



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:17 AM GMT

PDB ID : 3OAE
Title : Crystal structure of HPV16 L1 Pentamer bound to Heparin oligosaccharides
Authors : Chen, X.S.; Dasgupta, J.
Deposited on : 2010-08-05
Resolution : 2.80 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

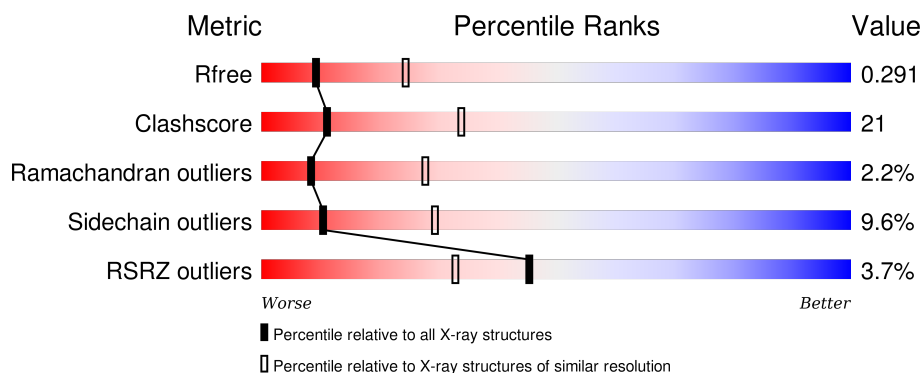
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	428	<div> <div>3%</div> <div>58% 34% 6% •</div> </div>
1	B	428	<div> <div>4%</div> <div>61% 31% 7% •</div> </div>
1	C	428	<div> <div>3%</div> <div>59% 33% 7% •</div> </div>
1	D	428	<div> <div>5%</div> <div>60% 33% 6% •</div> </div>
1	E	428	<div> <div>3%</div> <div>61% 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	JHM	A	507	-	-	X	X
2	JHM	A	519	-	-	-	X
2	JHM	C	501	-	-	X	-
2	JHM	C	509	-	-	X	X
2	JHM	D	511	-	-	-	X
2	JHM	E	513	-	-	X	-
2	JHM	E	527	-	-	X	-
3	IDS	C	502	-	-	X	X
3	IDS	C	504	-	-	X	-
3	IDS	D	510	-	-	-	X
3	IDS	D	512	-	-	-	X
3	IDS	D	516	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17030 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 Late major capsid protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3322	2116	556	630	20			
1	B	421	Total	C	N	O	S	0	0	0
			3322	2116	556	630	20			
1	C	421	Total	C	N	O	S	0	0	0
			3322	2116	556	630	20			
1	D	421	Total	C	N	O	S	0	0	0
			3322	2116	556	630	20			
1	E	421	Total	C	N	O	S	0	0	0
			3322	2116	556	630	20			

There are 55 discrepancies between the modelled and reference sequences:

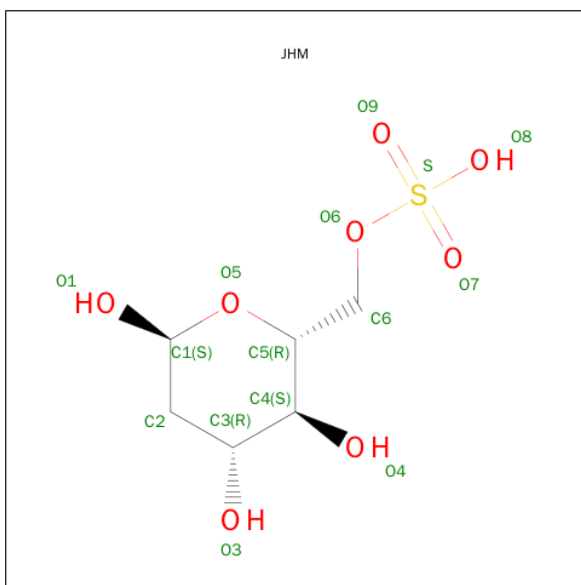
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	EXPRESSION TAG	UNP Q81007
A	19	SER	-	EXPRESSION TAG	UNP Q81007
A	20	ALA	-	EXPRESSION TAG	UNP Q81007
A	177	GLN	ASN	ENGINEERED MUTATION	UNP Q81007
A	181	GLN	ASN	ENGINEERED MUTATION	UNP Q81007
A	433	GLY	-	LINKER	UNP Q81007
A	434	GLY	-	LINKER	UNP Q81007
A	435	SER	-	LINKER	UNP Q81007
A	436	GLY	-	LINKER	UNP Q81007
A	437	GLY	-	LINKER	UNP Q81007
A	472	LEU	ALA	ENGINEERED MUTATION	UNP Q81007
B	18	GLY	-	EXPRESSION TAG	UNP Q81007
B	19	SER	-	EXPRESSION TAG	UNP Q81007
B	20	ALA	-	EXPRESSION TAG	UNP Q81007
B	177	GLN	ASN	ENGINEERED MUTATION	UNP Q81007
B	181	GLN	ASN	ENGINEERED MUTATION	UNP Q81007
B	433	GLY	-	LINKER	UNP Q81007
B	434	GLY	-	LINKER	UNP Q81007
B	435	SER	-	LINKER	UNP Q81007

Continued on next page...

Continued from previous page...

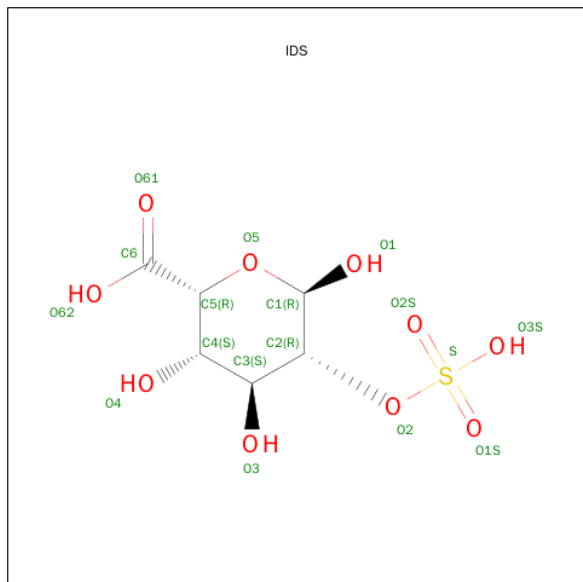
Chain	Residue	Modelled	Actual	Comment	Reference
B	436	GLY	-	LINKER	UNP Q81007
B	437	GLY	-	LINKER	UNP Q81007
B	472	LEU	ALA	ENGINEERED MUTATION	UNP Q81007
C	18	GLY	-	EXPRESSION TAG	UNP Q81007
C	19	SER	-	EXPRESSION TAG	UNP Q81007
C	20	ALA	-	EXPRESSION TAG	UNP Q81007
C	177	GLN	ASN	ENGINEERED MUTATION	UNP Q81007
C	181	GLN	ASN	ENGINEERED MUTATION	UNP Q81007
C	433	GLY	-	LINKER	UNP Q81007
C	434	GLY	-	LINKER	UNP Q81007
C	435	SER	-	LINKER	UNP Q81007
C	436	GLY	-	LINKER	UNP Q81007
C	437	GLY	-	LINKER	UNP Q81007
C	472	LEU	ALA	ENGINEERED MUTATION	UNP Q81007
D	18	GLY	-	EXPRESSION TAG	UNP Q81007
D	19	SER	-	EXPRESSION TAG	UNP Q81007
D	20	ALA	-	EXPRESSION TAG	UNP Q81007
D	177	GLN	ASN	ENGINEERED MUTATION	UNP Q81007
D	181	GLN	ASN	ENGINEERED MUTATION	UNP Q81007
D	433	GLY	-	LINKER	UNP Q81007
D	434	GLY	-	LINKER	UNP Q81007
D	435	SER	-	LINKER	UNP Q81007
D	436	GLY	-	LINKER	UNP Q81007
D	437	GLY	-	LINKER	UNP Q81007
D	472	LEU	ALA	ENGINEERED MUTATION	UNP Q81007
E	18	GLY	-	EXPRESSION TAG	UNP Q81007
E	19	SER	-	EXPRESSION TAG	UNP Q81007
E	20	ALA	-	EXPRESSION TAG	UNP Q81007
E	177	GLN	ASN	ENGINEERED MUTATION	UNP Q81007
E	181	GLN	ASN	ENGINEERED MUTATION	UNP Q81007
E	433	GLY	-	LINKER	UNP Q81007
E	434	GLY	-	LINKER	UNP Q81007
E	435	SER	-	LINKER	UNP Q81007
E	436	GLY	-	LINKER	UNP Q81007
E	437	GLY	-	LINKER	UNP Q81007
E	472	LEU	ALA	ENGINEERED MUTATION	UNP Q81007

- Molecule 2 is 2-DEOXY-6-O-SULFO-ALPHA-D-ARABINO-HEXOPYRANOSE (three-letter code: JHM) (formula: C₆H₁₂O₈S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	S	0	0
			15	6	8	1		
2	C	1	Total	C	O	S	0	0
			15	6	8	1		
2	B	1	Total	C	O	S	0	0
			15	6	8	1		
2	A	1	Total	C	O	S	0	0
			15	6	8	1		
2	C	1	Total	C	O	S	0	0
			15	6	8	1		
2	D	1	Total	C	O	S	0	0
			15	6	8	1		
2	E	1	Total	C	O	S	0	0
			15	6	8	1		
2	D	1	Total	C	O	S	0	0
			15	6	8	1		
2	E	1	Total	C	O	S	0	0
			15	6	8	1		
2	A	1	Total	C	O	S	0	0
			15	6	8	1		
2	E	1	Total	C	O	S	0	0
			15	6	8	1		
2	E	1	Total	C	O	S	0	0
			15	6	8	1		
2	E	1	Total	C	O	S	0	0
			15	6	8	1		
2	E	1	Total	C	O	S	0	0
			15	6	8	1		

- Molecule 3 is SUGAR (2-O-SULFO-BETA-L-ALTROPYRANURONIC ACID) (three-letter code: IDS) (formula: C₆H₁₀O₁₀S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	O	S	0	0
			15	6	8	1		
3	C	1	Total	C	O	S	0	0
			15	6	8	1		
3	B	1	Total	C	O	S	0	0
			15	6	8	1		
3	B	1	Total	C	O	S	0	0
			15	6	8	1		
3	D	1	Total	C	O	S	0	0
			15	6	8	1		
3	D	1	Total	C	O	S	0	0
			15	6	8	1		
3	E	1	Total	C	O	S	0	0
			15	6	8	1		
3	D	1	Total	C	O	S	0	0
			15	6	8	1		
3	E	1	Total	C	O	S	0	0
			15	6	8	1		
3	A	1	Total	C	O	S	0	0
			15	6	8	1		
3	E	1	Total	C	O	S	0	0
			15	6	8	1		
3	E	1	Total	C	O	S	0	0
			15	6	8	1		

Continued on next page...

