	1:E:250:ASN:HD21	1.93	0.66
1:E:296:ILE:O	1:E:300:LYS:HG2	1.95	0.66
1:B:56:ARG:HD3	4:B:610:NDP:O1X	1.95	0.65
1:C:267:GLY:O	1:D:271:ARG:NH2	2.29	0.65
1:C:359:ASP:OD2	1:C:361:THR:HG22	1.96	0.65
1:A:56:ARG:HD3	4:A:606:NDP:O1X	1.96	0.65
1:C:79:LEU:HD23	1:C:80:PRO:HD2	1.77	0.65
1:D:225:ASN:O	1:D:233:ARG:NH2	2.28	0.65
1:E:79:LEU:HD23	1:E:80:PRO:HD2	1.78	0.65
1:D:217:LYS:N	1:D:250:ASN:HD21	1.94	0.65
1:A:35:PHE:HA	1:B:206:ILE:HD11	1.79	0.65
1:A:81:GLN:HE22	1:A:92:ARG:NE	1.95	0.65
1:B:468:ASN:N	1:B:468:ASN:HD22	1.94	0.65
1:B:79:LEU:HD23	1:B:80:PRO:HD2	1.79	0.65
1:D:4:LYS:HE2	1:D:101:LEU:HA	1.77	0.65
1:E:67:LEU:HG	1:E:72:ILE:HD11	1.77	0.64
1:D:293:GLU:HA	1:D:296:ILE:HD11	1.78	0.64
1:A:349:TYR:CE2	1:B:391:PRO:HD2	2.33	0.64
1:C:296:ILE:O	1:C:300:LYS:HG2	1.97	0.64
1:B:104:ASP:C	1:B:106:SER:H	1.98	0.64
1:C:289:ARG:HG3	1:C:501:TRP:CE2	2.33	0.64
1:D:79:LEU:HD23	1:D:80:PRO:HD2	1.80	0.64
1:A:104:ASP:C	1:A:106:SER:H	1.99	0.64
1:A:267:GLY:O	1:B:271:ARG:NH2	2.31	0.64
1:D:315:ILE:HD13	3:D:616:F89:C18	2.28	0.64
1:B:217:LYS:N	1:B:250:ASN:HD21	1.96	0.63
1:C:67:LEU:HG	1:C:72:ILE:HD11	1.79	0.63
1:E:225:ASN:O	1:E:233:ARG:NH2	2.30	0.63
1:C:99:GLU:C	1:C:99:GLU:OE2	2.37	0.63
1:E:104:ASP:C	1:E:106:SER:H	2.01	0.63
1:A:304:ASN:HD21	1:A:306:ASN:HB2	1.62	0.63
1:A:67:LEU:HG	1:A:72:ILE:HD11	1.81	0.63
1:A:79:LEU:HD23	1:A:80:PRO:HD2	1.81	0.63
1:B:293:GLU:HA	1:B:296:ILE:HD11	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ASN:H	1:B:468:ASN:HD22	1.44	0.63
1:D:81:GLN:HE22	1:D:92:ARG:NE	1.96	0.63
1:A:225:ASN:O	1:A:233:ARG:NH2	2.31	0.63
3:E:621:F89:C6	4:E:622:NDP:H42N	2.29	0.63
1:C:217:LYS:N	1:C:250:ASN:HD21	1.95	0.63
1:C:93:ASN:HD21	1:C:95:GLU:HB3	1.64	0.63
1:D:260:ILE:N	1:D:260:ILE:HD12	2.13	0.63
1:E:151:PRO:HG2	1:E:154:PHE:CD2	2.33	0.63
1:E:304:ASN:HD21	1:E:306:ASN:HB2	1.63	0.63
1:E:81:GLN:HE22	1:E:92:ARG:NE	1.96	0.63
1:A:296:ILE:HD12	1:A:297:TRP:H	1.64	0.63
1:B:289:ARG:HG3	1:B:501:TRP:CE2	2.33	0.63
1:A:217:LYS:N	1:A:250:ASN:HD21	1.96	0.62
1:E:93:ASN:HD21	1:E:95:GLU:HB3	1.64	0.62
1:D:220:LYS:NZ	5:D:631:HOH:O	2.31	0.62
1:B:67:LEU:HG	1:B:72:ILE:HD11	1.82	0.62
1:C:468:ASN:N	1:C:468:ASN:HD22	1.98	0.62
1:E:52:LEU:HB3	1:E:113:CYS:SG	2.39	0.62
1:B:15:LEU:HB2	1:B:139:GLU:HG2	1.81	0.62
1:B:225:ASN:O	1:B:233:ARG:NH2	2.32	0.62
1:B:33:LEU:HB3	3:B:609:F89:HG1	1.80	0.62
1:D:136:VAL:HG12	1:D:138:LEU:CD2	2.29	0.62
1:A:289:ARG:HG3	1:A:501:TRP:CE2	2.34	0.62
1:E:289:ARG:NH1	1:E:289:ARG:HB3	2.15	0.62
1:D:297:TRP:CD1	1:D:302:ASP:HB3	2.35	0.62
1:A:99:GLU:OE2	1:A:99:GLU:C	2.38	0.61
1:C:304:ASN:HD21	1:C:306:ASN:HB2	1.65	0.61
1:E:296:ILE:HD12	1:E:297:TRP:N	2.15	0.61
1:E:468:ASN:HD22	1:E:468:ASN:N	1.96	0.61
1:D:67:LEU:HG	1:D:72:ILE:HD11	1.82	0.61
1:E:293:GLU:HA	1:E:296:ILE:HD11	1.82	0.61
1:A:293:GLU:HA	1:A:296:ILE:HD11	1.82	0.61
1:D:151:PRO:HG2	1:D:154:PHE:CD2	2.34	0.61
1:E:297:TRP:CG	1:E:308:LEU:HD21	2.35	0.61
1:A:468:ASN:HD22	1:A:468:ASN:N	1.98	0.61
1:C:225:ASN:O	1:C:233:ARG:NH2	2.33	0.61
1:E:260:ILE:HD12	1:E:260:ILE:N	2.15	0.61
1:E:297:TRP:CD1	1:E:302:ASP:HB3	2.35	0.61
1:B:296:ILE:HD12	1:B:297:TRP:H	1.65	0.61
1:E:468:ASN:HD22	1:E:468:ASN:H	1.48	0.61
1:A:296:ILE:HD12	1:A:297:TRP:N	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:VAL:HG12	1:A:138:LEU:CD2	2.31	0.61
1:B:419:ASN:ND2	1:B:457:ALA:HB3	2.16	0.61
1:E:378:ASN:ND2	1:E:381:ASP:HB2	2.16	0.61
1:B:296:ILE:HD12	1:B:297:TRP:N	2.15	0.61
1:C:151:PRO:HG2	1:C:154:PHE:CD2	2.36	0.61
3:C:613:F89:C6A	4:C:614:NDP:H42N	2.30	0.61
1:E:136:VAL:HG12	1:E:138:LEU:CD2	2.30	0.61
1:B:243:LEU:O	1:B:247:VAL:HG13	2.01	0.60
1:B:297:TRP:CG	1:B:308:LEU:HD21	2.36	0.60
1:D:490:LYS:HD2	1:D:502:GLU:O	2.02	0.60
1:D:99:GLU:OE2	1:D:99:GLU:C	2.39	0.60
1:B:136:VAL:HG12	1:B:138:LEU:CD2	2.30	0.60
1:C:136:VAL:HG12	1:C:138:LEU:CD2	2.30	0.60
1:D:468:ASN:N	1:D:468:ASN:HD22	1.99	0.60
1:D:296:ILE:HD12	1:D:297:TRP:N	2.17	0.60
1:E:99:GLU:C	1:E:99:GLU:OE2	2.39	0.60
1:A:103:ASN:O	1:A:104:ASP:C	2.40	0.60
3:A:605:F89:C6	4:A:606:NDP:H42N	2.30	0.60
1:C:104:ASP:HB3	1:C:107:ILE:HD13	1.84	0.60
1:A:297:TRP:CG	1:A:308:LEU:HD21	2.36	0.60
1:E:389:TRP:HB2	1:E:404:VAL:HG13	1.83	0.60
1:C:468:ASN:HD22	1:C:468:ASN:H	1.50	0.60
1:D:297:TRP:CG	1:D:308:LEU:HD21	2.37	0.60
1:E:104:ASP:HB3	1:E:107:ILE:HD13	1.83	0.60
1:A:419:ASN:ND2	1:A:457:ALA:HB3	2.17	0.60
3:D:617:F89:C6	4:D:618:NDP:H42N	2.32	0.60
1:E:179:GLU:OE2	1:E:179:GLU:HA	2.02	0.60
1:A:315:ILE:HG21	3:A:604:F89:C15	2.31	0.60
1:C:103:ASN:C	1:C:103:ASN:HD22	2.04	0.60
1:D:419:ASN:ND2	1:D:457:ALA:HB3	2.17	0.59
1:A:297:TRP:CD1	1:A:302:ASP:HB3	2.38	0.59
1:A:37:SER:HB2	3:A:605:F89:HB1	1.84	0.59
1:C:15:LEU:HB2	1:C:139:GLU:HG2	1.85	0.59
1:A:490:LYS:HD2	1:A:502:GLU:O	2.01	0.59
1:B:19:ILE:O	4:B:610:NDP:H2N	2.02	0.59
1:D:52:LEU:HB3	1:D:113:CYS:SG	2.42	0.59
1:D:93:ASN:HD21	1:D:95:GLU:HB3	1.67	0.59
1:C:378:ASN:ND2	1:C:381:ASP:HB2	2.17	0.59
1:E:103:ASN:O	1:E:104:ASP:C	2.41	0.59
1:D:15:LEU:HB2	1:D:139:GLU:HG2	1.84	0.59
1:D:33:LEU:CB	3:D:617:F89:HG1	2.30	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:296:ILE:HD12	1:E:297:TRP:H	1.66	0.59
1:C:104:ASP:C	1:C:106:SER:N	2.55	0.59
1:D:179:GLU:HA	1:D:179:GLU:OE2	2.02	0.59
1:D:304:ASN:HD21	1:D:306:ASN:HB2	1.65	0.59
1:B:260:ILE:N	1:B:260:ILE:HD12	2.18	0.59
1:D:296:ILE:HD12	1:D:297:TRP:H	1.67	0.59
1:E:315:ILE:HG21	3:E:620:F89:C15	2.32	0.59
1:B:93:ASN:HD21	1:B:95:GLU:HB3	1.67	0.59
1:E:334:GLU:OE2	1:E:357:HIS:HE1	1.85	0.59
1:A:151:PRO:HG2	1:A:154:PHE:CD2	2.38	0.59
1:A:206:ILE:HG12	1:B:34:LYS:HG2	1.84	0.59
1:C:35:PHE:HA	1:D:206:ILE:HD11	1.85	0.59
1:D:289:ARG:HB3	1:D:289:ARG:NH1	2.18	0.59
1:E:490:LYS:HD2	1:E:502:GLU:O	2.03	0.59
1:A:260:ILE:HD12	1:A:260:ILE:N	2.17	0.59
1:C:297:TRP:CG	1:C:308:LEU:HD21	2.38	0.58
1:D:468:ASN:HD22	1:D:468:ASN:H	1.51	0.58
1:B:104:ASP:C	1:B:106:SER:N	2.55	0.58
1:C:389:TRP:HB2	1:C:404:VAL:HG13	1.85	0.58
1:A:15:LEU:HB2	1:A:139:GLU:HG2	1.86	0.58
1:B:304:ASN:HD21	1:B:306:ASN:HB2	1.66	0.58
1:B:378:ASN:ND2	1:B:381:ASP:HB2	2.19	0.58
1:D:103:ASN:O	1:D:104:ASP:C	2.41	0.58
3:E:621:F89:C6A	4:E:622:NDP:H42N	2.33	0.58
1:B:289:ARG:NH1	1:B:289:ARG:HB3	2.18	0.58
1:A:104:ASP:C	1:A:106:SER:N	2.56	0.58
1:B:103:ASN:O	1:B:104:ASP:C	2.41	0.58
1:D:389:TRP:HB2	1:D:404:VAL:HG13	1.86	0.58
3:D:617:F89:C6A	4:D:618:NDP:H42N	2.34	0.58
1:B:103:ASN:HD22	1:B:103:ASN:C	2.05	0.58
1:B:490:LYS:HD2	1:B:502:GLU:O	2.03	0.58
1:C:289:ARG:NH1	1:C:289:ARG:HB3	2.17	0.58
1:E:103:ASN:C	1:E:103:ASN:HD22	2.06	0.58
1:A:289:ARG:HB3	1:A:289:ARG:NH1	2.17	0.58
1:D:126:ASN:HD21	1:D:177:LYS:CE	2.16	0.58
1:A:468:ASN:HD22	1:A:468:ASN:H	1.51	0.58
1:E:19:ILE:O	4:E:622:NDP:H2N	2.03	0.58
1:C:260:ILE:N	1:C:260:ILE:HD12	2.18	0.57
1:C:490:LYS:HD2	1:C:502:GLU:O	2.03	0.57
1:E:126:ASN:HD21	1:E:177:LYS:HE3	1.69	0.57
1:B:285:LYS:HD3	1:B:514:THR:HG22	1.84	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:HB3	1:B:113:CYS:SG	2.44	0.57
1:C:439:ALA:O	1:C:443:MET:HG3	2.04	0.57
1:D:114:GLY:HA2	1:D:119:TYR:CZ	2.39	0.57
1:D:126:ASN:HD21	1:D:177:LYS:HE3	1.69	0.57
1:B:179:GLU:HA	1:B:179:GLU:OE2	2.05	0.57
1:D:103:ASN:HD22	1:D:103:ASN:C	2.05	0.57
1:B:334:GLU:OE2	1:B:357:HIS:HE1	1.88	0.57
1:E:15:LEU:HB2	1:E:139:GLU:HG2	1.85	0.57
1:A:179:GLU:OE2	1:A:179:GLU:HA	2.05	0.57
1:A:285:LYS:HD3	1:A:514:THR:HG22	1.87	0.57
1:C:52:LEU:HB3	1:C:113:CYS:SG	2.45	0.57
1:B:151:PRO:HG2	1:B:154:PHE:CD2	2.38	0.57
3:B:609:F89:C10	3:B:609:F89:O1A	2.53	0.57
1:C:285:LYS:HD3	1:C:514:THR:HG22	1.86	0.57
1:C:293:GLU:HA	1:C:296:ILE:HD11	1.85	0.57
1:E:126:ASN:HD21	1:E:177:LYS:CE	2.17	0.57
1:A:126:ASN:HD21	1:A:177:LYS:CE	2.18	0.57
1:A:126:ASN:HD21	1:A:177:LYS:NZ	2.03	0.57
1:B:439:ALA:O	1:B:443:MET:HG3	2.05	0.57
1:C:297:TRP:CD1	1:C:302:ASP:HB3	2.40	0.57