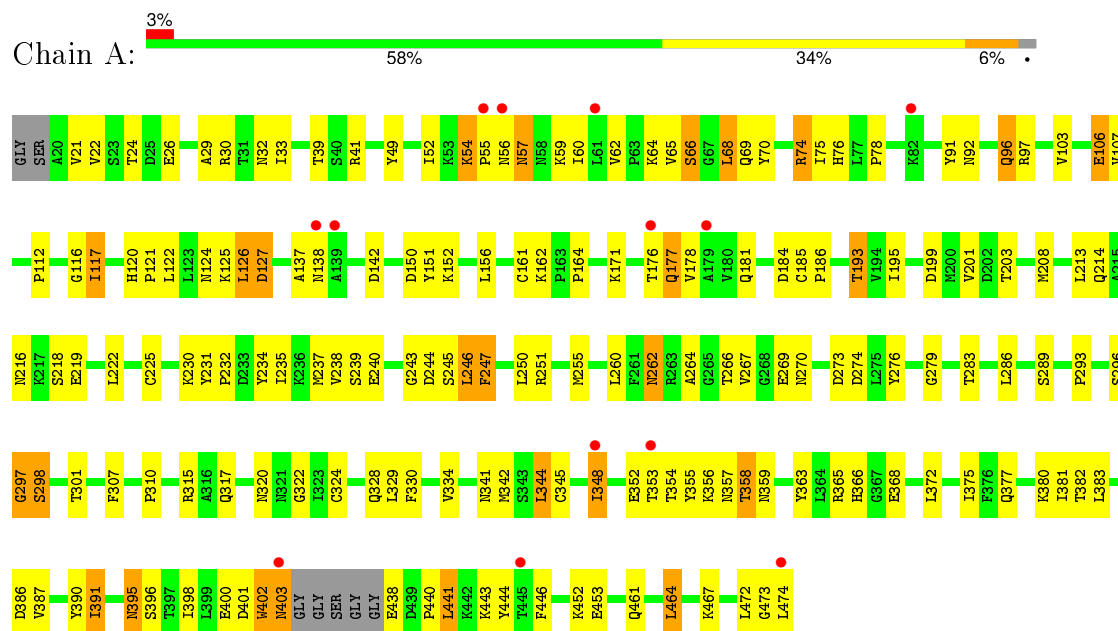
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	O	S	0	0
			15	6	8	1		
3	E	1	Total	C	O	S	0	0
			15	6	8	1		

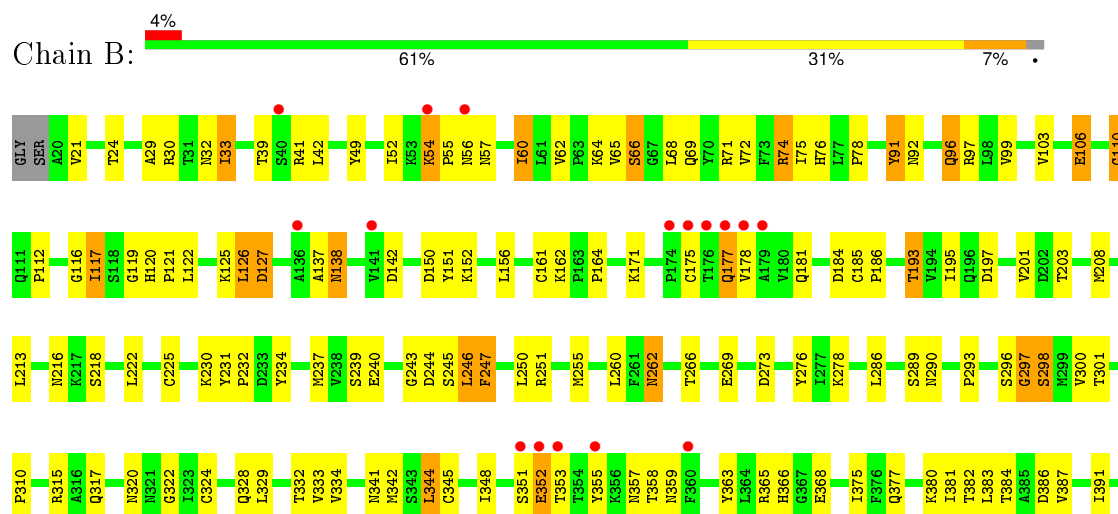
3 Residue-property plots

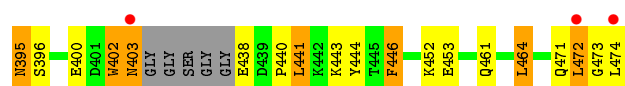
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Late major capsid protein L1

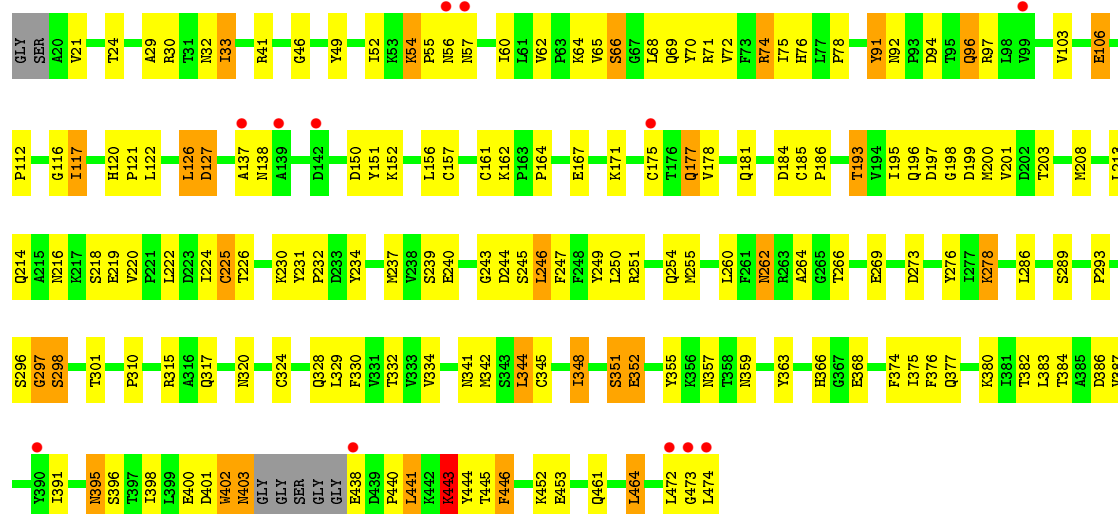


- Molecule 1: Late major capsid protein L1

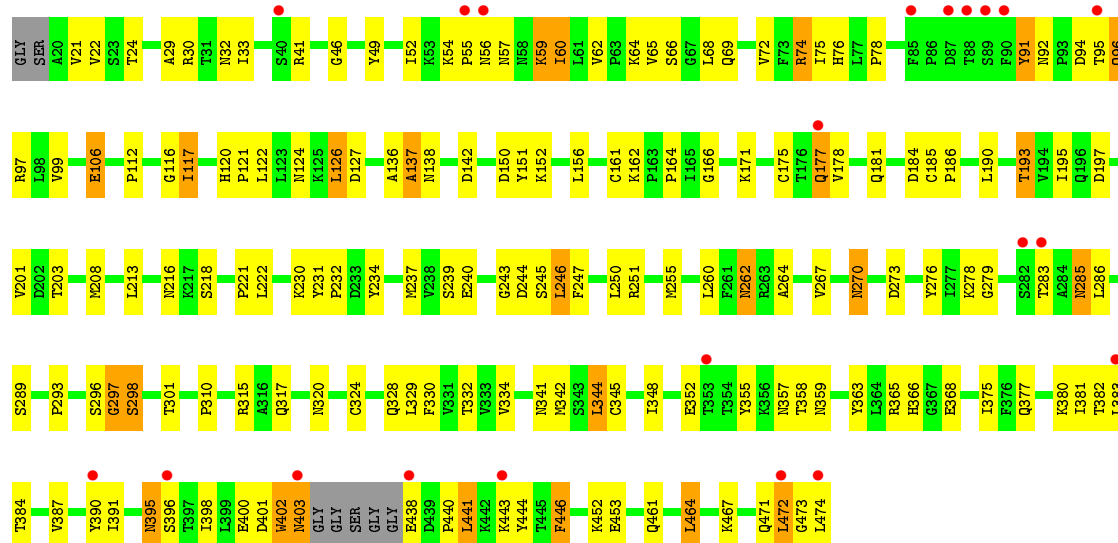




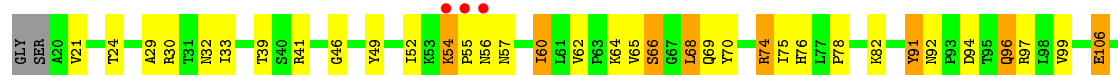
• Molecule 1: Late major capsid protein L1

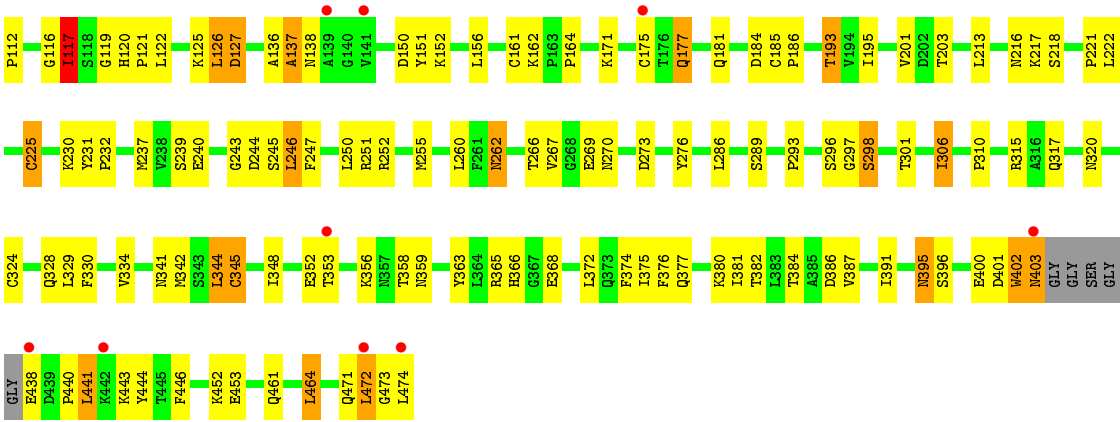


• Molecule 1: Late major capsid protein L1



• Molecule 1: Late major capsid protein L1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.62Å 101.25Å 128.18Å 90.00° 90.63° 90.00°	Depositor
Resolution (Å)	47.43 – 2.80 47.43 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.43-2.80) 93.6 (47.43-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.275 0.269 , 0.291	Depositor DCC
R_{free} test set	2872 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.9	EDS
Estimated twinning fraction	0.011 for -k,-h,-l 0.012 for k,h,-l 0.020 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 60076 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	17030	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: JHM, IDS

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	0.58	6/3407 (0.2%)	0.72	3/4632 (0.1%)
1	B	0.49	0/3407	0.70	2/4632 (0.0%)
1	C	0.53	2/3407 (0.1%)	0.71	1/4632 (0.0%)
1	D	0.55	3/3407 (0.1%)	0.71	3/4632 (0.1%)
1	E	0.52	1/3407 (0.0%)	0.72	0/4632
All	All	0.53	12/17035 (0.1%)	0.71	9/23160 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	59	LYS	CB-CG	-8.86	1.28	1.52
1	A	443	LYS	CD-CE	-6.59	1.34	1.51
1	A	57	ASN	CG-OD1	-6.35	1.09	1.24
1	D	285	ASN	CG-OD1	-6.11	1.10	1.24
1	C	443	LYS	CD-CE	-6.05	1.36	1.51
1	D	285	ASN	CG-ND2	-5.96	1.18	1.32
1	A	54	LYS	CD-CE	-5.70	1.37	1.51
1	C	443	LYS	CG-CD	-5.57	1.33	1.52
1	A	443	LYS	CB-CG	-5.56	1.37	1.52
1	E	225	CYS	CB-SG	-5.45	1.73	1.81
1	A	443	LYS	CG-CD	-5.43	1.33	1.52
1	A	54	LYS	CE-NZ	-5.16	1.36	1.49

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	443	LYS	CD-CE-NZ	-6.43	96.90	111.70
1	C	297	GLY	N-CA-C	-5.73	98.78	113.10
1	D	297	GLY	N-CA-C	-5.70	98.84	113.10
1	D	59	LYS	CA-CB-CG	5.59	125.71	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	ILE	CG1-CB-CG2	-5.53	99.24	111.40
1	A	297	GLY	N-CA-C	-5.46	99.45	113.10
1	B	297	GLY	N-CA-C	-5.34	99.76	113.10
1	B	110	GLY	N-CA-C	5.27	126.27	113.10
1	D	59	LYS	CB-CA-C	-5.20	100.00	110.40

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	3322	0	3227	148	4
1	B	3322	0	3227	146	0
1	C	3322	0	3227	166	2
1	D	3322	0	3227	140	2
1	E	3322	0	3226	142	0
2	A	30	0	19	20	0
2	B	15	0	9	0	0
2	C	45	0	30	25	2
2	D	30	0	19	2	0
2	E	90	0	58	23	1
3	A	15	0	4	1	0
3	B	30	0	8	0	0
3	C	30	0	8	24	0
3	D	45	0	12	10	3
3	E	90	0	24	7	2
All	All	17030	0	16325	694	8

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 21.

All (694) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:THR:HB	2:A:507:JHM:C1	1.48	1.40
1:A:358:THR:CB	2:A:507:JHM:H1	1.48	1.39
3:D:516:IDS:C4	2:E:513:JHM:O1	1.72	1.37
2:E:525:JHM:O1	3:E:528:IDS:C4	1.73	1.35
2:A:507:JHM:H6A	1:B:266:THR:CG2	1.63	1.26
2:C:501:JHM:H1	3:C:504:IDS:C6	1.64	1.26
2:A:507:JHM:C6	1:B:266:THR:HG21	1.71	1.21
1:E:452:LYS:NZ	2:E:527:JHM:H6A	1.56	1.17
1:A:358:THR:CG2	2:A:507:JHM:H1	1.75	1.16
3:D:516:IDS:C4	2:E:513:JHM:C1	2.24	1.14
1:C:198:GLY:O	3:C:502:IDS:O61	1.66	1.13
1:E:452:LYS:NZ	2:E:527:JHM:C6	2.13	1.12
1:A:54:LYS:HB3	1:A:57:ASN:HB3	1.23	1.12
1:C:97:ARG:HH21	1:C:403:ASN:HB2	1.13	1.10
1:E:452:LYS:HZ3	2:E:527:JHM:C6	1.67	1.07
1:E:452:LYS:HZ3	2:E:527:JHM:H6A	1.02	1.05
2:C:501:JHM:H1	3:C:504:IDS:C4	1.86	1.04
2:C:501:JHM:C2	3:C:504:IDS:O62	2.05	1.04
1:B:461:GLN:HE22	1:C:21:VAL:H	1.04	1.03
1:C:196:GLN:NE2	3:C:504:IDS:O61	1.91	1.03
2:C:501:JHM:H1	3:C:504:IDS:O62	1.57	1.03
1:C:54:LYS:HB3	1:C:57:ASN:HB3	1.40	1.01
1:E:175:CYS:HB3	1:E:177:GLN:OE1	1.61	0.98
1:D:56:ASN:HB3	3:D:516:IDS:O61	1.61	0.98
2:C:501:JHM:C1	3:C:504:IDS:O62	2.11	0.98
1:C:461:GLN:HE22	1:D:21:VAL:H	1.10	0.97
1:B:54:LYS:HB3	1:B:57:ASN:HB3	1.47	0.96
2:C:501:JHM:C1	3:C:504:IDS:C4	2.44	0.96
1:A:21:VAL:H	1:E:461:GLN:HE22	1.10	0.93
1:A:461:GLN:HE22	1:B:21:VAL:H	1.09	0.92
1:A:97:ARG:HH21	1:A:403:ASN:HB2	1.31	0.92
1:D:121:PRO:HD3	1:D:222:LEU:HD21	1.52	0.92
1:D:461:GLN:HE22	1:E:21:VAL:H	1.05	0.92
1:A:358:THR:HB	2:A:507:JHM:H1	0.96	0.91
1:B:29:ALA:HB3	1:B:380:LYS:HG3	1.55	0.89
3:D:516:IDS:O2S	2:E:513:JHM:O7	1.91	0.89
1:E:29:ALA:HB3	1:E:380:LYS:HG3	1.54	0.88
1:A:358:THR:HB	2:A:507:JHM:O5	1.74	0.88
2:C:501:JHM:H1	3:C:504:IDS:C5	2.04	0.87
1:D:443:LYS:HE2	1:D:443:LYS:HA	1.57	0.87
1:B:97:ARG:HH21	1:B:403:ASN:HB2	1.37	0.87
1:B:345:CYS:SG	1:C:216:ASN:HB2	2.14	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:PRO:HD3	1:C:222:LEU:HD21	1.58	0.86
1:A:29:ALA:HB3	1:A:380:LYS:HG3	1.58	0.86
1:B:121:PRO:HD3	1:B:222:LEU:HD21	1.58	0.86
1:C:200:MET:HG2	3:C:502:IDS:O62	1.76	0.85
1:B:443:LYS:HE2	1:B:443:LYS:HA	1.58	0.85
1:E:121:PRO:HD3	1:E:222:LEU:HD21	1.58	0.85
2:C:501:JHM:C1	3:C:504:IDS:C6	2.54	0.85
2:E:525:JHM:C1	3:E:528:IDS:C4	2.53	0.85
1:C:345:CYS:SG	1:D:216:ASN:HB2	2.17	0.85
1:C:121:PRO:HG3	1:D:289:SER:HB3	1.59	0.84
1:D:29:ALA:HB3	1:D:380:LYS:HG3	1.59	0.84
1:A:121:PRO:HD3	1:A:222:LEU:HD21	1.58	0.84
2:E:525:JHM:HO1	3:E:528:IDS:C4	1.90	0.84
1:A:216:ASN:HB2	1:E:345:CYS:SG	2.17	0.84
2:C:501:JHM:O1	3:C:504:IDS:C4	2.26	0.83
1:C:55:PRO:HG3	2:C:509:JHM:O5	1.77	0.83
1:A:345:CYS:SG	1:B:216:ASN:HB2	2.19	0.83
1:C:55:PRO:HG3	2:C:509:JHM:C1	2.10	0.82
1:A:358:THR:CB	2:A:507:JHM:C1	2.25	0.82
1:C:196:GLN:NE2	3:C:504:IDS:C6	2.42	0.82
1:C:97:ARG:NH2	1:C:403:ASN:HB2	1.95	0.81
1:A:121:PRO:HG3	1:B:289:SER:HB3	1.62	0.81
1:E:452:LYS:HZ2	2:E:527:JHM:C6	1.91	0.81
1:B:461:GLN:NE2	1:C:21:VAL:H	1.79	0.81
1:C:29:ALA:HB3	1:C:380:LYS:HG3	1.60	0.81
1:E:443:LYS:HE2	1:E:443:LYS:HA	1.63	0.81
1:C:196:GLN:HE22	3:C:504:IDS:C6	1.93	0.80
1:E:452:LYS:NZ	2:E:527:JHM:H6	1.95	0.80
1:A:54:LYS:HB3	1:A:57:ASN:CB	2.10	0.80
1:C:444:TYR:CE2	2:C:503:JHM:H2	2.16	0.80
1:C:445:THR:HG21	2:C:501:JHM:O8	1.81	0.80
1:D:97:ARG:HH21	1:D:403:ASN:HB2	1.47	0.79
1:C:461:GLN:NE2	1:D:21:VAL:H	1.80	0.78
2:C:501:JHM:H2	3:C:504:IDS:O62	1.83	0.78
1:E:358:THR:HG21	2:E:521:JHM:O3	1.83	0.78
1:D:345:CYS:SG	1:E:216:ASN:HB2	2.24	0.78
1:B:121:PRO:HG3	1:C:289:SER:HB3	1.66	0.77
2:E:523:JHM:H6A	3:E:526:IDS:O2S	1.86	0.76
1:A:366:HIS:HE1	1:A:368:GLU:OE1	1.69	0.76
1:D:440:PRO:HG2	1:D:441:LEU:HD12	1.68	0.76
1:A:21:VAL:H	1:E:461:GLN:NE2	1.83	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:SER:HB3	1:E:121:PRO:HG3	1.66	0.75
1:D:54:LYS:HB3	1:D:57:ASN:CB	2.17	0.75
1:D:461:GLN:NE2	1:E:21:VAL:H	1.82	0.74
1:D:54:LYS:HB3	1:D:57:ASN:HB3	1.69	0.74
1:C:196:GLN:CD	3:C:504:IDS:O61	2.25	0.74
1:C:55:PRO:HG3	2:C:509:JHM:H1	1.68	0.74
2:A:507:JHM:H6A	1:B:266:THR:HG21	0.80	0.74
1:C:444:TYR:HE2	2:C:503:JHM:C2	2.00	0.74
1:A:461:GLN:NE2	1:B:21:VAL:H	1.84	0.73
1:A:162:LYS:HB2	1:A:245:SER:HA	1.71	0.72
1:D:121:PRO:HG3	1:E:289:SER:HB3	1.70	0.72
1:D:162:LYS:HB2	1:D:245:SER:HA	1.71	0.72
1:D:122:LEU:O	1:D:218:SER:HB3	1.90	0.72
1:B:402:TRP:O	1:B:403:ASN:C	2.28	0.72
1:B:387:VAL:O	1:B:391:ILE:HD13	1.90	0.71
1:B:152:LYS:HB2	1:B:255:MET:HB2	1.72	0.71
1:C:122:LEU:O	1:C:218:SER:HB3	1.90	0.70
1:C:162:LYS:HB2	1:C:245:SER:HA	1.72	0.70
1:C:199:ASP:HA	3:C:502:IDS:O61	1.90	0.70
1:C:444:TYR:CE2	2:C:503:JHM:C2	2.75	0.70
1:E:122:LEU:O	1:E:218:SER:HB3	1.92	0.69
1:E:78:PRO:HD3	1:E:452:LYS:HA	1.73	0.69
1:C:55:PRO:HB3	2:C:509:JHM:C6	2.22	0.69
1:A:358:THR:HA	2:A:507:JHM:O5	1.92	0.69
1:E:152:LYS:HB2	1:E:255:MET:HB2	1.73	0.69
1:E:162:LYS:HB2	1:E:245:SER:HA	1.74	0.69
1:E:452:LYS:HZ2	2:E:527:JHM:H6	1.55	0.69
1:D:78:PRO:HD3	1:D:452:LYS:HA	1.75	0.69
1:A:358:THR:HG22	2:A:507:JHM:H1	1.69	0.68
1:A:122:LEU:O	1:A:218:SER:HB3	1.93	0.68
1:D:152:LYS:HB2	1:D:255:MET:HB2	1.74	0.68
1:E:97:ARG:HH21	1:E:403:ASN:HB2	1.58	0.68
1:C:443:LYS:HB3	1:C:443:LYS:HZ2	1.59	0.68
1:C:198:GLY:O	3:C:502:IDS:C6	2.42	0.68
1:B:122:LEU:O	1:B:218:SER:HB3	1.94	0.67
1:B:162:LYS:HB2	1:B:245:SER:HA	1.76	0.67
1:C:440:PRO:HG2	1:C:441:LEU:HD12	1.77	0.67
1:B:440:PRO:HG2	1:B:441:LEU:HD12	1.76	0.67
1:A:152:LYS:HB2	1:A:255:MET:HB2	1.76	0.67
1:A:176:THR:O	1:A:177:GLN:HG3	1.94	0.67
1:D:270:ASN:CG	3:D:510:IDS:O3	2.33	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:LYS:HB2	1:C:255:MET:HB2	1.76	0.67
1:C:117:ILE:HG21	1:D:293:PRO:HD3	1.77	0.67
1:A:78:PRO:HD3	1:A:452:LYS:HA	1.76	0.67
1:D:402:TRP:O	1:D:403:ASN:C	2.34	0.67
1:B:117:ILE:HG21	1:C:293:PRO:HD3	1.77	0.66
1:C:55:PRO:HB3	2:C:509:JHM:H6A	1.77	0.66
1:E:440:PRO:HG2	1:E:441:LEU:HD12	1.77	0.66
1:B:52:ILE:HB	1:B:62:VAL:HB	1.78	0.66
1:C:55:PRO:CG	2:C:509:JHM:O5	2.44	0.66
1:C:52:ILE:HB	1:C:62:VAL:HB	1.78	0.65
1:C:396:SER:O	1:C:400:GLU:HG3	1.96	0.65
1:C:66:SER:H	1:C:69:GLN:NE2	1.95	0.65
1:D:66:SER:H	1:D:69:GLN:NE2	1.95	0.65
1:A:440:PRO:HG2	1:A:441:LEU:HD12	1.77	0.65
1:C:363:TYR:CE2	1:D:185:CYS:HB2	2.32	0.65
1:C:402:TRP:O	1:C:403:ASN:C	2.34	0.65
1:B:78:PRO:HD3	1:B:452:LYS:HA	1.78	0.65
1:D:375:ILE:HG12	1:D:464:LEU:HD13	1.79	0.64
1:C:175:CYS:HB3	1:C:177:GLN:OE1	1.96	0.64
1:B:375:ILE:HG12	1:B:464:LEU:HD13	1.80	0.64
1:D:366:HIS:HE1	1:D:368:GLU:OE1	1.81	0.64
1:E:375:ILE:HG12	1:E:464:LEU:HD13	1.78	0.64
1:E:358:THR:CG2	2:E:521:JHM:O3	2.46	0.64
1:D:68:LEU:HD22	1:D:203:THR:HG22	1.77	0.64
1:E:181:GLN:HB2	1:E:184:ASP:OD1	1.98	0.64
1:A:348:ILE:HG22	1:A:359:ASN:OD1	1.97	0.64
1:B:396:SER:O	1:B:400:GLU:HG3	1.98	0.64
1:E:348:ILE:HG22	1:E:359:ASN:OD1	1.97	0.64
1:C:375:ILE:HG12	1:C:464:LEU:HD13	1.80	0.63
1:D:270:ASN:ND2	3:D:510:IDS:O3	2.30	0.63
1:A:185:CYS:HB2	1:E:363:TYR:CE2	2.33	0.63
1:C:199:ASP:CA	3:C:502:IDS:O61	2.47	0.63
1:D:267:VAL:HG11	1:D:270:ASN:ND2	2.12	0.63
1:D:126:LEU:HB3	1:D:262:ASN:HB3	1.81	0.63
1:B:92:ASN:O	1:B:96:GLN:HG2	1.99	0.63
1:E:366:HIS:HE1	1:E:368:GLU:OE1	1.82	0.63
1:A:52:ILE:HB	1:A:62:VAL:HB	1.80	0.63
1:D:443:LYS:HE2	1:D:443:LYS:CA	2.29	0.62
1:E:387:VAL:HG12	1:E:391:ILE:HD12	1.80	0.62
1:E:68:LEU:HD22	1:E:203:THR:HG22	1.80	0.62
1:C:387:VAL:O	1:C:391:ILE:HG12	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:CYS:HB3	1:D:177:GLN:OE1	2.00	0.62
1:A:402:TRP:O	1:A:403:ASN:C	2.34	0.62
1:D:440:PRO:HG2	1:D:441:LEU:CD1	2.30	0.62
1:A:126:LEU:HB3	1:A:262:ASN:HB3	1.82	0.61
1:A:68:LEU:HD22	1:A:203:THR:HG22	1.82	0.61
1:D:161:CYS:SG	1:D:244:ASP:HB3	2.41	0.61
1:B:68:LEU:HD22	1:B:203:THR:HG22	1.82	0.61
1:C:49:TYR:O	1:C:64:LYS:HE2	1.99	0.61
1:A:66:SER:H	1:A:69:GLN:NE2	1.98	0.61
1:A:92:ASN:O	1:A:96:GLN:HG2	1.99	0.61
1:A:216:ASN:OD1	1:A:218:SER:HB2	2.01	0.61
1:B:237:MET:SD	1:B:246:LEU:HD23	2.41	0.61
1:C:366:HIS:HE1	1:C:368:GLU:OE1	1.84	0.61
1:C:68:LEU:HD22	1:C:203:THR:HG22	1.82	0.60
1:D:240:GLU:HG2	1:D:243:GLY:H	1.66	0.60
1:D:49:TYR:O	1:D:64:LYS:HE2	2.00	0.60
1:A:161:CYS:SG	1:A:244:ASP:HB3	2.42	0.60
3:D:516:IDS:C4	2:E:513:JHM:O5	2.50	0.60
1:E:344:LEU:HD23	1:E:344:LEU:N	2.16	0.60
1:A:112:PRO:HB3	1:B:231:TYR:CD1	2.37	0.60
1:D:387:VAL:HG12	1:D:391:ILE:HD12	1.84	0.60
1:C:156:LEU:HG	1:C:334:VAL:HB	1.82	0.60
1:C:200:MET:CG	3:C:502:IDS:O62	2.48	0.60
1:E:92:ASN:O	1:E:96:GLN:HG2	2.00	0.60
1:E:156:LEU:HA	1:E:250:LEU:O	2.02	0.59
1:A:49:TYR:O	1:A:64:LYS:HE2	2.02	0.59
1:A:403:ASN:C	1:A:403:ASN:HD22	2.05	0.59
1:A:375:ILE:HG12	1:A:464:LEU:HD13	1.85	0.59
1:C:78:PRO:HD3	1:C:452:LYS:HA	1.84	0.59
1:C:126:LEU:HB3	1:C:262:ASN:HB3	1.84	0.59
1:A:363:TYR:CE2	1:B:185:CYS:HB2	2.38	0.59
1:B:66:SER:H	1:B:69:GLN:NE2	1.99	0.59
1:B:461:GLN:HE22	1:C:21:VAL:N	1.88	0.59
1:E:358:THR:HG21	2:E:521:JHM:C2	2.33	0.59
2:A:507:JHM:C6	1:B:266:THR:CG2	2.53	0.59
1:C:363:TYR:CD2	1:D:185:CYS:HB2	2.36	0.59
1:E:66:SER:H	1:E:69:GLN:NE2	2.00	0.59
1:C:112:PRO:HB3	1:D:231:TYR:CD1	2.38	0.59
1:A:54:LYS:HG2	1:A:56:ASN:OD1	2.02	0.59
2:E:523:JHM:C6	3:E:526:IDS:O2S	2.50	0.58
1:D:68:LEU:HD13	1:D:151:TYR:HD1	1.67	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:CYS:HB3	1:B:177:GLN:OE1	2.03	0.58
1:B:112:PRO:HB3	1:C:231:TYR:CD1	2.39	0.58
1:C:240:GLU:HG2	1:C:243:GLY:H	1.68	0.58
1:A:293:PRO:HD3	1:E:117:ILE:HG21	1.85	0.58
1:A:358:THR:CA	2:A:507:JHM:O5	2.51	0.58
1:C:196:GLN:OE1	1:C:445:THR:N	2.31	0.58
1:E:49:TYR:O	1:E:64:LYS:HE2	2.03	0.58
1:C:246:LEU:O	1:C:246:LEU:HD12	2.04	0.58
1:B:126:LEU:HB3	1:B:262:ASN:HB3	1.85	0.58
1:C:403:ASN:HD22	1:C:403:ASN:C	2.07	0.58
1:D:120:HIS:HA	1:D:222:LEU:HD22	1.86	0.58
1:B:49:TYR:O	1:B:64:LYS:HE2	2.04	0.58
1:B:216:ASN:OD1	1:B:218:SER:HB2	2.04	0.58
1:A:237:MET:SD	1:A:246:LEU:HD23	2.44	0.58
1:B:181:GLN:HB2	1:B:184:ASP:OD1	2.04	0.57
1:A:358:THR:CB	2:A:507:JHM:O5	2.43	0.57
1:C:324:CYS:HB3	1:C:328:GLN:O	2.04	0.57
1:C:441:LEU:HB3	1:C:444:TYR:HD1	1.70	0.57
1:D:97:ARG:HG3	1:D:383:LEU:HD11	1.86	0.57
1:A:363:TYR:CD2	1:B:185:CYS:HB2	2.40	0.57
1:C:444:TYR:HE2	2:C:503:JHM:H2A	1.69	0.57
1:A:246:LEU:HD12	1:A:246:LEU:O	2.05	0.57
1:E:126:LEU:HB3	1:E:262:ASN:HB3	1.86	0.57
1:D:285:ASN:HA	2:D:511:JHM:O8	2.03	0.57
1:C:196:GLN:NE2	2:C:503:JHM:O3	2.38	0.57
1:C:68:LEU:O	1:C:201:VAL:HG23	2.05	0.57
1:D:52:ILE:HB	1:D:62:VAL:HB	1.86	0.57