1:D:104:ASP:C	1:D:106:SER:N	2.56	0.57
1:D:19:ILE:O	4:D:618:NDP:H2N	2.05	0.57
1:B:389:TRP:HB2	1:B:404:VAL:HG13	1.87	0.56
1:D:334:GLU:OE2	1:D:357:HIS:HE1	1.87	0.56
1:D:217:LYS:H	1:D:250:ASN:ND2	2.03	0.56
1:E:114:GLY:HA2	1:E:119:TYR:CZ	2.39	0.56
1:A:320:GLY:O	1:A:335:GLU:O	2.23	0.56
1:A:291:ILE:HD13	1:A:436:ALA:HB3	1.86	0.56
1:A:439:ALA:O	1:A:443:MET:HG3	2.05	0.56
1:C:271:ARG:NH2	1:D:267:GLY:O	2.38	0.56
1:C:315:ILE:HG21	3:C:612:F89:C15	2.35	0.56
1:C:334:GLU:OE2	1:C:357:HIS:HE1	1.87	0.56
1:D:439:ALA:O	1:D:443:MET:HG3	2.05	0.56
1:A:93:ASN:HD21	1:A:95:GLU:HB3	1.68	0.56
1:B:468:ASN:H	1:B:468:ASN:ND2	2.04	0.56
1:D:104:ASP:HB3	1:D:107:ILE:HD13	1.87	0.56
1:A:126:ASN:ND2	1:A:177:LYS:NZ	2.53	0.56
1:A:115:GLY:HA3	4:A:606:NDP:PA	2.46	0.56
1:B:291:ILE:HD13	1:B:436:ALA:HB3	1.87	0.56
1:A:269:MET:HE1	1:B:269:MET:HE2	1.86	0.56
1:B:126:ASN:HD21	1:B:177:LYS:CE	2.18	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HD11	1:B:35:PHE:HA	1.87	0.56
1:D:291:ILE:HD13	1:D:436:ALA:HB3	1.87	0.56
1:D:495:ASN:OD1	1:D:497:GLU:HG2	2.06	0.56
1:E:217:LYS:H	1:E:250:ASN:ND2	2.04	0.56
1:E:243:LEU:O	1:E:247:VAL:HG13	2.05	0.56
1:B:487:LEU:O	1:B:488:LYS:HD3	2.05	0.56
1:C:103:ASN:O	1:C:104:ASP:C	2.43	0.56
1:E:285:LYS:HD3	1:E:514:THR:HG22	1.87	0.56
1:A:102:MET:CE	1:A:102:MET:HA	2.36	0.56
1:D:285:LYS:HD3	1:D:514:THR:HG22	1.87	0.56
1:E:123:LEU:HD13	1:E:128:VAL:HG11	1.88	0.56
1:B:102:MET:CE	1:B:102:MET:HA	2.36	0.56
1:A:104:ASP:HB3	1:A:107:ILE:HD13	1.87	0.55
1:E:104:ASP:C	1:E:106:SER:N	2.57	0.55
1:E:495:ASN:OD1	1:E:497:GLU:HG2	2.07	0.55
1:A:389:TRP:HB2	1:A:404:VAL:HG13	1.87	0.55
1:C:243:LEU:O	1:C:247:VAL:HG13	2.07	0.55
1:A:103:ASN:C	1:A:103:ASN:HD22	2.07	0.55
1:A:334:GLU:OE2	1:A:357:HIS:HE1	1.89	0.55
1:A:52:LEU:HB3	1:A:113:CYS:SG	2.47	0.55
1:B:126:ASN:HD21	1:B:177:LYS:HE3	1.71	0.55
1:B:297:TRP:CD1	1:B:302:ASP:HB3	2.42	0.55
3:C:612:F89:C10	3:C:612:F89:O1A	2.53	0.55
1:E:304:ASN:ND2	1:E:306:ASN:HB2	2.22	0.55
1:E:320:GLY:O	1:E:335:GLU:O	2.24	0.55
1:E:291:ILE:HD13	1:E:436:ALA:HB3	1.88	0.55
1:A:114:GLY:HA2	1:A:119:TYR:CZ	2.42	0.55
1:A:404:VAL:HG11	1:B:405:LEU:HD11	1.87	0.55
3:B:609:F89:C6	4:B:610:NDP:H42N	2.36	0.55
1:D:378:ASN:ND2	1:D:381:ASP:HB2	2.21	0.55
1:A:115:GLY:HA3	4:A:606:NDP:O1A	2.07	0.55
1:C:284:LYS:HZ1	1:C:432:PRO:HG2	1.72	0.55
1:C:487:LEU:O	1:C:488:LYS:HD3	2.07	0.55
1:C:126:ASN:HD21	1:C:177:LYS:HE3	1.72	0.55
1:A:233:ARG:NH1	1:A:242:ASP:OD1	2.40	0.54
3:C:612:F89:OE1	3:C:612:F89:HA	2.07	0.54
1:A:19:ILE:O	4:A:606:NDP:H2N	2.07	0.54
1:C:509:TYR:HA	5:C:669:HOH:O	2.08	0.54
1:E:284:LYS:HZ1	1:E:432:PRO:HG2	1.72	0.54
1:D:102:MET:HA	1:D:102:MET:CE	2.38	0.54
1:E:102:MET:CE	1:E:102:MET:HA	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLY:HA2	1:B:119:TYR:CZ	2.43	0.54
1:C:126:ASN:HD21	1:C:177:LYS:CE	2.20	0.54
1:C:211:LYS:HE3	5:C:682:HOH:O	2.06	0.54
1:D:123:LEU:HD13	1:D:128:VAL:HG11	1.89	0.54
1:B:315:ILE:HD13	3:B:608:F89:C18	2.37	0.54
1:B:320:GLY:O	1:B:335:GLU:O	2.26	0.54
1:C:136:VAL:HG12	1:C:138:LEU:HD23	1.90	0.54
1:D:243:LEU:O	1:D:247:VAL:HG13	2.07	0.54
1:E:439:ALA:O	1:E:443:MET:HG3	2.07	0.54
1:B:130:ARG:HD2	1:B:132:TYR:CE1	2.43	0.54
1:C:291:ILE:HD13	1:C:436:ALA:HB3	1.88	0.54
1:C:519:MET:HG2	1:C:520:ALA:N	2.23	0.54
1:D:315:ILE:HD12	3:D:616:F89:H8	1.90	0.54
1:E:123:LEU:HD13	1:E:128:VAL:CG1	2.38	0.54
1:C:123:LEU:HD13	1:C:128:VAL:HG11	1.89	0.53
1:D:126:ASN:ND2	1:D:177:LYS:NZ	2.56	0.53
1:E:75:ILE:O	4:E:622:NDP:H1B	2.08	0.53
1:A:123:LEU:HD13	1:A:128:VAL:HG11	1.90	0.53
3:B:608:F89:OE1	3:B:608:F89:HA	2.08	0.53
1:C:102:MET:HA	1:C:102:MET:CE	2.37	0.53
1:A:304:ASN:ND2	1:A:306:ASN:HB2	2.22	0.53
1:D:359:ASP:CG	1:D:361:THR:HG22	2.29	0.53
1:B:519:MET:HG2	1:B:520:ALA:N	2.23	0.53
1:D:126:ASN:HD21	1:D:177:LYS:NZ	2.06	0.53
1:D:304:ASN:C	1:D:304:ASN:ND2	2.61	0.53
1:E:126:ASN:ND2	1:E:177:LYS:NZ	2.57	0.53
1:A:215:ARG:NH1	5:A:652:HOH:O	2.41	0.53
1:C:130:ARG:HD2	1:C:132:TYR:CE1	2.43	0.53
1:C:320:GLY:O	1:C:335:GLU:O	2.25	0.53
1:A:243:LEU:O	1:A:247:VAL:HG13	2.09	0.53
1:C:304:ASN:ND2	1:C:304:ASN:C	2.60	0.53
1:D:83:GLU:HA	1:D:83:GLU:OE2	2.07	0.53
1:A:126:ASN:HD21	1:A:177:LYS:HE3	1.73	0.53
1:A:495:ASN:OD1	1:A:497:GLU:HG2	2.09	0.53
1:C:405:LEU:HD11	1:D:404:VAL:HG11	1.90	0.53
1:D:315:ILE:HG21	3:D:616:F89:C15	2.39	0.53
1:C:114:GLY:HA2	1:C:119:TYR:CZ	2.44	0.53
1:E:114:GLY:HA2	1:E:119:TYR:CE2	2.44	0.53
1:E:359:ASP:CG	1:E:361:THR:HG22	2.28	0.53
1:A:239:GLN:HG3	1:A:271:ARG:O	2.08	0.53
1:A:51:ALA:C	1:A:52:LEU:HD23	2.29	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ARG:NH1	1:D:242:ASP:OD1	2.40	0.53
1:A:519:MET:HG2	1:A:520:ALA:N	2.24	0.52
1:B:123:LEU:HD13	1:B:128:VAL:HG11	1.90	0.52
1:B:315:ILE:HG21	3:B:608:F89:C15	2.39	0.52
3:E:620:F89:OE1	3:E:620:F89:HA	2.08	0.52
1:B:126:ASN:HD21	1:B:177:LYS:NZ	2.07	0.52
1:B:284:LYS:HZ1	1:B:432:PRO:HG2	1.74	0.52
1:B:115:GLY:HA3	4:B:610:NDP:PA	2.49	0.52
1:E:136:VAL:HG12	1:E:138:LEU:HD23	1.92	0.52
1:B:126:ASN:ND2	1:B:177:LYS:NZ	2.57	0.52
1:B:495:ASN:OD1	1:B:497:GLU:HG2	2.10	0.52
1:C:495:ASN:OD1	1:C:497:GLU:HG2	2.10	0.52
1:B:217:LYS:H	1:B:250:ASN:ND2	2.05	0.52
1:D:114:GLY:HA2	1:D:119:TYR:CE2	2.44	0.52
1:D:37:SER:O	1:D:41:ASN:HB2	2.10	0.52
1:E:83:GLU:OE2	1:E:83:GLU:HA	2.10	0.52
1:B:41:ASN:HD21	1:B:69:ASN:HB2	1.75	0.52
1:C:103:ASN:C	1:C:103:ASN:ND2	2.62	0.52
1:A:217:LYS:H	1:A:250:ASN:ND2	2.06	0.52
1:A:83:GLU:OE2	1:A:83:GLU:HA	2.09	0.52
1:B:103:ASN:C	1:B:103:ASN:ND2	2.63	0.52
1:C:123:LEU:HD13	1:C:128:VAL:CG1	2.40	0.52
1:D:136:VAL:HG12	1:D:138:LEU:HD23	1.91	0.52
1:E:340:PRO:HG3	1:E:353:TYR:CB	2.40	0.52
1:E:51:ALA:C	1:E:52:LEU:HD23	2.30	0.52
1:B:104:ASP:HB3	1:B:107:ILE:HD13	1.91	0.52
1:B:136:VAL:HG12	1:B:138:LEU:HD23	1.91	0.52
2:A:603:UMP:OP1	1:B:383:ARG:NH1	2.43	0.52
1:E:183:LEU:HD21	5:E:643:HOH:O	2.08	0.52
1:E:468:ASN:H	1:E:468:ASN:ND2	2.07	0.52
1:E:423:ARG:NH1	2:E:619:UMP:OP3	2.38	0.52
1:E:11:ALA:HB2	3:E:621:F89:H3M2	1.92	0.52
1:C:113:CYS:O	3:C:613:F89:H6	2.10	0.52
1:A:359:ASP:CG	1:A:361:THR:HG22	2.30	0.52
3:A:604:F89:HA	3:A:604:F89:OE1	2.10	0.52
1:B:509:TYR:HA	5:B:621:HOH:O	2.10	0.52
1:C:83:GLU:OE2	1:C:83:GLU:HA	2.10	0.51
1:D:320:GLY:O	1:D:335:GLU:O	2.26	0.51
1:D:519:MET:HG2	1:D:520:ALA:N	2.25	0.51
1:D:51:ALA:C	1:D:52:LEU:HD23	2.31	0.51
1:C:126:ASN:ND2	1:C:177:LYS:NZ	2.59	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:ARG:NH1	1:E:242:ASP:OD1	2.41	0.51
1:C:468:ASN:H	1:C:468:ASN:ND2	2.08	0.51
1:C:75:ILE:O	4:C:614:NDP:H1B	2.11	0.51
1:E:388:ALA:O	1:E:401:PRO:HG2	2.09	0.51
1:A:288:ILE:HD11	1:A:440:ILE:HD11	1.92	0.51
1:E:315:ILE:HD12	3:E:620:F89:C8	2.41	0.51
1:B:304:ASN:ND2	1:B:306:ASN:HB2	2.26	0.51
1:D:304:ASN:ND2	1:D:306:ASN:HB2	2.25	0.51
1:B:115:GLY:HA3	4:B:610:NDP:O1A	2.11	0.51
1:C:4:LYS:HB3	1:C:101:LEU:HD23	1.92	0.51
1:A:136:VAL:HG12	1:A:138:LEU:HD23	1.92	0.51
1:E:288:ILE:HD11	1:E:440:ILE:HD11	1.92	0.51
1:A:340:PRO:HG3	1:A:353:TYR:CB	2.41	0.51
1:B:83:GLU:HA	1:B:83:GLU:OE2	2.10	0.51
1:E:126:ASN:HD21	1:E:177:LYS:NZ	2.07	0.51
1:A:304:ASN:C	1:A:304:ASN:ND2	2.61	0.51
1:C:217:LYS:H	1:C:250:ASN:ND2	2.07	0.51
1:D:33:LEU:HB3	3:D:617:F89:CG	2.34	0.50
1:E:103:ASN:C	1:E:103:ASN:ND2	2.65	0.50
1:E:304:ASN:C	1:E:304:ASN:ND2	2.63	0.50
1:A:41:ASN:HD21	1:A:69:ASN:HB2	1.75	0.50
1:D:287:ALA:HB1	5:D:654:HOH:O	2.10	0.50
1:E:130:ARG:HD2	1:E:132:TYR:CE1	2.47	0.50
1:A:103:ASN:ND2	1:A:103:ASN:C	2.65	0.50
1:B:51:ALA:C	1:B:52:LEU:HD23	2.32	0.50
1:C:239:GLN:HG3	1:C:271:ARG:O	2.11	0.50
1:D:123:LEU:HD13	1:D:128:VAL:CG1	2.41	0.50
1:D:75:ILE:O	4:D:618:NDP:H1B	2.11	0.50
1:C:304:ASN:ND2	1:C:306:ASN:HB2	2.26	0.50
1:D:103:ASN:C	1:D:103:ASN:ND2	2.64	0.50
1:E:4:LYS:HB3	1:E:101:LEU:HD23	1.93	0.50
1:A:123:LEU:HD13	1:A:128:VAL:CG1	2.42	0.50