1:C:273:ASP:HA	1:C:276:TYR:CE2	2.39	0.57
1:B:363:TYR:CE2	1:C:185:CYS:HB2	2.40	0.56
1:C:341:ASN:HD22	1:C:366:HIS:HB2	1.70	0.56
1:B:353:THR:O	1:D:278:LYS:HB2	2.05	0.56
1:E:381:ILE:HD12	1:E:381:ILE:N	2.20	0.56
1:D:55:PRO:HG2	1:D:56:ASN:H	1.71	0.56
1:A:185:CYS:SG	1:E:365:ARG:NH1	2.79	0.56
1:B:246:LEU:O	1:B:246:LEU:HD12	2.06	0.56
1:B:278:LYS:HB2	1:E:353:THR:O	2.05	0.56
1:B:366:HIS:HE1	1:B:368:GLU:OE1	1.89	0.56
1:C:196:GLN:OE1	3:C:504:IDS:O61	2.22	0.56
1:E:52:ILE:HB	1:E:62:VAL:HB	1.87	0.56
1:A:75:ILE:HB	1:A:329:LEU:HB3	1.87	0.56
1:E:273:ASP:HA	1:E:276:TYR:CE2	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:LEU:HB3	1:D:444:TYR:HD1	1.70	0.56
1:C:92:ASN:O	1:C:96:GLN:HG2	2.04	0.56
1:C:348:ILE:HG22	1:C:359:ASN:OD1	2.06	0.56
1:A:269:GLU:CD	1:E:52:ILE:HG12	2.26	0.56
1:D:166:GLY:HA3	1:D:195:ILE:HD11	1.88	0.56
1:C:54:LYS:HB3	1:C:57:ASN:CB	2.26	0.56
1:D:117:ILE:HG21	1:E:293:PRO:HD3	1.86	0.56
1:B:344:LEU:HD23	1:B:344:LEU:N	2.20	0.56
1:D:92:ASN:O	1:D:96:GLN:HG2	2.06	0.56
1:E:441:LEU:HB3	1:E:444:TYR:HD1	1.70	0.56
1:A:240:GLU:HG2	1:A:243:GLY:H	1.70	0.56
1:B:156:LEU:HG	1:B:334:VAL:HB	1.87	0.56
1:A:185:CYS:HB2	1:E:363:TYR:CD2	2.41	0.56
1:D:381:ILE:N	1:D:381:ILE:HD12	2.22	0.55
1:E:161:CYS:SG	1:E:244:ASP:HB3	2.46	0.55
1:A:57:ASN:OD1	1:A:59:LYS:HB3	2.07	0.55
1:B:384:THR:OG1	1:B:387:VAL:HG23	2.06	0.55
1:C:75:ILE:HB	1:C:329:LEU:HB3	1.88	0.55
1:A:117:ILE:HG21	1:B:293:PRO:HD3	1.88	0.55
1:D:273:ASP:HA	1:D:276:TYR:CE2	2.41	0.55
1:A:231:TYR:CD1	1:E:112:PRO:HB3	2.41	0.55
1:D:324:CYS:HB3	1:D:328:GLN:O	2.07	0.55
1:C:440:PRO:HG2	1:C:441:LEU:CD1	2.36	0.55
1:E:54:LYS:CB	1:E:57:ASN:HB3	2.37	0.55
1:E:402:TRP:O	1:E:403:ASN:C	2.45	0.55
1:E:440:PRO:HG2	1:E:441:LEU:CD1	2.37	0.55
1:B:395:ASN:HD22	1:B:395:ASN:C	2.09	0.55
1:E:30:ARG:HB3	1:E:377:GLN:NE2	2.21	0.55
1:E:156:LEU:HG	1:E:334:VAL:HB	1.89	0.55
1:D:156:LEU:HG	1:D:334:VAL:HB	1.89	0.55
1:B:324:CYS:HB3	1:B:328:GLN:O	2.07	0.55
1:A:356:LYS:HB3	1:A:358:THR:HG23	1.87	0.54
1:C:54:LYS:HG3	1:C:55:PRO:HD2	1.89	0.54
1:C:276:TYR:HE1	1:C:278:LYS:HE3	1.72	0.54
1:B:150:ASP:O	1:B:296:SER:HA	2.07	0.54
1:E:216:ASN:OD1	1:E:218:SER:HB2	2.07	0.54
1:B:193:THR:HG21	1:B:230:LYS:HD2	1.90	0.54
1:D:68:LEU:O	1:D:201:VAL:HG23	2.06	0.54
1:B:161:CYS:SG	1:B:244:ASP:HB3	2.48	0.54
1:E:396:SER:O	1:E:400:GLU:HG3	2.08	0.54
1:D:396:SER:O	1:D:400:GLU:HG3	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LYS:HG3	1:B:55:PRO:HD2	1.90	0.54
1:E:240:GLU:HG2	1:E:243:GLY:H	1.72	0.54
1:A:441:LEU:HB3	1:A:444:TYR:HD1	1.72	0.54
1:B:68:LEU:HD13	1:B:151:TYR:HD1	1.72	0.54
1:A:324:CYS:HB3	1:A:328:GLN:O	2.06	0.54
1:D:164:PRO:HG2	1:D:195:ILE:HB	1.90	0.54
1:E:75:ILE:HB	1:E:329:LEU:HB3	1.89	0.54
1:B:440:PRO:HG2	1:B:441:LEU:CD1	2.37	0.54
1:E:68:LEU:HD13	1:E:151:TYR:HD1	1.73	0.54
1:D:348:ILE:HG22	1:D:359:ASN:OD1	2.07	0.54
3:D:516:IDS:C4	2:E:513:JHM:H1	2.29	0.54
1:B:96:GLN:HB3	1:B:382:THR:HA	1.89	0.54
1:A:68:LEU:O	1:A:201:VAL:HG23	2.08	0.54
1:E:116:GLY:O	1:E:117:ILE:HB	2.08	0.54
1:D:112:PRO:HB3	1:E:231:TYR:CD1	2.42	0.54
1:C:120:HIS:ND1	1:C:121:PRO:HD2	2.23	0.54
1:D:54:LYS:HB3	1:D:57:ASN:HB2	1.88	0.54
1:D:344:LEU:HD23	1:D:344:LEU:N	2.23	0.54
1:D:46:GLY:HA3	1:D:65:VAL:HG23	1.89	0.53
1:D:56:ASN:CB	3:D:516:IDS:O61	2.48	0.53
1:B:348:ILE:HG22	1:B:359:ASN:OD1	2.08	0.53
1:D:395:ASN:HD22	1:D:395:ASN:C	2.12	0.53
1:B:54:LYS:HB3	1:B:57:ASN:CB	2.32	0.53
1:A:156:LEU:HG	1:A:334:VAL:HB	1.91	0.53
2:A:507:JHM:H6A	1:B:266:THR:CB	2.34	0.53
1:D:120:HIS:ND1	1:D:121:PRO:HD2	2.23	0.53
1:B:260:LEU:N	1:B:260:LEU:HD12	2.23	0.53
1:B:74:ARG:HD2	1:B:76:HIS:CE1	2.44	0.53
1:E:54:LYS:HB2	1:E:57:ASN:HB3	1.90	0.53
1:C:161:CYS:SG	1:C:244:ASP:HB3	2.49	0.53
1:C:150:ASP:O	1:C:296:SER:HA	2.09	0.53
1:A:440:PRO:HG2	1:A:441:LEU:CD1	2.38	0.52
1:E:324:CYS:HB3	1:E:328:GLN:O	2.09	0.52
1:A:273:ASP:HA	1:A:276:TYR:CE2	2.44	0.52
1:C:24:THR:HG23	1:C:320:ASN:HA	1.91	0.52
1:A:260:LEU:HD12	1:A:260:LEU:N	2.24	0.52
1:C:395:ASN:C	1:C:395:ASN:HD22	2.13	0.52
1:C:461:GLN:HE22	1:D:21:VAL:N	1.92	0.52
1:A:120:HIS:ND1	1:A:121:PRO:HD2	2.23	0.52
1:D:97:ARG:CG	1:D:383:LEU:HD11	2.40	0.52
1:B:240:GLU:HG2	1:B:243:GLY:H	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:525:JHM:H1	3:E:528:IDS:C4	2.36	0.52
1:B:68:LEU:O	1:B:201:VAL:HG23	2.08	0.52
1:A:156:LEU:HA	1:A:250:LEU:O	2.10	0.52
1:A:344:LEU:HD12	1:B:186:PRO:HG2	1.91	0.52
1:D:216:ASN:OD1	1:D:218:SER:HB2	2.09	0.52
1:E:401:ASP:O	1:E:402:TRP:O	2.27	0.52
1:D:156:LEU:HA	1:D:250:LEU:O	2.09	0.52
1:E:74:ARG:HD2	1:E:76:HIS:CE1	2.45	0.52
1:C:55:PRO:HG2	1:C:56:ASN:H	1.74	0.52
1:B:471:GLN:OE1	1:B:472:LEU:HD23	2.08	0.52
1:E:246:LEU:O	1:E:246:LEU:HD12	2.10	0.52
1:A:366:HIS:CE1	1:A:368:GLU:OE1	2.57	0.51
1:D:237:MET:SD	1:D:246:LEU:HD23	2.50	0.51
1:E:126:LEU:HG	1:E:127:ASP:OD2	2.10	0.51
1:E:150:ASP:O	1:E:296:SER:HA	2.10	0.51
1:D:150:ASP:O	1:D:296:SER:HA	2.11	0.51
1:A:269:GLU:OE1	1:E:365:ARG:NH2	2.44	0.51
1:B:151:TYR:CG	1:B:203:THR:HB	2.45	0.51
1:B:75:ILE:HB	1:B:329:LEU:HB3	1.91	0.51
1:A:387:VAL:O	1:A:391:ILE:HD13	2.10	0.51
1:D:260:LEU:HD12	1:D:260:LEU:N	2.26	0.51
1:E:395:ASN:C	1:E:395:ASN:HD22	2.12	0.51
1:E:380:LYS:C	1:E:381:ILE:HD12	2.31	0.51
1:C:216:ASN:OD1	1:C:218:SER:HB2	2.11	0.51
1:D:96:GLN:HB3	1:D:382:THR:HA	1.93	0.51
1:D:75:ILE:HB	1:D:329:LEU:HB3	1.92	0.51
1:B:30:ARG:HB3	1:B:377:GLN:NE2	2.26	0.51
1:B:441:LEU:HB3	1:B:444:TYR:HD1	1.75	0.51
1:A:395:ASN:HD22	1:A:395:ASN:C	2.12	0.51
1:D:151:TYR:CG	1:D:203:THR:HB	2.46	0.51
1:A:91:TYR:HD1	1:A:96:GLN:HG3	1.76	0.51
1:C:91:TYR:HD1	1:C:96:GLN:HG3	1.74	0.51
1:C:445:THR:CG2	1:C:446:PHE:N	2.73	0.51
1:B:55:PRO:HG2	1:B:56:ASN:H	1.76	0.51
1:C:30:ARG:HB3	1:C:377:GLN:NE2	2.26	0.51
1:B:91:TYR:HD1	1:B:96:GLN:HG3	1.76	0.51
1:E:151:TYR:CG	1:E:203:THR:HB	2.45	0.51
1:C:151:TYR:CG	1:C:203:THR:HB	2.46	0.51
1:B:395:ASN:ND2	1:B:395:ASN:C	2.64	0.51
1:A:193:THR:HG21	1:A:230:LYS:HD2	1.92	0.51
1:B:273:ASP:HA	1:B:276:TYR:CE2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PRO:HG2	1:A:56:ASN:H	1.76	0.50
1:D:403:ASN:C	1:D:403:ASN:HD22	2.13	0.50
1:E:65:VAL:HA	1:E:69:GLN:NE2	2.26	0.50
1:C:96:GLN:HB3	1:C:382:THR:HA	1.93	0.50
1:A:401:ASP:O	1:A:402:TRP:O	2.29	0.50
1:D:193:THR:HG21	1:D:230:LYS:HD2	1.93	0.50
1:B:120:HIS:HA	1:B:222:LEU:HD22	1.93	0.50
1:A:151:TYR:CG	1:A:203:THR:HB	2.46	0.50
1:E:164:PRO:HG2	1:E:195:ILE:HB	1.93	0.50
1:E:267:VAL:HG11	1:E:270:ASN:OD1	2.11	0.50
1:B:403:ASN:C	1:B:403:ASN:HD22	2.15	0.50
1:B:363:TYR:CD2	1:C:185:CYS:HB2	2.47	0.50
1:D:341:ASN:HD22	1:D:366:HIS:HB2	1.77	0.50
1:A:66:SER:H	1:A:69:GLN:HE21	1.59	0.50
1:A:358:THR:CA	2:A:507:JHM:C1	2.89	0.50
1:E:441:LEU:N	1:E:441:LEU:HD12	2.27	0.50
1:D:91:TYR:HD1	1:D:96:GLN:HG3	1.77	0.50
1:B:106:GLU:HG2	1:B:310:PRO:HA	1.93	0.50
1:B:24:THR:HG23	1:B:320:ASN:HA	1.93	0.50
1:C:384:THR:OG1	1:C:387:VAL:HG23	2.12	0.50
1:B:381:ILE:HD12	1:B:381:ILE:N	2.26	0.50
1:E:252:ARG:HD2	1:E:306:ILE:HD11	1.93	0.49
1:E:120:HIS:HA	1:E:222:LEU:HD22	1.93	0.49
1:C:106:GLU:HG2	1:C:310:PRO:HA	1.94	0.49
1:B:341:ASN:HD22	1:B:366:HIS:HB2	1.77	0.49
1:A:365:ARG:NH2	1:B:269:GLU:OE1	2.45	0.49
1:C:181:GLN:HB2	1:C:184:ASP:OD1	2.11	0.49
1:D:30:ARG:HB3	1:D:377:GLN:NE2	2.27	0.49
1:A:65:VAL:HA	1:A:69:GLN:NE2	2.28	0.49
1:C:74:ARG:HD2	1:C:76:HIS:CE1	2.47	0.49
1:A:380:LYS:C	1:A:381:ILE:HD13	2.33	0.49
2:A:519:JHM:H1	3:E:522:IDS:C6	2.41	0.49
1:C:237:MET:SD	1:C:246:LEU:HD23	2.52	0.49
1:A:344:LEU:HD23	1:A:344:LEU:N	2.28	0.49
1:A:222:LEU:O	1:A:225:CYS:HB3	2.12	0.49
1:D:66:SER:H	1:D:69:GLN:HE21	1.60	0.49
1:A:74:ARG:HD2	1:A:76:HIS:CE1	2.48	0.49
1:C:198:GLY:C	3:C:502:IDS:O61	2.49	0.49
1:A:116:GLY:O	1:A:117:ILE:HB	2.13	0.49
1:E:74:ARG:HG2	1:E:330:PHE:CE2	2.48	0.49
1:C:214:GLN:OE1	1:C:219:GLU:HB2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:VAL:HG23	1:B:381:ILE:CD1	2.42	0.49
1:A:186:PRO:HG2	1:E:344:LEU:HD12	1.94	0.49
1:E:96:GLN:HB3	1:E:382:THR:HA	1.94	0.49
1:E:55:PRO:HG2	1:E:56:ASN:H	1.77	0.49
1:A:120:HIS:HA	1:A:222:LEU:HD22	1.95	0.49
1:D:68:LEU:HD13	1:D:151:TYR:CD1	2.48	0.49
1:B:344:LEU:HD12	1:C:186:PRO:HG2	1.95	0.49
1:A:324:CYS:SG	1:A:329:LEU:HD23	2.53	0.49
1:E:193:THR:HG21	1:E:230:LYS:HD2	1.94	0.49
1:E:68:LEU:O	1:E:201:VAL:HG23	2.13	0.48
1:E:246:LEU:HD12	1:E:246:LEU:C	2.34	0.48
1:A:106:GLU:OE2	1:A:467:LYS:NZ	2.46	0.48
1:C:65:VAL:HA	1:C:69:GLN:NE2	2.28	0.48
1:D:65:VAL:HA	1:D:69:GLN:NE2	2.28	0.48
1:E:237:MET:SD	1:E:246:LEU:HD23	2.53	0.48
1:B:443:LYS:HE2	1:B:443:LYS:CA	2.31	0.48
1:E:356:LYS:C	1:E:358:THR:H	2.17	0.48
1:C:193:THR:HG21	1:C:230:LYS:HD2	1.94	0.48
1:C:344:LEU:HD12	1:D:186:PRO:HG2	1.96	0.48
1:C:116:GLY:O	1:C:117:ILE:HB	2.12	0.48
1:C:68:LEU:HD13	1:C:151:TYR:HD1	1.78	0.48
1:B:324:CYS:SG	1:B:329:LEU:HD23	2.53	0.48
1:A:24:THR:HG23	1:A:320:ASN:HA	1.96	0.48
1:C:260:LEU:HD12	1:C:260:LEU:N	2.29	0.48
1:A:68:LEU:HD13	1:A:151:TYR:HD1	1.78	0.48
1:C:156:LEU:HA	1:C:250:LEU:O	2.14	0.48
1:E:237:MET:O	1:E:240:GLU:HB3	2.14	0.48
1:A:150:ASP:O	1:A:296:SER:HA	2.14	0.48
1:C:120:HIS:HA	1:C:222:LEU:HD22	1.95	0.48
1:C:66:SER:H	1:C:69:GLN:HE21	1.62	0.48
1:E:341:ASN:HD22	1:E:366:HIS:HB2	1.79	0.48
1:B:246:LEU:C	1:B:246:LEU:HD12	2.34	0.48
1:C:97:ARG:HG3	1:C:383:LEU:HD11	1.95	0.47
1:E:120:HIS:ND1	1:E:121:PRO:HD2	2.28	0.47
1:B:341:ASN:ND2	1:B:366:HIS:CD2	2.82	0.47
1:A:395:ASN:ND2	1:A:395:ASN:C	2.68	0.47
1:D:297:GLY:O	1:D:298:SER:O	2.32	0.47
1:C:69:GLN:NE2	1:C:71:ARG:NH2	2.62	0.47
1:A:96:GLN:HB3	1:A:382:THR:HA	1.95	0.47
1:A:106:GLU:HG2	1:A:310:PRO:HA	1.97	0.47
1:C:344:LEU:HD23	1:C:344:LEU:N	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:520:IDS:C6	2:E:517:JHM:H1	2.44	0.47
1:C:225:CYS:SG	1:C:226:THR:HG23	2.54	0.47
1:D:384:THR:OG1	1:D:387:VAL:HG23	2.15	0.47
1:C:126:LEU:HG	1:C:127:ASP:OD2	2.15	0.47
1:A:441:LEU:N	1:A:441:LEU:HD12	2.29	0.47
1:A:30:ARG:HB3	1:A:377:GLN:NE2	2.30	0.47
1:D:24:THR:HG23	1:D:320:ASN:HA	1.96	0.47
1:A:164:PRO:HG2	1:A:195:ILE:HB	1.97	0.47
1:E:125:LYS:O	1:E:125:LYS:HD3	2.14	0.47
1:A:266:THR:HB	2:A:519:JHM:O7	2.15	0.47
1:A:181:GLN:HB2	1:A:184:ASP:OD1	2.15	0.47
1:D:181:GLN:HB2	1:D:184:ASP:OD1	2.14	0.47
1:B:380:LYS:C	1:B:381:ILE:HD12	2.35	0.47
1:D:68:LEU:CD1	1:D:151:TYR:HD1	2.27	0.47
1:C:164:PRO:HG2	1:C:195:ILE:HB	1.96	0.47
1:D:74:ARG:HG2	1:D:330:PHE:CZ	2.50	0.47