1:C:233:ARG:NH1	1:C:242:ASP:OD1	2.43	0.50
1:D:340:PRO:HG3	1:D:353:TYR:CB	2.41	0.50
1:E:308:LEU:HD12	1:E:313:VAL:HG11	1.94	0.50
1:C:4:LYS:H	1:C:101:LEU:CD2	2.24	0.50
1:C:115:GLY:HA3	4:C:614:NDP:O1A	2.12	0.50
1:D:193:LEU:N	1:D:193:LEU:HD23	2.27	0.50
1:D:41:ASN:HD21	1:D:69:ASN:HB2	1.76	0.50
1:E:41:ASN:HD21	1:E:69:ASN:HB2	1.75	0.50
1:E:519:MET:HG2	1:E:520:ALA:N	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:GLY:HA2	1:C:119:TYR:CE2	2.47	0.50
1:C:126:ASN:HD21	1:C:177:LYS:NZ	2.10	0.50
1:D:131:ILE:HB	1:D:175:PHE:HB2	1.94	0.50
1:E:487:LEU:O	1:E:488:LYS:HD3	2.12	0.50
1:A:405:LEU:HD11	1:B:404:VAL:HG11	1.93	0.50
1:D:468:ASN:ND2	1:D:468:ASN:H	2.10	0.50
1:E:239:GLN:HG3	1:E:271:ARG:O	2.12	0.50
1:B:490:LYS:HE2	1:B:505:GLU:HG3	1.94	0.49
1:D:239:GLN:HG3	1:D:271:ARG:O	2.11	0.49
3:D:616:F89:OE1	3:D:616:F89:HA	2.10	0.49
1:A:130:ARG:HD2	1:A:132:TYR:CE1	2.47	0.49
1:C:179:GLU:OE2	1:C:179:GLU:HA	2.12	0.49
1:C:51:ALA:C	1:C:52:LEU:HD23	2.32	0.49
1:D:115:GLY:HA3	4:D:618:NDP:O1A	2.11	0.49
1:E:308:LEU:HD12	1:E:313:VAL:CG1	2.42	0.49
1:B:4:LYS:HB3	1:B:101:LEU:HD23	1.93	0.49
1:C:288:ILE:HD11	1:C:440:ILE:HD11	1.93	0.49
1:C:133:LEU:HD22	1:C:134:THR:N	2.27	0.49
1:C:41:ASN:HD21	1:C:69:ASN:HB2	1.77	0.49
1:D:284:LYS:HZ1	1:D:432:PRO:HG2	1.76	0.49
1:D:113:CYS:O	3:D:617:F89:H6	2.11	0.49
1:A:487:LEU:O	1:A:488:LYS:HD3	2.13	0.49
1:E:402:CYS:SG	2:E:619:UMP:C6	3.05	0.49
1:C:308:LEU:HD12	1:C:313:VAL:HG11	1.95	0.49
1:A:378:ASN:ND2	1:A:381:ASP:HB2	2.27	0.49
1:A:468:ASN:ND2	1:A:468:ASN:H	2.09	0.49
1:B:315:ILE:HD12	3:B:608:F89:C8	2.43	0.49
1:C:19:ILE:O	4:C:614:NDP:H2N	2.12	0.49
1:B:233:ARG:NH1	1:B:242:ASP:OD1	2.43	0.49
1:B:308:LEU:HD12	1:B:313:VAL:HG11	1.93	0.49
2:C:611:UMP:OP1	1:D:383:ARG:NH1	2.46	0.49
1:B:113:CYS:O	3:B:609:F89:H6	2.11	0.49
1:B:359:ASP:CG	1:B:361:THR:HG22	2.33	0.49
1:D:288:ILE:HD11	1:D:440:ILE:HD11	1.94	0.49
1:A:131:ILE:HB	1:A:175:PHE:HB2	1.94	0.48
1:C:388:ALA:O	1:C:401:PRO:HG2	2.13	0.48
1:A:490:LYS:HE2	1:A:505:GLU:HG3	1.96	0.48
1:B:468:ASN:N	1:B:468:ASN:ND2	2.61	0.48
1:C:202:LEU:HG	1:D:38:LYS:HB3	1.94	0.48
1:E:131:ILE:HB	1:E:175:PHE:HB2	1.95	0.48
1:A:37:SER:HB2	3:A:605:F89:CB	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:LEU:HD12	1:B:313:VAL:CG1	2.44	0.48
1:A:280:LEU:HD11	1:A:286:VAL:HB	1.95	0.48
1:A:284:LYS:HZ1	1:A:432:PRO:HG2	1.77	0.48
1:B:193:LEU:HD23	1:B:193:LEU:N	2.28	0.48
1:B:37:SER:O	1:B:41:ASN:HB2	2.14	0.48
1:C:359:ASP:CG	1:C:361:THR:HG22	2.34	0.48
3:C:613:F89:C10	3:C:613:F89:O1A	2.53	0.48
1:C:405:LEU:HD23	1:C:405:LEU:C	2.34	0.48
1:D:4:LYS:H	1:D:101:LEU:CD2	2.26	0.48
1:E:113:CYS:O	3:E:621:F89:H6	2.13	0.48
1:B:239:GLN:HG3	1:B:271:ARG:O	2.13	0.48
1:C:308:LEU:HD12	1:C:313:VAL:CG1	2.43	0.48
1:C:423:ARG:NH1	2:C:611:UMP:OP3	2.42	0.48
1:C:56:ARG:O	1:C:59:TRP:HB3	2.14	0.48
1:E:133:LEU:HD22	1:E:134:THR:N	2.28	0.48
1:E:4:LYS:H	1:E:101:LEU:CD2	2.27	0.48
1:E:315:ILE:CG2	3:E:620:F89:C15	2.92	0.48
1:B:225:ASN:O	1:B:226:THR:C	2.53	0.48
1:E:25:LEU:HD11	3:E:621:F89:H10	1.95	0.48
1:B:288:ILE:HG23	1:B:501:TRP:HH2	1.79	0.48
1:B:62:ILE:N	1:B:62:ILE:HD13	2.28	0.48
1:A:114:GLY:HA2	1:A:119:TYR:CE2	2.49	0.47
1:D:294:GLU:O	1:D:297:TRP:HB3	2.14	0.47
1:D:343:GLY:HA2	1:D:346:TRP:HB2	1.96	0.47
1:E:37:SER:O	1:E:41:ASN:HB2	2.14	0.47
1:A:289:ARG:NH1	5:A:629:HOH:O	2.47	0.47
1:A:304:ASN:HD21	1:A:306:ASN:CB	2.27	0.47
1:B:131:ILE:HB	1:B:175:PHE:HB2	1.95	0.47
1:B:280:LEU:HD11	1:B:286:VAL:HB	1.96	0.47
1:D:115:GLY:HA3	4:D:618:NDP:PA	2.54	0.47
1:D:130:ARG:HD2	1:D:132:TYR:CE1	2.48	0.47
1:D:487:LEU:O	1:D:488:LYS:HD3	2.13	0.47
1:E:304:ASN:HD21	1:E:306:ASN:CB	2.26	0.47
1:A:297:TRP:CD2	1:A:308:LEU:HD21	2.50	0.47
1:B:96:ASP:O	1:B:99:GLU:HG3	2.14	0.47
1:C:404:VAL:HG11	1:D:405:LEU:HD11	1.97	0.47
1:D:388:ALA:O	1:D:401:PRO:HG2	2.15	0.47
1:A:269:MET:HE1	1:B:269:MET:CE	2.44	0.47
1:C:315:ILE:HD12	3:C:612:F89:C8	2.45	0.47
1:A:193:LEU:HD21	1:A:196:ILE:CD1	2.41	0.47
1:D:56:ARG:O	1:D:59:TRP:HB3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:LEU:HD11	1:E:286:VAL:HB	1.95	0.47
1:A:37:SER:O	1:A:41:ASN:HB2	2.14	0.47
1:B:123:LEU:HD13	1:B:128:VAL:CG1	2.44	0.47
1:D:4:LYS:HB3	1:D:101:LEU:HD23	1.94	0.47
1:C:199:THR:OG1	1:D:174:ILE:HD11	2.15	0.47
1:E:472:GLN:HG2	1:E:517:MET:HG2	1.97	0.47
1:B:297:TRP:CD2	1:B:308:LEU:HD21	2.49	0.47
1:C:62:ILE:HD13	1:C:62:ILE:N	2.30	0.47
1:A:75:ILE:O	4:A:606:NDP:H1B	2.14	0.47
1:A:62:ILE:N	1:A:62:ILE:HD13	2.30	0.47
1:B:79:LEU:HD23	1:B:80:PRO:CD	2.45	0.47
1:C:340:PRO:HG3	1:C:353:TYR:CB	2.44	0.47
1:C:206:ILE:HG12	1:D:34:LYS:HG2	1.96	0.47
1:E:56:ARG:O	1:E:59:TRP:HB3	2.15	0.47
1:A:101:LEU:O	1:A:103:ASN:N	2.46	0.47
1:B:423:ARG:NH1	2:B:607:UMP:OP3	2.43	0.47
3:D:616:F89:O1A	3:D:616:F89:C10	2.54	0.47
1:E:343:GLY:HA2	1:E:346:TRP:HB2	1.97	0.47
1:E:405:LEU:C	1:E:405:LEU:HD23	2.36	0.47
1:E:490:LYS:HE2	1:E:505:GLU:HG3	1.97	0.47
1:A:308:LEU:HD12	1:A:313:VAL:CG1	2.45	0.47
1:A:383:ARG:NH1	1:B:400:PRO:HD2	2.30	0.47
1:D:171:ASP:OD2	1:D:483:PRO:HD3	2.15	0.47
1:D:339:GLY:HA2	1:D:353:TYR:CE2	2.50	0.47
1:E:340:PRO:HG3	1:E:353:TYR:CG	2.50	0.47
1:E:248:LEU:HD13	1:E:465:ILE:HD12	1.97	0.47
1:E:315:ILE:HG21	3:E:620:F89:C14	2.45	0.47
1:A:4:LYS:HB3	1:A:101:LEU:HD23	1.94	0.46
1:A:459:PHE:CD2	1:B:459:PHE:CD2	3.03	0.46
1:C:193:LEU:HD21	1:C:196:ILE:CD1	2.41	0.46
1:C:53:ILE:HG23	1:C:75:ILE:HD13	1.97	0.46
1:D:233:ARG:NH1	1:D:242:ASP:OD2	2.48	0.46
1:E:288:ILE:HG23	1:E:501:TRP:HH2	1.80	0.46
1:E:62:ILE:HD13	1:E:62:ILE:N	2.29	0.46
1:E:92:ARG:O	4:E:622:NDP:H2A	2.15	0.46
1:E:96:ASP:O	1:E:99:GLU:HG3	2.15	0.46
3:B:609:F89:C6A	4:B:610:NDP:H42N	2.45	0.46
1:C:297:TRP:CD2	1:C:308:LEU:HD21	2.50	0.46
1:D:308:LEU:HD12	1:D:313:VAL:CG1	2.45	0.46
1:C:131:ILE:HB	1:C:175:PHE:HB2	1.95	0.46
1:C:295:LEU:O	1:C:299:ILE:HG13	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:LEU:HD22	1:D:134:THR:N	2.30	0.46
3:E:620:F89:C10	3:E:620:F89:O1A	2.55	0.46
1:A:254:ARG:HB2	1:B:380:LYS:HD2	1.97	0.46
1:A:340:PRO:HG3	1:A:353:TYR:CG	2.50	0.46
1:B:335:GLU:HB3	5:B:682:HOH:O	2.16	0.46
1:E:193:LEU:N	1:E:193:LEU:HD23	2.30	0.46
1:E:224:TYR:O	1:E:227:PRO:HG3	2.16	0.46
1:A:388:ALA:O	1:A:401:PRO:HG2	2.15	0.46
1:A:402:CYS:SG	2:A:603:UMP:C6	3.09	0.46
1:B:193:LEU:HD21	1:B:196:ILE:CD1	2.44	0.46
1:B:248:LEU:HD13	1:B:465:ILE:HD12	1.97	0.46
1:B:53:ILE:HG23	1:B:75:ILE:HD13	1.98	0.46
1:B:99:GLU:O	1:B:99:GLU:OE2	2.34	0.46
1:C:512:TYR:HB3	1:C:513:PRO:HD2	1.97	0.46
1:D:8:ILE:HG12	1:D:112:VAL:HB	1.97	0.46
1:B:56:ARG:O	1:B:59:TRP:HB3	2.16	0.46
1:C:224:TYR:O	1:C:227:PRO:HG3	2.15	0.46
1:A:315:ILE:HG21	3:A:604:F89:C16	2.45	0.46
1:B:4:LYS:H	1:B:101:LEU:CD2	2.28	0.46
1:C:10:VAL:HG22	1:C:11:ALA:N	2.31	0.46
1:C:225:ASN:O	1:C:226:THR:C	2.54	0.46
1:C:293:GLU:HG2	1:C:311:LYS:HB3	1.97	0.46
1:C:53:ILE:HG23	1:C:75:ILE:CD1	2.46	0.46
1:D:224:TYR:O	1:D:227:PRO:HG3	2.15	0.46
1:E:297:TRP:CD2	1:E:308:LEU:HD21	2.50	0.46
1:A:293:GLU:HG2	1:A:311:LYS:HB3	1.98	0.46
1:A:248:LEU:HD13	1:A:465:ILE:HD12	1.98	0.46
1:B:79:LEU:HA	1:B:80:PRO:HD3	1.83	0.46
1:E:14:VAL:HG13	1:E:15:LEU:HG	1.98	0.46
1:C:472:GLN:HG2	1:C:517:MET:HG2	1.97	0.46
1:C:96:ASP:O	1:C:99:GLU:HG3	2.14	0.46
1:D:288:ILE:HG23	1:D:501:TRP:HH2	1.81	0.46
1:D:470:LEU:HD12	1:D:470:LEU:HA	1.80	0.46
1:D:62:ILE:N	1:D:62:ILE:HD13	2.31	0.46
1:A:288:ILE:HG23	1:A:501:TRP:HH2	1.81	0.46
1:A:4:LYS:H	1:A:101:LEU:CD2	2.29	0.46
1:A:315:ILE:HD12	3:A:604:F89:C8	2.46	0.46
1:E:428:GLY:O	1:E:517:MET:HE3	2.16	0.46
1:B:52:LEU:HD23	1:B:52:LEU:N	2.31	0.45
1:D:405:LEU:C	1:D:405:LEU:HD23	2.36	0.45
1:E:380:LYS:HE3	1:E:412:ASN:ND2	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLY:HA2	1:B:119:TYR:CE2	2.51	0.45
1:B:340:PRO:HG3	1:B:353:TYR:CB	2.46	0.45
3:B:608:F89:O1A	3:B:608:F89:C10	2.54	0.45
1:C:468:ASN:N	1:C:468:ASN:ND2	2.63	0.45
1:D:372:ILE:O	1:D:376:LYS:HG2	2.16	0.45
1:D:423:ARG:NH1	2:D:615:UMP:OP3	2.39	0.45
1:A:383:ARG:NH1	2:B:607:UMP:OP1	2.50	0.45
1:C:280:LEU:HD11	1:C:286:VAL:HB	1.98	0.45
1:D:340:PRO:HG3	1:D:353:TYR:CG	2.51	0.45
1:A:359:ASP:OD2	1:A:361:THR:CG2	2.61	0.45
1:D:193:LEU:HD21	1:D:196:ILE:CD1	2.43	0.45
1:E:8:ILE:HG12	1:E:112:VAL:HB	1.99	0.45
1:A:96:ASP:O	1:A:99:GLU:HG3	2.17	0.45
1:C:163:PHE:HA	1:C:276:GLU:HB3	1.98	0.45
1:C:372:ILE:O	1:C:376:LYS:HG2	2.17	0.45
1:C:519:MET:HA	5:C:624:HOH:O	2.17	0.45
1:D:308:LEU:HD12	1:D:313:VAL:HG11	1.98	0.45
1:B:37:SER:HB2	3:B:609:F89:HB1	1.99	0.45
1:C:490:LYS:HE2	1:C:505:GLU:HG3	1.98	0.45
1:D:10:VAL:HG22	1:D:11:ALA:N	2.31	0.45
1:D:163:PHE:HA	1:D:276:GLU:HB3	1.98	0.45
1:D:311:LYS:NZ	5:D:677:HOH:O	2.49	0.45
1:E:468:ASN:N	1:E:468:ASN:ND2	2.63	0.45
1:A:225:ASN:O	1:A:226:THR:C	2.54	0.45
1:A:284:LYS:HZ3	1:A:517:MET:HE1	1.81	0.45
1:A:53:ILE:HG23	1:A:75:ILE:HD13	1.98	0.45
3:A:605:F89:C10	3:A:605:F89:O1A	2.53	0.45
1:B:101:LEU:O	1:B:103:ASN:N	2.47	0.45
1:B:10:VAL:HG22	1:B:11:ALA:N	2.32	0.45
1:B:163:PHE:HA	1:B:276:GLU:HB3	1.98	0.45
1:B:293:GLU:HG2	1:B:311:LYS:HB3	1.99	0.45
1:C:93:ASN:OD1	1:C:96:ASP:HB2	2.17	0.45
1:E:138:LEU:HD23	1:E:138:LEU:N	2.32	0.45
1:E:359:ASP:OD2	1:E:361:THR:CG2	2.62	0.45
1:A:269:MET:HE2	1:B:269:MET:HE1	1.97	0.45
1:C:37:SER:O	1:C:41:ASN:HB2	2.16	0.45
1:C:8:ILE:HG12	1:C:112:VAL:HB	1.99	0.45
1:D:490:LYS:HE2	1:D:505:GLU:HG3	1.97	0.45
1:E:293:GLU:HG2	1:E:311:LYS:HB3	1.98	0.45
1:A:154:PHE:CE1	1:A:177:LYS:HB2	2.52	0.45
1:A:8:ILE:HG12	1:A:112:VAL:HB	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:GLU:HG2	1:B:497:GLU:H	1.58	0.45
1:D:280:LEU:HD11	1:D:286:VAL:HB	1.97	0.45
1:A:52:LEU:N	1:A:52:LEU:HD23	2.32	0.45
1:A:383:ARG:CZ	1:B:400:PRO:HG2	2.47	0.45
1:B:264:SER:CB	1:B:464:HIS:HB3	2.47	0.45
1:D:304:ASN:HD21	1:D:306:ASN:CB	2.29	0.45
1:D:79:LEU:HD23	1:D:80:PRO:CD	2.47	0.45
1:E:93:ASN:OD1	1:E:96:ASP:HB2	2.17	0.45
1:A:294:GLU:O	1:A:297:TRP:HB3	2.17	0.44
1:B:304:ASN:ND2	1:B:304:ASN:C	2.63	0.44
1:C:304:ASN:HD21	1:C:306:ASN:CB	2.29	0.44
1:C:308:LEU:HD12	1:C:313:VAL:HB	1.99	0.44
1:C:38:LYS:HB3	1:D:202:LEU:HG	1.98	0.44
1:C:402:CYS:SG	2:C:611:UMP:C6	3.11	0.44
1:D:472:GLN:HG2	1:D:517:MET:HG2	1.98	0.44
1:E:193:LEU:HD21	1:E:196:ILE:CD1	2.44	0.44
1:E:295:LEU:O	1:E:299:ILE:HG13	2.16	0.44
1:A:380:LYS:HE3	1:A:412:ASN:ND2	2.32	0.44
1:C:101:LEU:O	1:C:103:ASN:N	2.50	0.44
1:D:308:LEU:HD12	1:D:313:VAL:HB	1.99	0.44
1:D:81:GLN:NE2	1:D:92:ARG:NE	2.64	0.44
1:A:133:LEU:HD22	1:A:134:THR:N	2.32	0.44
1:B:288:ILE:HD11	1:B:440:ILE:HD11	1.98	0.44
1:C:193:LEU:HD23	1:C:193:LEU:N	2.31	0.44
1:C:99:GLU:C	1:C:101:LEU:N	2.69	0.44
1:D:99:GLU:C	1:D:101:LEU:N	2.69	0.44
1:E:10:VAL:HG22	1:E:11:ALA:N	2.32	0.44
1:E:226:THR:N	1:E:227:PRO:HD3	2.33	0.44
1:A:308:LEU:HD12	1:A:313:VAL:HG11	1.98	0.44
1:C:288:ILE:HG23	1:C:501:TRP:HH2	1.80	0.44
1:D:56:ARG:HG3	1:D:79:LEU:HD12	1.99	0.44
1:E:100:ASN:HB2	1:E:110:ILE:HD11	1.99	0.44
1:E:96:ASP:O	1:E:99:GLU:CG	2.66	0.44
1:A:371:LEU:O	1:A:374:THR:HG22	2.18	0.44
1:A:405:LEU:HD23	1:A:405:LEU:C	2.37	0.44
1:A:53:ILE:HG23	1:A:75:ILE:CD1	2.47	0.44
1:B:388:ALA:O	1:B:401:PRO:HG2	2.17	0.44
1:C:37:SER:HB2	3:C:613:F89:HB1	1.98	0.44
1:A:114:GLY:HA3	4:A:606:NDP:H5N	2.00	0.44
1:A:472:GLN:HG2	1:A:517:MET:HG2	2.00	0.44
3:A:604:F89:C10	3:A:604:F89:O1A	2.54	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:LEU:HD22	1:C:133:LEU:C	2.38	0.44
1:C:181:LYS:O	1:C:182:THR:HB	2.17	0.44
1:C:380:LYS:HE3	1:C:412:ASN:ND2	2.33	0.44
1:C:470:LEU:HD12	1:C:470:LEU:HA	1.79	0.44
1:E:339:GLY:HA2	1:E:353:TYR:CE2	2.53	0.44
1:A:193:LEU:N	1:A:193:LEU:HD23	2.32	0.44
1:A:233:ARG:NH1	1:A:242:ASP:OD2	2.50	0.44
1:A:79:LEU:HD23	1:A:80:PRO:CD	2.46	0.44
1:D:154:PHE:CE1	1:D:177:LYS:HB2	2.53	0.44
1:D:126:ASN:ND2	1:D:177:LYS:HZ2	2.16	0.44
1:D:297:TRP:CD2	1:D:308:LEU:HD21	2.51	0.44
1:D:248:LEU:HD13	1:D:465:ILE:HD12	2.00	0.44
1:D:512:TYR:HB3	1:D:513:PRO:HD2	1.99	0.44
1:E:163:PHE:HA	1:E:276:GLU:HB3	2.00	0.44
1:A:56:ARG:O	1:A:59:TRP:HB3	2.17	0.44
1:B:183:LEU:O	1:B:184:GLN:HB3	2.18	0.44
1:B:470:LEU:HD12	1:B:470:LEU:HA	1.79	0.44
1:C:34:LYS:HB2	1:C:34:LYS:HE3	1.77	0.44
1:E:308:LEU:HD12	1:E:313:VAL:HB	1.99	0.44
1:E:372:ILE:O	1:E:376:LYS:HG2	2.18	0.44
3:A:605:F89:C6A	4:A:606:NDP:H42N	2.47	0.44
1:C:114:GLY:HA3	4:C:614:NDP:H5N	2.00	0.44
1:C:154:PHE:CE1	1:C:177:LYS:HB2	2.52	0.44
1:E:512:TYR:HB3	1:E:513:PRO:HD2	1.99	0.44
1:E:52:LEU:N	1:E:52:LEU:HD23	2.32	0.44
1:B:372:ILE:O	1:B:376:LYS:HG2	2.18	0.43
1:C:183:LEU:O	1:C:184:GLN:HB3	2.18	0.43
1:D:428:GLY:O	1:D:517:MET:HE3	2.17	0.43
1:E:115:GLY:HA3	4:E:622:NDP:O1A	2.17	0.43
1:E:181:LYS:O	1:E:182:THR:HB	2.18	0.43
1:B:53:ILE:HG23	1:B:75:ILE:CD1	2.49	0.43
1:C:56:ARG:HG3	1:C:79:LEU:HD12	1.99	0.43
3:D:617:F89:O1A	3:D:617:F89:C10	2.53	0.43
1:E:154:PHE:CE1	1:E:177:LYS:HB2	2.53	0.43
1:E:53:ILE:HG23	1:E:75:ILE:HD13	2.00	0.43
1:B:512:TYR:HB3	1:B:513:PRO:HD2	1.99	0.43
1:B:56:ARG:HG3	1:B:79:LEU:HD12	2.00	0.43
1:C:96:ASP:O	1:C:99:GLU:CG	2.66	0.43
1:C:174:ILE:HD11	1:D:199:THR:OG1	2.18	0.43
1:D:293:GLU:HG2	1:D:311:LYS:HB3	1.99	0.43
1:E:99:GLU:C	1:E:101:LEU:N	2.69	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LEU:O	1:A:184:GLN:HB3	2.19	0.43
1:A:113:CYS:O	3:A:605:F89:H6	2.18	0.43
1:B:304:ASN:HD21	1:B:306:ASN:CB	2.30	0.43
1:A:383:ARG:HH12	1:B:400:PRO:HD2	1.82	0.43
1:B:78:SER:O	1:B:79:LEU:C	2.57	0.43
1:C:104:ASP:CB	1:C:107:ILE:HD13	2.48	0.43
1:D:468:ASN:N	1:D:468:ASN:ND2	2.65	0.43
1:A:224:TYR:O	1:A:227:PRO:HG3	2.18	0.43
1:A:308:LEU:HD12	1:A:313:VAL:HB	2.01	0.43
1:C:79:LEU:HA	1:C:80:PRO:HD3	1.81	0.43
1:D:96:ASP:O	1:D:99:GLU:HG3	2.17	0.43
1:E:133:LEU:HD13	1:E:135:ARG:HG2	2.00	0.43
1:A:163:PHE:HA	1:A:276:GLU:HB3	2.00	0.43
1:A:115:GLY:CA	4:A:606:NDP:PA	3.07	0.43
1:B:102:MET:O	1:B:103:ASN:HB3	2.18	0.43
1:B:181:LYS:O	1:B:182:THR:HB	2.18	0.43
1:B:93:ASN:OD1	1:B:96:ASP:HB2	2.18	0.43
1:D:359:ASP:OD2	1:D:361:THR:CG2	2.62	0.43
1:E:101:LEU:O	1:E:103:ASN:N	2.50	0.43
1:E:81:GLN:NE2	1:E:92:ARG:NE	2.65	0.43
1:A:31:GLU:HG2	1:B:207:PHE:CE1	2.54	0.43
1:D:101:LEU:O	1:D:103:ASN:N	2.49	0.43
1:D:429:LEU:CD2	1:D:519:MET:HB2	2.49	0.43
1:E:225:ASN:O	1:E:226:THR:C	2.56	0.43
1:E:75:ILE:HG22	4:E:622:NDP:C4A	2.49	0.43
1:A:400:PRO:HG2	1:B:383:ARG:CZ	2.49	0.43
1:A:429:LEU:CD2	1:A:519:MET:HB2	2.49	0.43
1:B:154:PHE:CE1	1:B:177:LYS:HB2	2.53	0.43
1:C:248:LEU:HD13	1:C:465:ILE:HD12	1.99	0.43
1:D:203:LEU:HA	1:D:203:LEU:HD12	1.90	0.43
1:C:115:GLY:O	1:C:116:GLU:C	2.57	0.43
1:C:343:GLY:HA2	1:C:346:TRP:HB2	2.01	0.43
1:C:78:SER:O	1:C:79:LEU:C	2.57	0.43
1:D:34:LYS:HE3	1:D:34:LYS:HB2	1.82	0.43
1:D:52:LEU:N	1:D:52:LEU:HD23	2.33	0.43
1:D:78:SER:O	1:D:79:LEU:C	2.57	0.43
1:A:126:ASN:ND2	1:A:177:LYS:HZ2	2.17	0.43
1:A:181:LYS:O	1:A:182:THR:HB	2.19	0.43
1:A:372:ILE:O	1:A:376:LYS:HG2	2.19	0.43
1:B:101:LEU:C	1:B:103:ASN:H	2.22	0.43
1:B:343:GLY:HA2	1:B:346:TRP:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LYS:NZ	1:B:48:LYS:O	2.42	0.43
1:C:247:VAL:HG21	1:C:465:ILE:HG13	2.01	0.43
1:D:53:ILE:HG23	1:D:75:ILE:HD13	2.01	0.43
1:C:383:ARG:NH1	2:D:615:UMP:OP1	2.52	0.42
1:C:428:GLY:O	1:C:517:MET:HE3	2.18	0.42
1:E:126:ASN:ND2	1:E:177:LYS:HZ2	2.17	0.42
1:A:512:TYR:HB3	1:A:513:PRO:HD2	2.01	0.42
1:B:472:GLN:HG2	1:B:517:MET:HG2	1.99	0.42
1:C:429:LEU:CD2	1:C:519:MET:HB2	2.49	0.42
1:D:225:ASN:O	1:D:226:THR:C	2.57	0.42
1:A:226:THR:N	1:A:227:PRO:HD3	2.34	0.42
1:A:380:LYS:HD2	1:B:254:ARG:HB2	2.01	0.42
1:A:81:GLN:NE2	1:A:92:ARG:NE	2.65	0.42
1:B:323:GLU:OE2	1:B:323:GLU:N	2.44	0.42
1:B:81:GLN:NE2	1:B:92:ARG:NE	2.63	0.42
1:C:14:VAL:HG13	1:C:15:LEU:HG	2.00	0.42
1:C:339:GLY:HA2	1:C:353:TYR:CE2	2.54	0.42
1:C:340:PRO:HG3	1:C:353:TYR:CG	2.53	0.42