1:C:65:VAL:HA	1:C:69:GLN:HE22	1.79	0.47
1:D:106:GLU:HG2	1:D:310:PRO:HA	1.97	0.47
1:D:279:GLY:HA3	1:D:283:THR:O	2.14	0.47
1:D:380:LYS:C	1:D:381:ILE:HD12	2.35	0.47
1:E:91:TYR:HD1	1:E:96:GLN:HG3	1.79	0.47
1:A:341:ASN:HD22	1:A:366:HIS:HB2	1.80	0.47
1:A:54:LYS:HG3	1:A:55:PRO:HD2	1.96	0.46
1:D:65:VAL:HA	1:D:69:GLN:HE22	1.80	0.46
1:A:201:VAL:O	1:A:203:THR:HG23	2.15	0.46
1:D:441:LEU:HD12	1:D:441:LEU:N	2.30	0.46
1:A:176:THR:C	1:A:177:GLN:HG3	2.35	0.46
1:C:237:MET:O	1:C:240:GLU:HB3	2.14	0.46
1:E:471:GLN:OE1	1:E:472:LEU:HD23	2.14	0.46
1:B:119:GLY:O	1:B:222:LEU:HD22	2.16	0.46
1:A:341:ASN:ND2	1:A:366:HIS:CD2	2.83	0.46
1:A:171:LYS:HG3	1:A:186:PRO:HB2	1.97	0.46
1:B:69:GLN:NE2	1:B:71:ARG:NH2	2.64	0.46
1:C:246:LEU:C	1:C:246:LEU:HD12	2.36	0.46
1:E:171:LYS:HG3	1:E:186:PRO:HB2	1.96	0.46
1:B:297:GLY:O	1:B:298:SER:O	2.33	0.46
1:C:441:LEU:N	1:C:441:LEU:HD12	2.30	0.46
1:D:363:TYR:CE2	1:E:185:CYS:HB2	2.51	0.46
3:D:516:IDS:C6	2:E:513:JHM:H1	2.45	0.46
1:C:355:TYR:HE2	1:C:357:ASN:ND2	2.14	0.46
2:A:507:JHM:C5	1:B:266:THR:HG21	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:VAL:HG23	1:B:381:ILE:HD13	1.97	0.46
1:E:443:LYS:CA	1:E:443:LYS:HE2	2.32	0.46
1:D:344:LEU:HD12	1:E:186:PRO:HG2	1.97	0.46
1:C:201:VAL:O	1:C:203:THR:HG23	2.16	0.46
1:B:156:LEU:HA	1:B:250:LEU:O	2.15	0.46
1:A:74:ARG:HG2	1:A:330:PHE:CZ	2.51	0.46
1:E:297:GLY:O	1:E:298:SER:O	2.33	0.46
1:A:279:GLY:HA3	1:A:283:THR:O	2.15	0.46
1:D:341:ASN:ND2	1:D:366:HIS:CD2	2.84	0.45
1:E:106:GLU:HB2	1:E:464:LEU:HG	1.98	0.45
1:D:120:HIS:HA	1:D:222:LEU:CD2	2.46	0.45
1:B:117:ILE:CG2	1:C:293:PRO:HD3	2.46	0.45
1:B:52:ILE:HG12	1:C:269:GLU:CD	2.36	0.45
1:B:365:ARG:NH2	1:C:269:GLU:OE1	2.48	0.45
1:B:106:GLU:HB2	1:B:464:LEU:HG	1.98	0.45
1:E:70:TYR:OH	1:E:232:PRO:HD3	2.16	0.45
1:C:171:LYS:HG3	1:C:186:PRO:HB2	1.97	0.45
1:A:355:TYR:HE2	1:A:357:ASN:ND2	2.14	0.45
1:E:395:ASN:C	1:E:395:ASN:ND2	2.70	0.45
1:A:358:THR:HG22	2:A:507:JHM:C1	2.42	0.45
1:B:201:VAL:O	1:B:203:THR:HG23	2.16	0.45
1:C:220:VAL:HB	1:C:224:ILE:HD11	1.99	0.45
1:E:24:THR:HG23	1:E:320:ASN:HA	1.98	0.45
1:A:97:ARG:HG3	1:A:383:LEU:HD11	1.98	0.45
1:C:395:ASN:O	1:C:398:ILE:HG12	2.17	0.45
1:E:106:GLU:HG2	1:E:310:PRO:HA	1.97	0.45
1:A:239:SER:O	1:A:240:GLU:C	2.55	0.45
1:B:333:VAL:HG12	1:B:334:VAL:N	2.32	0.45
1:C:342:MET:HB2	1:D:208:MET:SD	2.57	0.45
1:E:239:SER:O	1:E:240:GLU:C	2.55	0.45
1:C:74:ARG:HG2	1:C:330:PHE:CZ	2.51	0.45
1:A:396:SER:O	1:A:400:GLU:HG3	2.17	0.45
1:B:300:VAL:O	1:C:254:GLN:HA	2.17	0.45
1:E:384:THR:OG1	1:E:387:VAL:HG23	2.17	0.45
1:E:151:TYR:CD2	1:E:203:THR:HB	2.52	0.45
1:C:74:ARG:HG2	1:C:330:PHE:CE2	2.52	0.45
1:D:171:LYS:HG3	1:D:186:PRO:HB2	1.99	0.45
1:D:358:THR:HA	1:E:266:THR:CG2	2.47	0.45
1:C:55:PRO:CB	2:C:509:JHM:O5	2.65	0.44
1:E:341:ASN:ND2	1:E:366:HIS:CD2	2.85	0.44
1:A:262:ASN:HD22	1:A:262:ASN:HA	1.54	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ASN:OD1	1:C:94:ASP:HB2	2.17	0.44
1:C:33:ILE:H	1:C:33:ILE:HG12	1.67	0.44
1:C:106:GLU:HB2	1:C:464:LEU:HG	1.98	0.44
1:A:65:VAL:HA	1:A:69:GLN:HE22	1.81	0.44
1:B:237:MET:O	1:B:240:GLU:HB3	2.17	0.44
1:D:395:ASN:ND2	1:D:395:ASN:C	2.70	0.44
1:C:222:LEU:O	1:C:225:CYS:HB3	2.17	0.44
1:D:99:VAL:HG23	1:D:381:ILE:CD1	2.46	0.44
1:B:65:VAL:HA	1:B:69:GLN:NE2	2.33	0.44
1:C:395:ASN:C	1:C:395:ASN:ND2	2.69	0.44
1:B:125:LYS:O	1:B:125:LYS:HD3	2.16	0.44
1:A:235:ILE:H	1:A:235:ILE:HD12	1.83	0.44
1:A:54:LYS:CG	1:A:56:ASN:OD1	2.66	0.44
1:D:461:GLN:HE22	1:E:21:VAL:N	1.90	0.44
1:E:356:LYS:C	1:E:358:THR:N	2.69	0.44
1:B:239:SER:O	1:B:240:GLU:C	2.55	0.44
1:E:74:ARG:HG2	1:E:330:PHE:CZ	2.52	0.44
1:E:99:VAL:HG23	1:E:381:ILE:HD13	2.00	0.44
1:E:222:LEU:O	1:E:225:CYS:HB3	2.18	0.44
1:E:260:LEU:HD12	1:E:260:LEU:N	2.32	0.44
1:D:106:GLU:OE2	1:D:467:LYS:NZ	2.48	0.44
1:A:208:MET:SD	1:E:342:MET:HB2	2.57	0.44
1:C:97:ARG:CG	1:C:383:LEU:HD11	2.48	0.44
1:A:237:MET:O	1:A:240:GLU:HB3	2.17	0.44
1:A:246:LEU:HD12	1:A:246:LEU:C	2.37	0.44
1:B:290:ASN:HA	1:B:290:ASN:HD22	1.60	0.44
1:E:99:VAL:HG23	1:E:381:ILE:CD1	2.47	0.44
1:A:126:LEU:HG	1:A:127:ASP:OD2	2.17	0.44
1:B:126:LEU:HG	1:B:127:ASP:OD2	2.17	0.44
1:B:342:MET:HB2	1:C:208:MET:SD	2.57	0.44
1:E:136:ALA:O	1:E:137:ALA:O	2.36	0.44
1:B:116:GLY:O	1:B:117:ILE:HB	2.18	0.44
1:C:324:CYS:SG	1:C:329:LEU:HD23	2.57	0.44
1:D:116:GLY:O	1:D:117:ILE:HB	2.17	0.44
1:D:355:TYR:HE2	1:D:357:ASN:ND2	2.16	0.44
1:D:471:GLN:OE1	1:D:472:LEU:HD23	2.18	0.44
2:C:501:JHM:H2A	3:C:504:IDS:O62	2.09	0.43
1:D:99:VAL:HG23	1:D:381:ILE:HD13	2.00	0.43
1:E:66:SER:H	1:E:69:GLN:HE21	1.64	0.43
1:B:164:PRO:HG2	1:B:195:ILE:HB	1.99	0.43
1:A:70:TYR:OH	1:A:232:PRO:HD3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:LEU:O	1:D:246:LEU:HD12	2.17	0.43
1:D:92:ASN:OD1	1:D:94:ASP:HB2	2.18	0.43
1:D:74:ARG:HG2	1:D:330:PHE:CE2	2.52	0.43
1:A:22:VAL:HB	1:A:26:GLU:HG3	2.00	0.43
1:C:239:SER:O	1:C:240:GLU:C	2.57	0.43
1:E:54:LYS:HB3	1:E:57:ASN:CB	2.48	0.43
1:A:125:LYS:O	1:A:125:LYS:HD3	2.18	0.43
1:B:60:ILE:H	1:B:60:ILE:HG13	1.39	0.43
1:C:443:LYS:HB2	1:C:443:LYS:HE3	1.53	0.43
1:B:33:ILE:HG12	1:B:33:ILE:H	1.70	0.43
1:B:391:ILE:HD12	1:B:391:ILE:N	2.33	0.43
1:C:351:SER:HB2	1:C:352:GLU:H	1.63	0.43
1:E:39:THR:HG23	1:E:372:LEU:HB2	2.01	0.43
1:D:262:ASN:HA	1:D:262:ASN:HD22	1.51	0.43
1:E:262:ASN:HA	1:E:262:ASN:HD22	1.53	0.43
1:D:363:TYR:CD2	1:E:185:CYS:HB2	2.53	0.43
1:C:70:TYR:OH	1:C:232:PRO:HD3	2.18	0.43
1:B:222:LEU:O	1:B:225:CYS:HB3	2.18	0.43
1:B:262:ASN:HD22	1:B:262:ASN:HA	1.48	0.43
1:A:274:ASP:O	1:E:217:LYS:HE2	2.18	0.43
1:A:297:GLY:O	1:A:298:SER:O	2.36	0.43
1:B:66:SER:H	1:B:69:GLN:HE21	1.66	0.43
1:E:324:CYS:SG	1:E:329:LEU:HD23	2.58	0.43
1:A:74:ARG:HG2	1:A:330:PHE:CE2	2.53	0.43
1:D:60:ILE:H	1:D:60:ILE:HD12	1.84	0.43
1:B:171:LYS:HG3	1:B:186:PRO:HB2	2.01	0.43
1:D:365:ARG:NH2	1:E:269:GLU:OE1	2.51	0.43
1:C:55:PRO:HB3	2:C:509:JHM:O5	2.19	0.42
1:C:443:LYS:H	1:C:443:LYS:HG3	0.98	0.42
1:B:441:LEU:N	1:B:441:LEU:HD12	2.34	0.42
1:D:237:MET:O	1:D:240:GLU:HB3	2.18	0.42
1:E:65:VAL:HA	1:E:69:GLN:HE22	1.82	0.42
1:A:342:MET:HB2	1:B:208:MET:SD	2.59	0.42
1:C:197:ASP:CB	1:C:446:PHE:HA	2.48	0.42
1:D:151:TYR:CD2	1:D:203:THR:HB	2.54	0.42
1:D:136:ALA:O	1:D:137:ALA:O	2.37	0.42
1:B:39:THR:HB	1:B:42:LEU:HD21	2.01	0.42
1:A:266:THR:HG23	1:E:358:THR:HA	2.02	0.42
1:D:201:VAL:O	1:D:203:THR:HG23	2.19	0.42
1:B:151:TYR:CD2	1:B:203:THR:HB	2.55	0.42
1:A:103:VAL:O	1:A:103:VAL:HG12	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:HIS:HB2	1:E:221:PRO:HA	2.00	0.42
1:B:193:THR:CG2	1:B:230:LYS:HD2	2.49	0.42
1:B:120:HIS:HA	1:B:222:LEU:CD2	2.50	0.42
1:D:106:GLU:HB2	1:D:464:LEU:HG	2.00	0.42
1:A:22:VAL:HG22	1:A:390:TYR:CE1	2.54	0.42
1:D:60:ILE:CD1	1:D:60:ILE:H	2.32	0.42
1:B:138:ASN:HD22	1:B:138:ASN:HA	1.66	0.42
1:E:366:HIS:CE1	1:E:368:GLU:OE1	2.68	0.42
1:A:96:GLN:HE21	1:A:96:GLN:HB3	1.57	0.42
1:E:46:GLY:HA3	1:E:65:VAL:HG23	2.01	0.42
1:D:239:SER:O	1:D:240:GLU:C	2.57	0.42
1:C:157:CYS:O	1:C:249:TYR:HA	2.19	0.42
1:C:117:ILE:CG2	1:D:293:PRO:HD3	2.48	0.42
1:C:341:ASN:ND2	1:C:366:HIS:CD2	2.88	0.42
1:B:357:ASN:ND2	1:C:264:ALA:HB1	2.35	0.42
1:B:103:VAL:HG12	1:B:103:VAL:O	2.20	0.42
1:D:124:ASN:OD1	1:D:264:ALA:HB3	2.20	0.42
1:B:97:ARG:HG3	1:B:383:LEU:HD11	2.01	0.42
1:B:68:LEU:CD1	1:B:151:TYR:HD1	2.33	0.42
1:E:54:LYS:HB3	1:E:57:ASN:HB3	2.02	0.42
1:B:24:THR:CG2	1:B:320:ASN:HA	2.50	0.42
1:E:60:ILE:H	1:E:60:ILE:HD12	1.84	0.42
1:B:110:GLY:O	1:C:167:GLU:OE2	2.37	0.41
1:C:64:LYS:HD2	3:C:502:IDS:C4	2.49	0.41
1:C:401:ASP:O	1:C:402:TRP:O	2.38	0.41
1:D:285:ASN:HA	2:D:511:JHM:S	2.60	0.41
1:D:232:PRO:HB2	1:D:234:TYR:CE1	2.56	0.41
1:A:234:TYR:O	1:A:238:VAL:HG23	2.21	0.41
1:A:293:PRO:HD3	1:E:117:ILE:CG2	2.51	0.41
1:B:333:VAL:CG1	1:B:334:VAL:N	2.83	0.41
1:A:199:ASP:CG	1:A:230:LYS:HE2	2.41	0.41
1:D:74:ARG:HD2	1:D:76:HIS:CE1	2.55	0.41
1:B:351:SER:HB2	1:B:352:GLU:H	1.66	0.41
1:A:107:VAL:O	1:A:307:PHE:HB3	2.20	0.41
1:D:120:HIS:HA	1:D:121:PRO:HD3	1.92	0.41
1:C:276:TYR:CE1	1:C:278:LYS:HE3	2.53	0.41
1:C:96:GLN:HE21	1:C:96:GLN:HB3	1.61	0.41
1:D:72:VAL:HG22	1:D:332:THR:HG23	2.03	0.41
1:B:197:ASP:CB	1:B:446:PHE:HA	2.50	0.41
1:C:297:GLY:O	1:C:298:SER:O	2.39	0.41
1:B:355:TYR:HE2	1:B:357:ASN:ND2	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:HG11	1:A:270:ASN:HA	2.03	0.41
1:A:214:GLN:OE1	1:A:219:GLU:HB2	2.21	0.41
1:C:103:VAL:HG12	1:C:103:VAL:O	2.20	0.41
1:A:247:PHE:CZ	1:A:322:GLY:HA2	2.56	0.41
1:E:119:GLY:O	1:E:222:LEU:HD22	2.20	0.41
1:A:120:HIS:HA	1:A:121:PRO:HD3	1.94	0.41
1:B:365:ARG:NH1	1:C:185:CYS:SG	2.93	0.41
1:E:92:ASN:OD1	1:E:94:ASP:HB2	2.21	0.41
1:D:395:ASN:O	1:D:398:ILE:HG13	2.20	0.41
1:B:232:PRO:HB2	1:B:234:TYR:CE1	2.56	0.41
1:B:72:VAL:HG22	1:B:332:THR:HG23	2.02	0.41
1:E:66:SER:O	1:E:69:GLN:HG3	2.21	0.41
1:A:193:THR:CG2	1:A:230:LYS:HD2	2.51	0.41
1:A:39:THR:HG23	1:A:372:LEU:HB2	2.03	0.41
1:D:190:LEU:HD12	1:D:190:LEU:HA	1.96	0.41
1:C:403:ASN:ND2	1:C:403:ASN:C	2.74	0.40
1:E:201:VAL:O	1:E:203:THR:HG23	2.21	0.40
1:B:68:LEU:HD13	1:B:151:TYR:CD1	2.54	0.40
1:C:232:PRO:HB2	1:C:234:TYR:CE1	2.55	0.40
1:A:357:ASN:O	1:B:266:THR:HG23	2.22	0.40
1:B:120:HIS:ND1	1:B:121:PRO:HD2	2.36	0.40
1:D:401:ASP:O	1:D:402:TRP:O	2.38	0.40
1:D:324:CYS:SG	1:D:329:LEU:HD23	2.61	0.40
1:D:197:ASP:CB	1:D:446:PHE:HA	2.52	0.40
1:C:197:ASP:HB2	1:C:446:PHE:HA	2.04	0.40
1:B:247:PHE:CZ	1:B:322:GLY:HA2	2.56	0.40
1:B:358:THR:HA	1:C:266:THR:CG2	2.51	0.40
1:E:374:PHE:HB2	1:E:376:PHE:CE1	2.56	0.40
1:D:246:LEU:C	1:D:246:LEU:HD12	2.41	0.40
1:A:395:ASN:O	1:A:398:ILE:HG13	2.21	0.40
1:C:72:VAL:HG22	1:C:332:THR:HG23	2.03	0.40
1:D:120:HIS:HB2	1:D:221:PRO:HA	2.04	0.40
1:C:46:GLY:HA3	1:C:65:VAL:HG23	2.03	0.40
1:A:201:VAL:HG21	1:A:334:VAL:CG1	2.52	0.40
1:D:22:VAL:HG22	1:D:390:TYR:CE1	2.56	0.40
1:A:124:ASN:OD1	1:A:264:ALA:HB3	2.21	0.40
1:C:374:PHE:HB2	1:C:376:PHE:CE1	2.57	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:LYS:NZ	3:E:526:IDS:O3[2_556]	1.87	0.33
1:A:354:THR:OG1	2:C:509:JHM:O8[2_545]	1.92	0.28
1:A:353:THR:OG1	3:D:510:IDS:O2[2_545]	1.97	0.23
1:A:354:THR:OG1	2:C:509:JHM:O6[2_545]	2.08	0.12
1:C:278:LYS:CG	3:D:510:IDS:O61[2_545]	2.10	0.10
1:C:278:LYS:CB	3:D:510:IDS:O61[2_545]	2.11	0.09
1:D:59:LYS:NZ	3:E:526:IDS:C3[2_556]	2.13	0.07
1:A:59:LYS:NZ	2:E:523:JHM:C2[2_546]	2.16	0.04