1:D:247:VAL:HG21	1:D:465:ILE:HG13	2.02	0.42
1:D:315:ILE:HD13	3:D:616:F89:C13	2.48	0.42
1:D:93:ASN:OD1	1:D:96:ASP:HB2	2.19	0.42
1:E:104:ASP:CB	1:E:107:ILE:HD13	2.48	0.42
1:E:209:ILE:CD1	1:E:209:ILE:N	2.70	0.42
3:E:621:F89:C10	3:E:621:F89:O1A	2.53	0.42
1:A:10:VAL:HG22	1:A:11:ALA:N	2.34	0.42
1:A:115:GLY:HA2	4:A:606:NDP:O5D	2.19	0.42
1:A:264:SER:CB	1:A:464:HIS:HB3	2.49	0.42
1:A:497:GLU:H	1:A:497:GLU:HG2	1.60	0.42
1:B:8:ILE:HG12	1:B:112:VAL:HB	2.02	0.42
1:B:114:GLY:HA3	4:B:610:NDP:H5N	2.01	0.42
1:B:295:LEU:O	1:B:299:ILE:HG13	2.19	0.42
1:B:247:VAL:HG21	1:B:465:ILE:HG13	2.00	0.42
1:E:133:LEU:CD1	1:E:135:ARG:HG2	2.49	0.42
1:E:247:VAL:HG21	1:E:465:ILE:HG13	2.01	0.42
1:E:294:GLU:O	1:E:297:TRP:HB3	2.19	0.42
1:E:264:SER:CB	1:E:464:HIS:HB3	2.50	0.42
1:A:284:LYS:NZ	1:A:517:MET:HE1	2.34	0.42
1:B:34:LYS:HB2	1:B:34:LYS:HE3	1.82	0.42
1:C:115:GLY:HA3	4:C:614:NDP:PA	2.59	0.42
1:E:183:LEU:O	1:E:184:GLN:HB3	2.19	0.42
1:A:203:LEU:HD11	1:B:172:PHE:CE2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:LEU:CD2	1:B:519:MET:HB2	2.50	0.42
1:C:233:ARG:NH1	1:C:242:ASP:OD2	2.53	0.42
1:C:371:LEU:O	1:C:374:THR:HG22	2.20	0.42
1:D:181:LYS:O	1:D:182:THR:HB	2.20	0.42
1:D:264:SER:CB	1:D:464:HIS:HB3	2.50	0.42
1:E:248:LEU:HA	1:E:248:LEU:HD12	1.91	0.42
1:E:34:LYS:HB2	1:E:34:LYS:HE3	1.80	0.42
1:E:371:LEU:O	1:E:374:THR:HG22	2.20	0.42
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.90	0.42
1:A:33:LEU:HD22	3:A:605:F89:H14	2.02	0.42
1:C:100:ASN:HB2	1:C:110:ILE:HD11	2.01	0.42
1:C:248:LEU:HD13	1:C:465:ILE:CD1	2.50	0.42
1:D:497:GLU:H	1:D:497:GLU:HG2	1.59	0.42
1:E:133:LEU:C	1:E:133:LEU:HD22	2.40	0.42
1:E:207:PHE:HB3	1:E:210:ARG:HB2	2.02	0.42
1:E:56:ARG:HG3	1:E:79:LEU:HD12	2.00	0.42
1:E:53:ILE:HG23	1:E:75:ILE:CD1	2.49	0.42
1:A:223:ILE:HD11	1:A:249:GLU:OE1	2.20	0.42
1:A:295:LEU:O	1:A:299:ILE:HG13	2.20	0.42
1:A:284:LYS:NZ	1:A:517:MET:CE	2.83	0.42
1:A:96:ASP:O	1:A:99:GLU:CG	2.68	0.42
1:B:220:LYS:NZ	5:B:705:HOH:O	2.52	0.42
1:C:248:LEU:HD12	1:C:248:LEU:HA	1.91	0.42
1:A:101:LEU:C	1:A:103:ASN:H	2.22	0.42
1:B:96:ASP:O	1:B:99:GLU:CG	2.68	0.42
1:E:361:THR:O	1:E:361:THR:HG23	2.20	0.42
1:E:79:LEU:HD23	1:E:80:PRO:CD	2.46	0.42
1:A:310:GLU:C	1:A:312:LYS:H	2.24	0.42
1:A:461:GLY:HA3	1:B:407:GLN:OE1	2.20	0.42
1:A:47:ASN:HD22	1:A:47:ASN:HA	1.66	0.42
1:B:226:THR:N	1:B:227:PRO:HD3	2.35	0.42
1:B:371:LEU:O	1:B:374:THR:HG22	2.20	0.42
1:C:126:ASN:ND2	1:C:177:LYS:HZ2	2.17	0.42
1:C:220:LYS:NZ	5:C:690:HOH:O	2.51	0.42
1:C:238:PHE:O	1:C:242:ASP:HB2	2.20	0.42
1:C:39:ILE:CG2	1:C:40:THR:N	2.83	0.42
1:C:284:LYS:NZ	1:C:517:MET:HE1	2.35	0.42
1:D:183:LEU:O	1:D:184:GLN:HB3	2.19	0.42
1:E:429:LEU:CD2	1:E:519:MET:HB2	2.50	0.42
1:A:238:PHE:O	1:A:242:ASP:HB2	2.20	0.41
1:B:133:LEU:HD13	1:B:135:ARG:HG2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:ILE:N	1:D:209:ILE:CD1	2.70	0.41
1:D:39:ILE:CG2	1:D:40:THR:N	2.82	0.41
1:A:126:ASN:CG	1:A:177:LYS:HZ1	2.24	0.41
1:C:101:LEU:C	1:C:103:ASN:H	2.23	0.41
1:C:138:LEU:N	1:C:138:LEU:HD23	2.35	0.41
1:D:371:LEU:O	1:D:374:THR:HG22	2.20	0.41
1:B:133:LEU:HD22	1:B:134:THR:N	2.34	0.41
1:B:224:TYR:O	1:B:227:PRO:HG3	2.20	0.41
1:A:207:PHE:CE1	1:B:31:GLU:HG2	2.55	0.41
1:D:138:LEU:HD23	1:D:138:LEU:N	2.35	0.41
1:C:271:ARG:HD3	1:D:212:MET:CE	2.50	0.41
1:E:133:LEU:HD13	1:E:135:ARG:CG	2.50	0.41
1:E:470:LEU:HA	1:E:470:LEU:HD12	1.81	0.41
1:A:102:MET:O	1:A:103:ASN:HB3	2.20	0.41
1:B:133:LEU:HD13	1:B:135:ARG:CG	2.49	0.41
1:C:81:GLN:NE2	1:C:92:ARG:NE	2.64	0.41
1:D:133:LEU:HD22	1:D:133:LEU:C	2.41	0.41
1:D:380:LYS:HE3	1:D:412:ASN:ND2	2.36	0.41
1:D:479:ARG:HD3	1:D:512:TYR:CG	2.55	0.41
1:D:96:ASP:O	1:D:99:GLU:CG	2.69	0.41
1:E:233:ARG:NH1	1:E:242:ASP:OD2	2.52	0.41
1:E:39:ILE:CG2	1:E:40:THR:N	2.83	0.41
1:A:343:GLY:HA2	1:A:346:TRP:HB2	2.02	0.41
1:B:99:GLU:C	1:B:101:LEU:N	2.72	0.41
1:C:226:THR:N	1:C:227:PRO:HD3	2.36	0.41
1:C:497:GLU:H	1:C:497:GLU:HG2	1.58	0.41
1:D:101:LEU:C	1:D:103:ASN:H	2.24	0.41
1:D:37:SER:HB2	3:D:617:F89:HB1	2.03	0.41
1:E:208:GLY:C	1:E:210:ARG:N	2.74	0.41
1:E:62:ILE:HG22	1:E:62:ILE:O	2.20	0.41
1:A:93:ASN:OD1	1:A:96:ASP:HB2	2.20	0.41
1:B:115:GLY:CA	4:B:610:NDP:PA	3.09	0.41
1:C:25:LEU:HD11	3:C:613:F89:H10	2.03	0.41
1:E:102:MET:O	1:E:103:ASN:HB3	2.21	0.41
1:C:102:MET:O	1:C:103:ASN:HB3	2.21	0.41
1:C:19:ILE:HD11	1:C:145:THR:HG22	2.03	0.41
3:C:612:F89:O	3:C:612:F89:HB2	2.20	0.41
1:D:104:ASP:CB	1:D:107:ILE:HD13	2.50	0.41
1:E:248:LEU:HD13	1:E:465:ILE:CD1	2.50	0.41
1:A:269:MET:CE	1:B:269:MET:CE	2.98	0.41
1:B:248:LEU:HD13	1:B:465:ILE:CD1	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLN:NE2	1:C:92:ARG:CZ	2.84	0.41
1:D:102:MET:O	1:D:103:ASN:HB3	2.21	0.41
1:D:220:LYS:NZ	1:D:220:LYS:HB2	2.36	0.41
1:E:310:GLU:C	1:E:312:LYS:H	2.23	0.41
1:E:62:ILE:HD12	3:E:621:F89:C18	2.51	0.41
1:A:248:LEU:HD13	1:A:465:ILE:CD1	2.51	0.41
1:B:308:LEU:HD12	1:B:313:VAL:HB	2.03	0.41
1:B:340:PRO:HG3	1:B:353:TYR:CG	2.56	0.41
1:B:402:CYS:SG	2:B:607:UMP:C6	3.14	0.41
1:E:340:PRO:HG3	1:E:353:TYR:HB2	2.03	0.41
1:E:78:SER:O	1:E:79:LEU:C	2.58	0.41
1:A:333:ARG:HG2	1:A:333:ARG:HH11	1.85	0.41
1:A:78:SER:O	1:A:79:LEU:C	2.59	0.41
1:B:181:LYS:HB2	1:B:182:THR:H	1.47	0.41
1:B:405:LEU:HD23	1:B:405:LEU:C	2.41	0.41
1:C:354:LYS:HD2	1:C:358:ASP:OD2	2.21	0.41
1:D:53:ILE:HG23	1:D:75:ILE:CD1	2.51	0.41
1:E:203:LEU:HD12	1:E:203:LEU:HA	1.93	0.41
1:A:133:LEU:HD13	1:A:135:ARG:HG2	2.03	0.41
1:A:99:GLU:C	1:A:101:LEU:N	2.71	0.41
1:B:138:LEU:N	1:B:138:LEU:HD23	2.36	0.41
1:B:294:GLU:O	1:B:297:TRP:HB3	2.21	0.41
1:B:310:GLU:C	1:B:312:LYS:H	2.25	0.41
1:D:223:ILE:HD11	1:D:249:GLU:OE1	2.21	0.41
1:A:14:VAL:HG13	1:A:15:LEU:HG	2.03	0.40
1:A:339:GLY:HA2	1:A:353:TYR:CE2	2.56	0.40
1:C:480:THR:HA	1:C:481:PRO:HD3	1.96	0.40
1:C:79:LEU:HD23	1:C:80:PRO:CD	2.45	0.40
1:D:238:PHE:O	1:D:242:ASP:HB2	2.21	0.40
1:D:310:GLU:C	1:D:312:LYS:H	2.23	0.40
1:E:101:LEU:C	1:E:103:ASN:H	2.24	0.40
1:E:62:ILE:HD11	3:E:621:F89:H8	2.02	0.40
1:A:158:TYR:O	1:A:173:MET:CB	2.70	0.40
1:B:133:LEU:CD1	1:B:135:ARG:HG2	2.51	0.40
1:C:182:THR:O	1:C:183:LEU:C	2.60	0.40
1:C:52:LEU:HD23	1:C:52:LEU:N	2.35	0.40
1:D:14:VAL:HG13	1:D:15:LEU:HG	2.02	0.40
1:E:238:PHE:O	1:E:242:ASP:HB2	2.20	0.40
1:A:264:SER:HB3	1:A:464:HIS:HB3	2.03	0.40
1:B:380:LYS:HE3	1:B:412:ASN:ND2	2.36	0.40
1:D:361:THR:HG23	1:D:361:THR:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:LEU:CD1	1:D:404:VAL:HG11	2.51	0.40
1:E:182:THR:O	1:E:183:LEU:C	2.60	0.40
1:A:138:LEU:N	1:A:138:LEU:HD23	2.36	0.40
1:A:400:PRO:HD2	1:B:383:ARG:NH1	2.37	0.40
1:A:58:THR:O	1:A:61:SER:HB2	2.22	0.40
1:B:3:GLU:HA	1:B:3:GLU:OE2	2.22	0.40
1:C:247:VAL:O	1:C:251:GLY:N	2.51	0.40
1:E:220:LYS:NZ	1:E:220:LYS:HB2	2.36	0.40
1:A:207:PHE:HB3	1:A:210:ARG:HB2	2.04	0.40
1:B:354:LYS:HD2	1:B:358:ASP:OD2	2.22	0.40
1:D:92:ARG:O	4:D:618:NDP:H2A	2.22	0.40
1:E:260:ILE:CD1	1:E:260:ILE:N	2.83	0.40
1:E:308:LEU:HD12	1:E:313:VAL:CB	2.52	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	517/521 (99%)	472 (91%)	36 (7%)	9 (2%)	11	34
1	B	517/521 (99%)	472 (91%)	36 (7%)	9 (2%)	11	34
1	C	517/521 (99%)	470 (91%)	38 (7%)	9 (2%)	11	34
1	D	517/521 (99%)	473 (92%)	35 (7%)	9 (2%)	11	34
1	E	517/521 (99%)	469 (91%)	39 (8%)	9 (2%)	11	34
All	All	2585/2605 (99%)	2356 (91%)	184 (7%)	45 (2%)	11	34

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	102	MET
1	A	179	GLU
1	A	182	THR
1	B	84	ALA
1	B	102	MET
1	B	179	GLU
1	B	182	THR
1	C	84	ALA
1	C	102	MET
1	C	179	GLU
1	C	182	THR
1	D	84	ALA
1	D	102	MET
1	D	179	GLU
1	D	182	THR
1	E	84	ALA
1	E	102	MET
1	E	179	GLU
1	E	182	THR
1	A	103	ASN
1	A	335	GLU
1	B	103	ASN
1	B	335	GLU
1	C	103	ASN
1	C	335	GLU
1	D	103	ASN
1	D	335	GLU
1	E	103	ASN
1	E	335	GLU
1	A	183	LEU
1	B	183	LEU
1	C	183	LEU
1	D	183	LEU
1	E	183	LEU
1	A	184	GLN
1	B	184	GLN
1	C	184	GLN
1	D	184	GLN
1	E	184	GLN
1	C	341	ILE
1	D	341	ILE
1	E	341	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	341	ILE
1	B	341	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	468/470 (100%)	432 (92%)	36 (8%)	15	38
1	B	468/470 (100%)	431 (92%)	37 (8%)	14	37
1	C	468/470 (100%)	432 (92%)	36 (8%)	15	38
1	D	468/470 (100%)	433 (92%)	35 (8%)	16	40
1	E	468/470 (100%)	434 (93%)	34 (7%)	16	41
All	All	2340/2350 (100%)	2162 (92%)	178 (8%)	15	39

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	41	ASN
1	A	79	LEU
1	A	81	GLN
1	A	99	GLU
1	A	102	MET
1	A	103	ASN
1	A	104	ASP
1	A	126	ASN
1	A	128	VAL
1	A	133	LEU
1	A	138	LEU
1	A	142	GLU
1	A	176	GLU
1	A	179	GLU
1	A	181	LYS
1	A	202	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	203	LEU
1	A	209	ILE
1	A	220	LYS
1	A	247	VAL
1	A	248	LEU
1	A	289	ARG
1	A	295	LEU
1	A	296	ILE
1	A	304	ASN
1	A	371	LEU
1	A	383	ARG
1	A	427	LEU
1	A	468	ASN
1	A	470	LEU
1	A	471	THR
1	A	474	LYS
1	A	506	LEU
1	A	514	THR
1	A	516	LYS
1	B	4	LYS
1	B	41	ASN
1	B	79	LEU
1	B	81	GLN
1	B	99	GLU
1	B	102	MET
1	B	103	ASN
1	B	104	ASP
1	B	126	ASN
1	B	128	VAL
1	B	133	LEU
1	B	138	LEU
1	B	142	GLU
1	B	176	GLU
1	B	179	GLU
1	B	181	LYS
1	B	202	LEU
1	B	203	LEU
1	B	209	ILE
1	B	220	LYS
1	B	247	VAL
1	B	248	LEU
1	B	289	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	295	LEU
1	B	296	ILE
1	B	304	ASN
1	B	311	LYS
1	B	371	LEU
1	B	383	ARG
1	B	427	LEU
1	B	468	ASN
1	B	470	LEU
1	B	471	THR
1	B	474	LYS
1	B	506	LEU
1	B	514	THR
1	B	516	LYS
1	C	4	LYS
1	C	41	ASN
1	C	79	LEU
1	C	81	GLN
1	C	99	GLU
1	C	102	MET
1	C	103	ASN
1	C	104	ASP
1	C	126	ASN
1	C	128	VAL
1	C	133	LEU
1	C	138	LEU
1	C	142	GLU
1	C	176	GLU
1	C	179	GLU
1	C	181	LYS
1	C	203	LEU
1	C	209	ILE
1	C	220	LYS
1	C	247	VAL
1	C	248	LEU
1	C	289	ARG
1	C	295	LEU
1	C	296	ILE
1	C	304	ASN
1	C	311	LYS
1	C	371	LEU
1	C	383	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	427	LEU
1	C	468	ASN
1	C	470	LEU
1	C	471	THR
1	C	474	LYS
1	C	506	LEU
1	C	514	THR
1	C	516	LYS
1	D	4	LYS
1	D	41	ASN
1	D	79	LEU
1	D	81	GLN
1	D	99	GLU
1	D	102	MET
1	D	103	ASN
1	D	104	ASP
1	D	126	ASN
1	D	128	VAL
1	D	133	LEU
1	D	138	LEU
1	D	142	GLU
1	D	176	GLU
1	D	179	GLU
1	D	181	LYS
1	D	203	LEU
1	D	209	ILE
1	D	220	LYS
1	D	247	VAL
1	D	248	LEU
1	D	295	LEU
1	D	296	ILE
1	D	304	ASN
1	D	311	LYS
1	D	371	LEU
1	D	383	ARG
1	D	427	LEU
1	D	468	ASN
1	D	470	LEU
1	D	471	THR
1	D	474	LYS
1	D	506	LEU
1	D	514	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	516	LYS
1	E	4	LYS
1	E	41	ASN
1	E	79	LEU
1	E	81	GLN
1	E	99	GLU
1	E	102	MET
1	E	103	ASN
1	E	104	ASP
1	E	126	ASN
1	E	128	VAL
1	E	133	LEU
1	E	138	LEU
1	E	142	GLU
1	E	176	GLU
1	E	179	GLU
1	E	181	LYS
1	E	203	LEU
1	E	209	ILE
1	E	220	LYS
1	E	247	VAL
1	E	248	LEU
1	E	289	ARG
1	E	295	LEU
1	E	304	ASN
1	E	371	LEU
1	E	383	ARG
1	E	427	LEU
1	E	468	ASN
1	E	470	LEU
1	E	471	THR
1	E	474	LYS
1	E	506	LEU
1	E	514	THR
1	E	516	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	41	ASN
1	A	47	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	69	ASN
1	A	81	GLN
1	A	103	ASN
1	A	126	ASN
1	A	167	ASN
1	A	250	ASN
1	A	256	ASN
1	A	268	GLN
1	A	304	ASN
1	A	306	ASN
1	A	336	ASN
1	A	357	HIS
1	A	412	ASN
1	A	419	ASN
1	A	422	GLN
1	A	468	ASN
1	A	476	GLN
1	B	24	GLN
1	B	41	ASN
1	B	47	ASN
1	B	81	GLN
1	B	103	ASN
1	B	126	ASN
1	B	167	ASN
1	B	250	ASN
1	B	256	ASN
1	B	268	GLN
1	B	304	ASN
1	B	306	ASN
1	B	336	ASN
1	B	357	HIS
1	B	378	ASN
1	B	412	ASN
1	B	419	ASN
1	B	422	GLN
1	B	468	ASN
1	B	476	GLN
1	C	24	GLN
1	C	41	ASN
1	C	47	ASN
1	C	69	ASN
1	C	81	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	103	ASN
1	C	126	ASN
1	C	167	ASN
1	C	192	GLN
1	C	250	ASN
1	C	256	ASN
1	C	268	GLN
1	C	304	ASN
1	C	306	ASN
1	C	336	ASN
1	C	357	HIS
1	C	378	ASN
1	C	412	ASN
1	C	419	ASN
1	C	422	GLN
1	C	468	ASN
1	C	476	GLN
1	D	24	GLN
1	D	41	ASN
1	D	47	ASN
1	D	81	GLN
1	D	103	ASN
1	D	126	ASN
1	D	167	ASN
1	D	192	GLN
1	D	250	ASN
1	D	256	ASN
1	D	268	GLN
1	D	304	ASN
1	D	306	ASN
1	D	336	ASN
1	D	357	HIS
1	D	378	ASN
1	D	412	ASN
1	D	419	ASN
1	D	422	GLN
1	D	468	ASN
1	D	476	GLN
1	E	24	GLN
1	E	41	ASN
1	E	47	ASN
1	E	69	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	81	GLN
1	E	103	ASN
1	E	126	ASN
1	E	167	ASN
1	E	250	ASN
1	E	256	ASN
1	E	268	GLN
1	E	304	ASN
1	E	306	ASN
1	E	336	ASN
1	E	357	HIS
1	E	378	ASN
1	E	412	ASN
1	E	419	ASN
1	E	422	GLN
1	E	468	ASN
1	E	476	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

20 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	UMP	A	603	-	17,21,21	3.55	5 (29%)	23,31,31	2.64	4 (17%)
3	F89	A	604	-	34,41,41	3.87	7 (20%)	42,60,60	4.09	14 (33%)
3	F89	A	605	-	34,41,41	3.88	7 (20%)	42,60,60	4.14	13 (30%)
4	NDP	A	606	-	43,52,52	1.63	5 (11%)	49,80,80	1.88	11 (22%)
2	UMP	B	607	-	17,21,21	3.56	4 (23%)	23,31,31	2.62	4 (17%)
3	F89	B	608	-	34,41,41	3.88	7 (20%)	42,60,60	4.12	14 (33%)
3	F89	B	609	-	34,41,41	3.87	7 (20%)	42,60,60	4.16	12 (28%)
4	NDP	B	610	-	43,52,52	1.61	6 (13%)	49,80,80	1.88	10 (20%)
2	UMP	C	611	-	17,21,21	3.53	4 (23%)	23,31,31	2.61	4 (17%)
3	F89	C	612	-	34,41,41	3.88	7 (20%)	42,60,60	4.12	13 (30%)
3	F89	C	613	-	34,41,41	3.87	7 (20%)	42,60,60	4.14	13 (30%)
4	NDP	C	614	-	43,52,52	1.65	8 (18%)	49,80,80	1.89	9 (18%)
2	UMP	D	615	-	17,21,21	3.56	5 (29%)	23,31,31	2.63	4 (17%)
3	F89	D	616	-	34,41,41	3.88	7 (20%)	42,60,60	4.14	14 (33%)
3	F89	D	617	-	34,41,41	3.87	7 (20%)	42,60,60	4.13	12 (28%)
4	NDP	D	618	-	43,52,52	1.63	6 (13%)	49,80,80	1.88	10 (20%)
2	UMP	E	619	-	17,21,21	3.55	5 (29%)	23,31,31	2.62	4 (17%)
3	F89	E	620	-	34,41,41	3.87	7 (20%)	42,60,60	4.06	13 (30%)
3	F89	E	621	-	34,41,41	3.87	7 (20%)	42,60,60	4.14	13 (30%)
4	NDP	E	622	-	43,52,52	1.65	8 (18%)	49,80,80	1.87	11 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UMP	A	603	-	-	0/6/22/22	0/2/2/2
3	F89	A	604	-	-	0/12/30/30	0/5/5/5
3	F89	A	605	-	-	0/12/30/30	0/5/5/5
4	NDP	A	606	-	-	0/30/77/77	0/5/5/5
2	UMP	B	607	-	-	0/6/22/22	0/2/2/2
3	F89	B	608	-	-	0/12/30/30	0/5/5/5
3	F89	B	609	-	-	0/12/30/30	0/5/5/5
4	NDP	B	610	-	-	0/30/77/77	0/5/5/5
2	UMP	C	611	-	-	0/6/22/22	0/2/2/2
3	F89	C	612	-	-	0/12/30/30	0/5/5/5
3	F89	C	613	-	-	0/12/30/30	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NDP	C	614	-	-	0/30/77/77	0/5/5/5
2	UMP	D	615	-	-	0/6/22/22	0/2/2/2
3	F89	D	616	-	-	0/12/30/30	0/5/5/5
3	F89	D	617	-	-	0/12/30/30	0/5/5/5
4	NDP	D	618	-	-	0/30/77/77	0/5/5/5
2	UMP	E	619	-	-	0/6/22/22	0/2/2/2
3	F89	E	620	-	-	0/12/30/30	0/5/5/5
3	F89	E	621	-	-	0/12/30/30	0/5/5/5
4	NDP	E	622	-	-	0/30/77/77	0/5/5/5

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	612	F89	C19-N	-15.96	1.33	1.46
3	B	608	F89	C19-N	-15.93	1.33	1.46
3	E	620	F89	C19-N	-15.88	1.33	1.46
3	D	616	F89	C19-N	-15.88	1.33	1.46
3	A	604	F89	C19-N	-15.88	1.33	1.46
3	E	621	F89	C19-N	-15.88	1.33	1.46
3	A	605	F89	C19-N	-15.88	1.33	1.46
3	D	617	F89	C19-N	-15.84	1.33	1.46
3	C	613	F89	C19-N	-15.81	1.33	1.46
3	B	609	F89	C19-N	-15.79	1.33	1.46
3	B	609	F89	C19-C15	-11.41	1.33	1.50
3	E	621	F89	C19-C15	-11.39	1.33	1.50
3	A	605	F89	C19-C15	-11.38	1.33	1.50
3	C	613	F89	C19-C15	-11.37	1.33	1.50
3	D	616	F89	C19-C15	-11.37	1.33	1.50
3	B	608	F89	C19-C15	-11.36	1.33	1.50
3	C	612	F89	C19-C15	-11.36	1.33	1.50
3	D	617	F89	C19-C15	-11.33	1.33	1.50
3	E	620	F89	C19-C15	-11.30	1.33	1.50
3	A	604	F89	C19-C15	-11.29	1.33	1.50
3	D	616	F89	C16-C	-6.02	1.39	1.48
3	B	609	F89	C16-C	-5.99	1.39	1.48
3	D	617	F89	C16-C	-5.98	1.39	1.48
3	A	605	F89	C16-C	-5.98	1.39	1.48
3	A	604	F89	C16-C	-5.93	1.39	1.48
3	B	608	F89	C16-C	-5.92	1.39	1.48
3	C	612	F89	C16-C	-5.92	1.39	1.48
3	E	620	F89	C16-C	-5.91	1.39	1.48
3	C	613	F89	C16-C	-5.90	1.39	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	621	F89	C16-C	-5.89	1.39	1.48