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	417/428 (97%)	378 (91%)	29 (7%)	10 (2%)	7	25
1	B	417/428 (97%)	378 (91%)	29 (7%)	10 (2%)	7	25
1	C	417/428 (97%)	375 (90%)	34 (8%)	8 (2%)	10	32
1	D	417/428 (97%)	377 (90%)	30 (7%)	10 (2%)	7	25
1	E	417/428 (97%)	377 (90%)	32 (8%)	8 (2%)	10	32
All	All	2085/2140 (97%)	1885 (90%)	154 (7%)	46 (2%)	8	28

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	ALA
1	A	298	SER
1	A	402	TRP
1	B	137	ALA
1	B	298	SER
1	C	137	ALA
1	C	298	SER
1	C	402	TRP
1	D	137	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	298	SER
1	D	402	TRP
1	E	137	ALA
1	E	298	SER
1	E	402	TRP
1	A	117	ILE
1	A	126	LEU
1	B	126	LEU
1	B	402	TRP
1	B	473	GLY
1	C	117	ILE
1	C	126	LEU
1	C	473	GLY
1	D	126	LEU
1	D	473	GLY
1	E	117	ILE
1	E	126	LEU
1	E	473	GLY
1	A	41	ARG
1	A	473	GLY
1	B	41	ARG
1	C	41	ARG
1	D	41	ARG
1	E	41	ARG
1	A	177	GLN
1	B	177	GLN
1	D	117	ILE
1	A	142	ASP
1	B	117	ILE
1	B	142	ASP
1	C	177	GLN
1	E	177	GLN
1	D	142	ASP
1	D	177	GLN
1	A	178	VAL
1	D	178	VAL
1	B	178	VAL