2	D	615	UMP	C2'-C1'	-4.69	1.39	1.52
2	A	603	UMP	C2'-C1'	-4.69	1.39	1.52
2	B	607	UMP	C2'-C1'	-4.68	1.39	1.52
2	C	611	UMP	C2'-C1'	-4.68	1.39	1.52
2	E	619	UMP	C2'-C1'	-4.67	1.39	1.52
4	B	610	NDP	C4N-C5N	-3.91	1.40	1.49
4	A	606	NDP	C4N-C5N	-3.89	1.40	1.49
4	C	614	NDP	C4N-C5N	-3.81	1.40	1.49
4	D	618	NDP	C4N-C5N	-3.73	1.41	1.49
4	E	622	NDP	C4N-C5N	-3.72	1.41	1.49
3	C	613	F89	C-N	-2.70	1.33	1.36
3	A	605	F89	C-N	-2.69	1.33	1.36
3	B	609	F89	C-N	-2.59	1.33	1.36
3	D	617	F89	C-N	-2.56	1.33	1.36
3	D	616	F89	C-N	-2.54	1.33	1.36
3	E	621	F89	C-N	-2.53	1.33	1.36
3	B	608	F89	C-N	-2.52	1.33	1.36
3	E	620	F89	C-N	-2.49	1.33	1.36
3	C	612	F89	C-N	-2.43	1.33	1.36
3	A	604	F89	C-N	-2.43	1.33	1.36
4	D	618	NDP	P2B-O2X	-2.37	1.45	1.54
4	A	606	NDP	P2B-O2X	-2.33	1.45	1.54
4	C	614	NDP	P2B-O2X	-2.33	1.45	1.54
4	E	622	NDP	P2B-O2X	-2.30	1.45	1.54
4	B	610	NDP	P2B-O2X	-2.29	1.45	1.54
4	E	622	NDP	C2N-C3N	2.01	1.40	1.34
4	C	614	NDP	C6N-N1N	2.01	1.43	1.37
4	C	614	NDP	C2N-C3N	2.02	1.40	1.34
4	E	622	NDP	C6N-N1N	2.04	1.43	1.37
4	D	618	NDP	C6N-N1N	2.05	1.43	1.37
2	E	619	UMP	O4'-C1'	2.05	1.47	1.42
2	A	603	UMP	O4'-C1'	2.13	1.47	1.42
2	D	615	UMP	O4'-C1'	2.17	1.47	1.42
4	E	622	NDP	O4D-C1D	2.18	1.47	1.42
4	C	614	NDP	O4D-C1D	2.19	1.47	1.42
4	B	610	NDP	O4D-C1D	2.27	1.47	1.42
2	A	603	UMP	P-OP1	2.56	1.59	1.50
2	C	611	UMP	P-OP1	2.59	1.59	1.50
2	B	607	UMP	P-OP1	2.61	1.59	1.50
2	D	615	UMP	P-OP1	2.79	1.60	1.50
2	E	619	UMP	P-OP1	2.92	1.60	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	605	F89	C3-N2	3.44	1.40	1.34
4	D	618	NDP	P2B-O1X	3.46	1.62	1.50
3	D	617	F89	C3-N2	3.47	1.40	1.34
3	B	609	F89	C3-N2	3.47	1.40	1.34
3	E	621	F89	C3-N2	3.48	1.40	1.34
3	C	612	F89	C3-N2	3.48	1.40	1.34
4	B	610	NDP	P2B-O1X	3.49	1.62	1.50
3	C	613	F89	C3-N2	3.49	1.40	1.34
3	B	608	F89	C3-N2	3.50	1.40	1.34
3	E	620	F89	C3-N2	3.51	1.40	1.34
3	D	616	F89	C3-N2	3.52	1.40	1.34
3	A	604	F89	C3-N2	3.53	1.40	1.34
4	E	622	NDP	P2B-O1X	3.64	1.63	1.50
4	A	606	NDP	P2B-O1X	3.65	1.63	1.50
4	C	614	NDP	P2B-O1X	3.66	1.63	1.50
4	B	610	NDP	C6N-C5N	3.82	1.40	1.33
4	A	606	NDP	C6N-C5N	3.85	1.40	1.33
4	D	618	NDP	C6N-C5N	3.95	1.40	1.33
4	E	622	NDP	C6N-C5N	4.07	1.40	1.33
4	C	614	NDP	C6N-C5N	4.07	1.40	1.33
3	B	609	F89	C1-N2	4.08	1.40	1.33
3	A	605	F89	C1-N2	4.09	1.40	1.33
3	E	621	F89	C1-N2	4.10	1.40	1.33
3	B	608	F89	C1-N2	4.11	1.40	1.33
3	C	612	F89	C1-N2	4.12	1.40	1.33
3	C	613	F89	C1-N2	4.12	1.40	1.33
3	D	617	F89	C1-N2	4.14	1.40	1.33
3	A	604	F89	C1-N2	4.16	1.40	1.33
3	D	616	F89	C1-N2	4.17	1.40	1.33
3	E	620	F89	C1-N2	4.17	1.40	1.33
4	B	610	NDP	O4B-C1B	5.10	1.48	1.41
4	A	606	NDP	O4B-C1B	5.36	1.48	1.41
4	C	614	NDP	O4B-C1B	5.37	1.48	1.41
4	D	618	NDP	O4B-C1B	5.46	1.48	1.41
4	E	622	NDP	O4B-C1B	5.48	1.48	1.41
3	D	617	F89	C6-C5	5.96	1.52	1.35
3	E	621	F89	C6-C5	6.01	1.52	1.35
3	B	608	F89	C6-C5	6.02	1.52	1.35
3	A	605	F89	C6-C5	6.03	1.52	1.35
3	A	604	F89	C6-C5	6.04	1.52	1.35
3	C	613	F89	C6-C5	6.04	1.52	1.35
3	C	612	F89	C6-C5	6.04	1.52	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	616	F89	C6-C5	6.05	1.52	1.35
3	B	609	F89	C6-C5	6.05	1.52	1.35
3	E	620	F89	C6-C5	6.12	1.52	1.35
2	C	611	UMP	C6-C5	6.99	1.53	1.38
2	B	607	UMP	C6-C5	7.04	1.53	1.38
2	E	619	UMP	C6-C5	7.07	1.53	1.38
2	D	615	UMP	C6-C5	7.08	1.53	1.38
2	A	603	UMP	C6-C5	7.08	1.53	1.38
2	A	603	UMP	C6-N1	10.88	1.50	1.35
2	E	619	UMP	C6-N1	10.91	1.50	1.35
2	D	615	UMP	C6-N1	10.92	1.50	1.35
2	C	611	UMP	C6-N1	10.93	1.50	1.35
2	B	607	UMP	C6-N1	11.00	1.50	1.35

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	609	F89	C19-N-C	-11.09	109.15	113.04
3	A	605	F89	C19-N-C	-11.04	109.17	113.04
3	D	616	F89	C19-N-C	-10.99	109.19	113.04
3	C	613	F89	C19-N-C	-10.94	109.21	113.04
3	D	617	F89	C19-N-C	-10.91	109.22	113.04
3	B	608	F89	C19-N-C	-10.88	109.23	113.04
3	C	612	F89	C19-N-C	-10.86	109.24	113.04
3	E	621	F89	C19-N-C	-10.78	109.26	113.04
3	A	604	F89	C19-N-C	-10.75	109.27	113.04
3	E	620	F89	C19-N-C	-10.62	109.32	113.04
4	C	614	NDP	N3A-C2A-N1A	-9.60	120.50	128.86
4	D	618	NDP	N3A-C2A-N1A	-9.55	120.55	128.86
4	E	622	NDP	N3A-C2A-N1A	-9.50	120.58	128.86
4	A	606	NDP	N3A-C2A-N1A	-9.49	120.59	128.86
4	B	610	NDP	N3A-C2A-N1A	-9.48	120.60	128.86
3	E	620	F89	C15-C16-C	-6.49	105.24	108.89
3	B	608	F89	C15-C16-C	-6.33	105.33	108.89
3	C	612	F89	C15-C16-C	-6.31	105.34	108.89
3	D	616	F89	C15-C16-C	-6.26	105.37	108.89
3	A	604	F89	C15-C16-C	-6.22	105.40	108.89
3	C	613	F89	C15-C16-C	-6.15	105.43	108.89
3	A	605	F89	C15-C16-C	-6.13	105.44	108.89
3	B	609	F89	C15-C16-C	-6.12	105.45	108.89
3	D	617	F89	C15-C16-C	-6.01	105.51	108.89
3	E	621	F89	C15-C16-C	-5.90	105.57	108.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	613	F89	C1A-C1-N2	-4.23	120.06	124.12
3	E	621	F89	C1A-C1-N2	-4.15	120.13	124.12
3	D	617	F89	C1A-C1-N2	-4.12	120.16	124.12
3	B	609	F89	C1A-C1-N2	-4.10	120.19	124.12
3	C	612	F89	C1A-C1-N2	-4.05	120.23	124.12
3	A	605	F89	C1A-C1-N2	-4.01	120.27	124.12
3	E	620	F89	C1A-C1-N2	-3.99	120.29	124.12
3	A	604	F89	C1A-C1-N2	-3.97	120.31	124.12
3	B	608	F89	C1A-C1-N2	-3.93	120.34	124.12
3	D	616	F89	C1A-C1-N2	-3.92	120.35	124.12
2	D	615	UMP	C5-C6-N1	-3.82	111.91	120.67
2	C	611	UMP	C5-C6-N1	-3.81	111.93	120.67
2	A	603	UMP	C5-C6-N1	-3.80	111.96	120.67
2	B	607	UMP	C5-C6-N1	-3.79	111.97	120.67
2	E	619	UMP	C5-C6-N1	-3.78	112.00	120.67
3	C	612	F89	N4-C3-N2	-3.26	119.00	125.60
3	B	608	F89	N4-C3-N2	-3.26	119.00	125.60
3	D	616	F89	N4-C3-N2	-3.25	119.02	125.60
3	A	604	F89	N4-C3-N2	-3.24	119.04	125.60
3	A	605	F89	N4-C3-N2	-3.24	119.05	125.60
3	B	609	F89	N4-C3-N2	-3.24	119.05	125.60
3	E	620	F89	N4-C3-N2	-3.23	119.07	125.60
3	E	621	F89	C19-C15-C16	-3.21	107.74	109.73
3	C	613	F89	N4-C3-N2	-3.21	119.10	125.60
3	D	617	F89	C19-C15-C16	-3.21	107.74	109.73
3	E	621	F89	N4-C3-N2	-3.20	119.12	125.60
3	D	617	F89	N4-C3-N2	-3.17	119.19	125.60
3	B	609	F89	C19-C15-C16	-3.11	107.80	109.73
3	C	613	F89	C19-C15-C16	-3.09	107.82	109.73
3	A	605	F89	C19-C15-C16	-3.08	107.82	109.73
4	B	610	NDP	O5B-PA-O1A	-3.00	97.13	109.25
4	C	614	NDP	O5B-PA-O1A	-2.99	97.17	109.25
3	D	616	F89	C19-C15-C16	-2.98	107.88	109.73
4	E	622	NDP	O5B-PA-O1A	-2.97	97.25	109.25
4	A	606	NDP	O5B-PA-O1A	-2.92	97.46	109.25
4	D	618	NDP	O5B-PA-O1A	-2.90	97.55	109.25
3	B	608	F89	C19-C15-C16	-2.86	107.96	109.73
3	A	604	F89	C19-C15-C16	-2.84	107.97	109.73
3	C	612	F89	C19-C15-C16	-2.83	107.98	109.73
3	E	620	F89	C19-C15-C16	-2.64	108.09	109.73
4	B	610	NDP	O2A-PA-O5B	-2.47	96.49	108.14
4	A	606	NDP	O3X-P2B-O1X	-2.46	100.86	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	606	NDP	O2A-PA-O5B	-2.45	96.57	108.14
4	C	614	NDP	O3X-P2B-O1X	-2.44	100.97	110.50
4	E	622	NDP	O3X-P2B-O1X	-2.42	101.05	110.50
4	B	610	NDP	O3X-P2B-O1X	-2.41	101.05	110.50
4	D	618	NDP	O3X-P2B-O1X	-2.40	101.09	110.50
4	E	622	NDP	C3N-C2N-N1N	-2.39	119.61	123.08
4	C	614	NDP	O2A-PA-O5B	-2.38	96.89	108.14
4	D	618	NDP	C3N-C2N-N1N	-2.38	119.63	123.08
4	D	618	NDP	O2A-PA-O5B	-2.37	96.93	108.14
4	A	606	NDP	C3N-C2N-N1N	-2.35	119.67	123.08
4	B	610	NDP	C3N-C2N-N1N	-2.33	119.70	123.08
4	E	622	NDP	O2A-PA-O5B	-2.33	97.15	108.14
4	C	614	NDP	C3N-C2N-N1N	-2.32	119.71	123.08
3	C	613	F89	C5-C6-C6A	-2.07	118.03	121.35
3	A	605	F89	C5-C6-C6A	-2.05	118.06	121.35
3	E	620	F89	C7-C6A-C6	-2.04	118.35	123.18
3	B	609	F89	C5-C6-C6A	-2.04	118.09	121.35
3	B	608	F89	C7-C6A-C6	-2.03	118.37	123.18
3	A	604	F89	C5-C6-C6A	-2.03	118.10	121.35
3	A	604	F89	C7-C6A-C6	-2.02	118.39	123.18
3	E	621	F89	C5-C6-C6A	-2.02	118.12	121.35
3	D	616	F89	C7-C6A-C6	-2.01	118.41	123.18
3	D	616	F89	C5-C6-C6A	-2.01	118.13	121.35
3	B	608	F89	C5-C6-C6A	-2.00	118.15	121.35
3	C	612	F89	C5-C6-C6A	-2.00	118.15	121.35
3	D	617	F89	C5-C6-C6A	-2.00	118.15	121.35
4	E	622	NDP	O2X-P2B-O1X	2.00	118.33	110.50
3	E	621	F89	C3M-C3-N2	2.00	120.48	117.20
4	D	618	NDP	O2X-P2B-O1X	2.01	118.36	110.50
4	B	610	NDP	O2N-PN-O5D	2.01	117.65	108.14
4	A	606	NDP	O2N-PN-O5D	2.02	117.66	108.14
3	A	604	F89	C3M-C3-N2	2.04	120.54	117.20
3	C	612	F89	C3M-C3-N2	2.05	120.56	117.20
4	E	622	NDP	O2N-PN-O5D	2.05	117.82	108.14
3	E	621	F89	CA-N-C	2.06	125.01	122.03
4	A	606	NDP	O2X-P2B-O1X	2.07	118.61	110.50
3	E	620	F89	C3M-C3-N4	2.08	120.62	117.22
3	A	605	F89	C3M-C3-N4	2.10	120.64	117.22
3	A	605	F89	CA-N-C	2.10	125.06	122.03
3	B	609	F89	CA-N-C	2.10	125.07	122.03
3	D	617	F89	CA-N-C	2.10	125.07	122.03
3	C	613	F89	CA-N-C	2.11	125.07	122.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	618	NDP	O4D-C1D-N1N	2.11	112.33	108.07
3	D	616	F89	C3M-C3-N2	2.13	120.69	117.20
3	B	608	F89	C3M-C3-N2	2.14	120.71	117.20
3	C	613	F89	C3M-C3-N2	2.17	120.76	117.20
2	B	607	UMP	O4'-C1'-N1	2.19	111.47	107.78
2	C	611	UMP	O4'-C1'-N1	2.20	111.49	107.78
2	E	619	UMP	O4'-C1'-N1	2.24	111.56	107.78
4	E	622	NDP	O4D-C1D-N1N	2.28	112.67	108.07
2	D	615	UMP	O4'-C1'-N1	2.31	111.68	107.78
4	A	606	NDP	O4D-C1D-N1N	2.34	112.78	108.07
2	A	603	UMP	O4'-C1'-N1	2.35	111.74	107.78
4	B	610	NDP	O2N-PN-O1N	2.37	124.54	112.28
4	A	606	NDP	O2N-PN-O1N	2.37	124.56	112.28
4	E	622	NDP	O2A-PA-O1A	2.39	124.65	112.28
4	C	614	NDP	O4D-C1D-N1N	2.40	112.89	108.07
4	E	622	NDP	O2N-PN-O1N	2.40	124.68	112.28
4	D	618	NDP	O2A-PA-O1A	2.40	124.69	112.28
4	A	606	NDP	O2A-PA-O1A	2.40	124.72	112.28
3	E	621	F89	C16-C-N	2.41	107.97	106.47
4	C	614	NDP	O2N-PN-O1N	2.41	124.75	112.28
4	D	618	NDP	O2N-PN-O1N	2.43	124.84	112.28
4	C	614	NDP	O2A-PA-O1A	2.43	124.85	112.28
4	B	610	NDP	O2A-PA-O1A	2.44	124.93	112.28
3	A	604	F89	C16-C-N	2.62	108.10	106.47
4	B	610	NDP	O4D-C1D-N1N	2.62	113.34	108.07
4	E	622	NDP	O2X-P2B-O2B	2.62	117.91	106.00
3	D	617	F89	C16-C-N	2.62	108.11	106.47
4	C	614	NDP	O2X-P2B-O2B	2.63	117.94	106.00
3	B	608	F89	C1A-C1B-C6A	2.64	120.89	118.81
3	C	612	F89	C16-C-N	2.66	108.13	106.47
4	A	606	NDP	O2X-P2B-O2B	2.68	118.18	106.00
3	C	613	F89	C16-C-N	2.68	108.14	106.47
4	D	618	NDP	O2X-P2B-O2B	2.68	118.19	106.00
3	C	612	F89	C1A-C1B-C6A	2.68	120.93	118.81
2	D	615	UMP	OP3-P-OP2	2.69	118.46	107.61
4	B	610	NDP	O2X-P2B-O2B	2.69	118.25	106.00
2	E	619	UMP	OP3-P-OP2	2.69	118.48	107.61
3	D	616	F89	C1A-C1B-C6A	2.71	120.95	118.81
3	B	608	F89	C16-C-N	2.71	108.16	106.47
3	B	609	F89	C16-C-N	2.71	108.16	106.47
3	A	605	F89	C16-C-N	2.72	108.17	106.47
2	B	607	UMP	OP3-P-OP2	2.73	118.61	107.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	UMP	OP3-P-OP2	2.73	118.61	107.61
3	E	620	F89	C16-C-N	2.75	108.19	106.47
2	C	611	UMP	OP3-P-OP2	2.75	118.72	107.61
3	D	616	F89	C16-C-N	2.79	108.21	106.47
3	A	604	F89	C1A-C1B-C6A	2.81	121.03	118.81
3	E	620	F89	C1A-C1B-C6A	2.88	121.09	118.81
3	E	620	F89	C17-C16-C	2.92	134.18	129.65
3	E	621	F89	C17-C16-C	2.95	134.23	129.65
3	D	617	F89	C1A-C1B-C6A	2.96	121.15	118.81
3	A	605	F89	C17-C16-C	2.96	134.24	129.65
3	A	604	F89	C17-C16-C	2.98	134.27	129.65
3	C	613	F89	C1A-C1B-C6A	2.99	121.18	118.81
3	E	621	F89	C1A-C1B-C6A	3.00	121.18	118.81
3	D	617	F89	C17-C16-C	3.00	134.30	129.65
3	C	612	F89	C17-C16-C	3.02	134.33	129.65
3	B	609	F89	C17-C16-C	3.03	134.35	129.65
3	C	613	F89	C17-C16-C	3.06	134.40	129.65
3	D	616	F89	C17-C16-C	3.07	134.41	129.65
3	B	608	F89	C17-C16-C	3.08	134.42	129.65
3	A	605	F89	C1A-C1B-C6A	3.09	121.25	118.81
3	B	609	F89	C1A-C1B-C6A	3.11	121.27	118.81
3	E	620	F89	C1B-C1A-C4A	3.21	121.05	117.85
3	B	609	F89	C1B-C1A-C4A	3.24	121.07	117.85
3	A	605	F89	C1B-C1A-C4A	3.24	121.08	117.85
3	E	621	F89	C1B-C1A-C4A	3.28	121.11	117.85
3	C	613	F89	C1B-C1A-C4A	3.29	121.12	117.85
3	A	604	F89	C1B-C1A-C4A	3.31	121.14	117.85
3	D	617	F89	C1B-C1A-C4A	3.32	121.16	117.85
3	C	612	F89	C1B-C1A-C4A	3.39	121.22	117.85
3	B	608	F89	C1B-C1A-C4A	3.39	121.22	117.85
3	B	608	F89	CA-N-C	3.39	126.93	122.03
3	D	616	F89	C1B-C1A-C4A	3.42	121.25	117.85
3	C	612	F89	CA-N-C	3.48	127.06	122.03
3	D	616	F89	CA-N-C	3.52	127.11	122.03
3	E	620	F89	CA-N-C	3.54	127.14	122.03
3	A	604	F89	CA-N-C	3.62	127.26	122.03
2	C	611	UMP	C4-N3-C2	10.98	123.56	114.13
2	B	607	UMP	C4-N3-C2	11.05	123.63	114.13
2	E	619	UMP	C4-N3-C2	11.08	123.65	114.13
2	D	615	UMP	C4-N3-C2	11.09	123.66	114.13
2	A	603	UMP	C4-N3-C2	11.14	123.70	114.13
3	E	620	F89	C15-C19-N	20.47	109.16	102.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	F89	C15-C19-N	20.77	109.25	102.18
3	C	612	F89	C15-C19-N	20.94	109.31	102.18
3	B	608	F89	C15-C19-N	20.95	109.32	102.18
3	D	616	F89	C15-C19-N	21.02	109.34	102.18
3	A	605	F89	C15-C19-N	21.16	109.39	102.18
3	C	613	F89	C15-C19-N	21.17	109.39	102.18
3	D	617	F89	C15-C19-N	21.23	109.41	102.18
3	B	609	F89	C15-C19-N	21.26	109.42	102.18
3	E	621	F89	C15-C19-N	21.33	109.45	102.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 122 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	UMP	2	0
3	A	604	F89	7	0
3	A	605	F89	9	0
4	A	606	NDP	10	0
2	B	607	UMP	3	0
3	B	608	F89	6	0
3	B	609	F89	7	0
4	B	610	NDP	8	0
2	C	611	UMP	3	0
3	C	612	F89	7	0
3	C	613	F89	8	0
4	C	614	NDP	8	0
2	D	615	UMP	2	0
3	D	616	F89	8	0
3	D	617	F89	9	0
4	D	618	NDP	8	0
2	E	619	UMP	2	0
3	E	620	F89	7	0
3	E	621	F89	10	0
4	E	622	NDP	8	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	519/521 (99%)	-0.28	9 (1%) 70 69	16, 30, 54, 76	0
1	B	519/521 (99%)	-0.25	9 (1%) 70 69	16, 29, 51, 76	0
1	C	519/521 (99%)	-0.32	9 (1%) 70 69	17, 31, 52, 76	0
1	D	519/521 (99%)	-0.29	13 (2%) 58 55	18, 31, 55, 76	0
1	E	519/521 (99%)	-0.19	14 (2%) 55 51	19, 32, 55, 76	0
All	All	2595/2605 (99%)	-0.27	54 (2%) 64 61	16, 31, 54, 76	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	521	VAL	6.1
1	D	521	VAL	6.0
1	B	180	LYS	5.1
1	D	182	THR	5.0
1	B	521	VAL	5.0
1	C	182	THR	4.9
1	B	182	THR	4.8
1	E	180	LYS	4.8
1	A	182	THR	4.8
1	C	180	LYS	4.6
1	E	182	THR	4.2
1	A	180	LYS	4.2
1	D	180	LYS	3.8
1	E	521	VAL	3.8
1	C	183	LEU	3.7
1	E	183	LEU	3.7
1	D	183	LEU	3.7
1	A	183	LEU	3.4
1	D	102	MET	3.4
1	A	179	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	179	GLU	3.3
1	C	521	VAL	3.3
1	B	102	MET	3.3
1	E	102	MET	3.2
1	C	179	GLU	3.1
1	E	520	ALA	3.1
1	B	183	LEU	3.0
1	C	82	ASP	3.0
1	D	179	GLU	3.0
1	D	520	ALA	2.9
1	C	102	MET	2.9
1	D	181	LYS	2.8
1	E	184	GLN	2.7
1	A	102	MET	2.7
1	E	181	LYS	2.6
1	B	179	GLU	2.6
1	A	181	LYS	2.5
1	B	103	ASN	2.5
1	C	3	GLU	2.4
1	C	181	LYS	2.4
1	D	84	ALA	2.4
1	E	84	ALA	2.4
1	D	82	ASP	2.3
1	E	82	ASP	2.3
1	D	3	GLU	2.2
1	A	520	ALA	2.2
1	B	3	GLU	2.2
1	D	184	GLN	2.1
1	E	328	ILE	2.1
1	B	520	ALA	2.1
1	E	519	MET	2.1
1	D	47	ASN	2.1
1	A	331	GLY	2.0
1	E	178	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	F89	C	613	37/37	0.91	0.23	4.16	42,50,56,56	0
3	F89	A	605	37/37	0.93	0.25	3.87	42,50,56,56	0
3	F89	D	617	37/37	0.91	0.23	3.70	42,50,56,56	0
2	UMP	C	611	20/20	0.95	0.21	3.39	49,61,68,68	0
3	F89	B	609	37/37	0.92	0.24	3.00	42,50,56,56	0
2	UMP	A	603	20/20	0.96	0.24	2.79	50,63,68,69	0
3	F89	C	612	37/37	0.85	0.27	2.34	42,50,56,56	0
2	UMP	B	607	20/20	0.95	0.22	2.08	47,61,67,67	0
3	F89	E	621	37/37	0.91	0.21	2.06	42,50,56,56	0
3	F89	B	608	37/37	0.86	0.28	1.82	42,50,56,56	0
3	F89	A	604	37/37	0.83	0.27	1.67	42,50,56,56	0
2	UMP	D	615	20/20	0.94	0.20	1.64	52,64,69,69	0
3	F89	E	620	37/37	0.84	0.36	1.59	42,50,56,56	0
3	F89	D	616	37/37	0.84	0.28	1.25	42,50,56,56	0
2	UMP	E	619	20/20	0.95	0.17	1.25	54,64,69,69	0
4	NDP	A	606	48/48	0.98	0.17	0.70	29,38,48,50	0
4	NDP	B	610	48/48	0.98	0.17	0.39	29,38,49,50	0
4	NDP	C	614	48/48	0.95	0.17	0.18	31,43,53,54	0
4	NDP	D	618	48/48	0.96	0.17	0.13	33,42,52,52	0
4	NDP	E	622	48/48	0.96	0.14	-0.61	33,43,52,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.