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	368/370 (100%)	334 (91%)	34 (9%)	11	32
1	B	368/370 (100%)	335 (91%)	33 (9%)	12	34
1	C	368/370 (100%)	329 (89%)	39 (11%)	8	24
1	D	368/370 (100%)	335 (91%)	33 (9%)	12	34
1	E	368/370 (100%)	330 (90%)	38 (10%)	9	26
All	All	1840/1850 (100%)	1663 (90%)	177 (10%)	10	29

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	33	ILE
1	A	60	ILE
1	A	66	SER
1	A	68	LEU
1	A	74	ARG
1	A	96	GLN
1	A	106	GLU
1	A	127	ASP
1	A	138	ASN
1	A	193	THR
1	A	213	LEU
1	A	246	LEU
1	A	247	PHE
1	A	251	ARG
1	A	262	ASN
1	A	286	LEU
1	A	301	THR
1	A	315	ARG
1	A	317	GLN
1	A	344	LEU
1	A	348	ILE
1	A	352	GLU
1	A	358	THR
1	A	386	ASP
1	A	395	ASN
1	A	403	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	438	GLU
1	A	441	LEU
1	A	446	PHE
1	A	453	GLU
1	A	464	LEU
1	A	472	LEU
1	A	474	LEU
1	B	32	ASN
1	B	33	ILE
1	B	54	LYS
1	B	60	ILE
1	B	66	SER
1	B	74	ARG
1	B	91	TYR
1	B	96	GLN
1	B	106	GLU
1	B	127	ASP
1	B	138	ASN
1	B	193	THR
1	B	213	LEU
1	B	246	LEU
1	B	247	PHE
1	B	251	ARG
1	B	262	ASN
1	B	286	LEU
1	B	301	THR
1	B	315	ARG
1	B	317	GLN
1	B	344	LEU
1	B	352	GLU
1	B	386	ASP
1	B	395	ASN
1	B	403	ASN
1	B	438	GLU
1	B	441	LEU
1	B	446	PHE
1	B	453	GLU
1	B	464	LEU
1	B	472	LEU
1	B	474	LEU
1	C	32	ASN
1	C	33	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	54	LYS
1	C	60	ILE
1	C	66	SER
1	C	74	ARG
1	C	91	TYR
1	C	96	GLN
1	C	106	GLU
1	C	127	ASP
1	C	138	ASN
1	C	178	VAL
1	C	193	THR
1	C	213	LEU
1	C	225	CYS
1	C	246	LEU
1	C	247	PHE
1	C	251	ARG
1	C	262	ASN
1	C	278	LYS
1	C	286	LEU
1	C	301	THR
1	C	315	ARG
1	C	317	GLN
1	C	344	LEU
1	C	348	ILE
1	C	351	SER
1	C	352	GLU
1	C	386	ASP
1	C	395	ASN
1	C	403	ASN
1	C	438	GLU
1	C	441	LEU
1	C	443	LYS
1	C	446	PHE
1	C	453	GLU
1	C	464	LEU
1	C	472	LEU
1	C	474	LEU
1	D	32	ASN
1	D	33	ILE
1	D	60	ILE
1	D	74	ARG
1	D	91	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	95	THR
1	D	96	GLN
1	D	106	GLU
1	D	127	ASP
1	D	138	ASN
1	D	193	THR
1	D	213	LEU
1	D	246	LEU
1	D	247	PHE
1	D	251	ARG
1	D	262	ASN
1	D	270	ASN
1	D	286	LEU
1	D	301	THR
1	D	315	ARG
1	D	317	GLN
1	D	342	MET
1	D	344	LEU
1	D	352	GLU
1	D	395	ASN
1	D	403	ASN
1	D	438	GLU
1	D	441	LEU
1	D	446	PHE
1	D	453	GLU
1	D	464	LEU
1	D	472	LEU
1	D	474	LEU
1	E	32	ASN
1	E	33	ILE
1	E	54	LYS
1	E	60	ILE
1	E	66	SER
1	E	68	LEU
1	E	74	ARG
1	E	82	LYS
1	E	91	TYR
1	E	96	GLN
1	E	106	GLU
1	E	117	ILE
1	E	127	ASP
1	E	138	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	193	THR
1	E	213	LEU
1	E	246	LEU
1	E	247	PHE
1	E	251	ARG
1	E	262	ASN
1	E	286	LEU
1	E	301	THR
1	E	306	ILE
1	E	315	ARG
1	E	317	GLN
1	E	344	LEU
1	E	345	CYS
1	E	352	GLU
1	E	386	ASP
1	E	395	ASN
1	E	403	ASN
1	E	438	GLU
1	E	441	LEU
1	E	446	PHE
1	E	453	GLU
1	E	464	LEU
1	E	472	LEU
1	E	474	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	69	GLN
1	A	138	ASN
1	A	153	GLN
1	A	192	ASN
1	A	259	HIS
1	A	262	ASN
1	A	290	ASN
1	A	341	ASN
1	A	366	HIS
1	A	395	ASN
1	A	403	ASN
1	A	461	GLN
1	B	32	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	69	GLN
1	B	96	GLN
1	B	138	ASN
1	B	153	GLN
1	B	259	HIS
1	B	262	ASN
1	B	290	ASN
1	B	341	ASN
1	B	366	HIS
1	B	395	ASN
1	B	403	ASN
1	B	461	GLN
1	C	32	ASN
1	C	69	GLN
1	C	138	ASN
1	C	153	GLN
1	C	262	ASN
1	C	290	ASN
1	C	341	ASN
1	C	366	HIS
1	C	395	ASN
1	C	403	ASN
1	C	461	GLN
1	D	32	ASN
1	D	69	GLN
1	D	96	GLN
1	D	138	ASN
1	D	153	GLN
1	D	192	ASN
1	D	262	ASN
1	D	270	ASN
1	D	290	ASN
1	D	341	ASN
1	D	366	HIS
1	D	395	ASN
1	D	403	ASN
1	D	461	GLN
1	E	32	ASN
1	E	69	GLN
1	E	138	ASN
1	E	153	GLN
1	E	262	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	290	ASN
1	E	341	ASN
1	E	366	HIS
1	E	395	ASN
1	E	403	ASN
1	E	461	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

28 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	JHM	A	507	-	15,15,15	1.14	2 (13%)	20,22,22	1.25	3 (15%)
2	JHM	A	519	3	15,15,15	1.14	2 (13%)	20,22,22	1.25	3 (15%)
3	IDS	A	520	2	12,15,17	2.16	1 (8%)	12,22,26	1.07	1 (8%)
2	JHM	B	505	3	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
3	IDS	B	506	2	12,15,17	2.17	1 (8%)	12,22,26	1.05	1 (8%)
3	IDS	B	508	-	12,15,17	2.16	1 (8%)	12,22,26	1.06	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	JHM	C	501	3	15,15,15	1.15	2 (13%)	20,22,22	1.24	3 (15%)
3	IDS	C	502	2	12,15,17	2.15	1 (8%)	12,22,26	1.05	1 (8%)
2	JHM	C	503	3	15,15,15	1.16	2 (13%)	20,22,22	1.25	3 (15%)
3	IDS	C	504	2	12,15,17	2.15	1 (8%)	12,22,26	1.05	1 (8%)
2	JHM	C	509	-	15,15,15	1.15	2 (13%)	20,22,22	1.26	3 (15%)
3	IDS	D	510	-	12,15,17	2.16	1 (8%)	12,22,26	1.05	1 (8%)
2	JHM	D	511	3	15,15,15	1.15	2 (13%)	20,22,22	1.25	3 (15%)
3	IDS	D	512	2	12,15,17	2.14	1 (8%)	12,22,26	1.06	1 (8%)
2	JHM	D	515	3	15,15,15	1.15	2 (13%)	20,22,22	1.25	3 (15%)
3	IDS	D	516	2	12,15,17	2.16	1 (8%)	12,22,26	1.06	1 (8%)
2	JHM	E	513	3	15,15,15	1.13	2 (13%)	20,22,22	1.24	3 (15%)
3	IDS	E	514	2	12,15,17	2.13	1 (8%)	12,22,26	1.07	1 (8%)
2	JHM	E	517	3	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
3	IDS	E	518	2	12,15,17	2.15	1 (8%)	12,22,26	1.06	1 (8%)
2	JHM	E	521	3	15,15,15	1.15	2 (13%)	20,22,22	1.24	3 (15%)
3	IDS	E	522	2	12,15,17	2.14	1 (8%)	12,22,26	1.06	1 (8%)
2	JHM	E	523	3	15,15,15	1.14	2 (13%)	20,22,22	1.25	3 (15%)
3	IDS	E	524	2	12,15,17	2.15	1 (8%)	12,22,26	1.07	1 (8%)
2	JHM	E	525	3	15,15,15	1.13	2 (13%)	20,22,22	1.24	3 (15%)
3	IDS	E	526	2	12,15,17	2.15	1 (8%)	12,22,26	1.07	1 (8%)
2	JHM	E	527	3	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
3	IDS	E	528	2	12,15,17	2.15	1 (8%)	12,22,26	1.08	1 (8%)

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	JHM	A	507	-	-	0/6/22/22	0/1/1/1
2	JHM	A	519	3	-	0/6/22/22	0/1/1/1
3	IDS	A	520	2	-	0/5/22/29	0/1/1/1
2	JHM	B	505	3	-	0/6/22/22	0/1/1/1
3	IDS	B	506	2	-	0/5/22/29	0/1/1/1
3	IDS	B	508	-	-	0/5/22/29	0/1/1/1
2	JHM	C	501	3	-	0/6/22/22	0/1/1/1
3	IDS	C	502	2	-	0/5/22/29	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	JHM	C	503	3	-	0/6/22/22	0/1/1/1
3	IDS	C	504	2	-	0/5/22/29	0/1/1/1
2	JHM	C	509	-	-	0/6/22/22	0/1/1/1
3	IDS	D	510	-	-	0/5/22/29	0/1/1/1
2	JHM	D	511	3	-	0/6/22/22	0/1/1/1
3	IDS	D	512	2	-	0/5/22/29	0/1/1/1
2	JHM	D	515	3	-	0/6/22/22	0/1/1/1
3	IDS	D	516	2	-	0/5/22/29	0/1/1/1
2	JHM	E	513	3	-	0/6/22/22	0/1/1/1
3	IDS	E	514	2	-	0/5/22/29	0/1/1/1
2	JHM	E	517	3	-	0/6/22/22	0/1/1/1
3	IDS	E	518	2	-	0/5/22/29	0/1/1/1
2	JHM	E	521	3	-	0/6/22/22	0/1/1/1
3	IDS	E	522	2	-	0/5/22/29	0/1/1/1
2	JHM	E	523	3	-	0/6/22/22	0/1/1/1
3	IDS	E	524	2	-	0/5/22/29	0/1/1/1
2	JHM	E	525	3	-	0/6/22/22	0/1/1/1
3	IDS	E	526	2	-	0/5/22/29	0/1/1/1
2	JHM	E	527	3	-	0/6/22/22	0/1/1/1
3	IDS	E	528	2	-	0/5/22/29	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	506	IDS	O2-C2	-6.74	1.37	1.47
3	D	510	IDS	O2-C2	-6.70	1.37	1.47
3	B	508	IDS	O2-C2	-6.70	1.37	1.47
3	E	524	IDS	O2-C2	-6.69	1.37	1.47
3	A	520	IDS	O2-C2	-6.68	1.37	1.47
3	D	516	IDS	O2-C2	-6.67	1.37	1.47
3	E	528	IDS	O2-C2	-6.66	1.37	1.47
3	E	518	IDS	O2-C2	-6.65	1.37	1.47
3	C	502	IDS	O2-C2	-6.65	1.37	1.47
3	C	504	IDS	O2-C2	-6.65	1.37	1.47
3	D	512	IDS	O2-C2	-6.64	1.37	1.47
3	E	526	IDS	O2-C2	-6.64	1.37	1.47
3	E	522	IDS	O2-C2	-6.62	1.37	1.47
3	E	514	IDS	O2-C2	-6.61	1.37	1.47
2	A	507	JHM	C3-C4	2.15	1.55	1.52
2	E	517	JHM	C3-C4	2.21	1.55	1.52
2	E	513	JHM	C3-C4	2.21	1.55	1.52
2	E	525	JHM	C3-C4	2.22	1.55	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	505	JHM	C3-C4	2.24	1.55	1.52
2	C	501	JHM	C3-C4	2.25	1.55	1.52
2	E	527	JHM	C3-C4	2.26	1.55	1.52
2	E	521	JHM	C3-C4	2.26	1.55	1.52
2	E	523	JHM	C3-C4	2.27	1.55	1.52
2	A	519	JHM	C3-C4	2.27	1.55	1.52
2	D	511	JHM	C3-C4	2.34	1.55	1.52
2	C	509	JHM	C3-C4	2.34	1.55	1.52
2	D	515	JHM	C3-C4	2.35	1.55	1.52
2	C	503	JHM	C3-C4	2.38	1.55	1.52
2	E	527	JHM	O1-C1	2.52	1.45	1.39
2	C	509	JHM	O1-C1	2.54	1.45	1.39
2	E	525	JHM	O1-C1	2.56	1.45	1.39
2	D	515	JHM	O1-C1	2.56	1.45	1.39
2	A	519	JHM	O1-C1	2.58	1.45	1.39
2	E	513	JHM	O1-C1	2.58	1.45	1.39
2	E	523	JHM	O1-C1	2.59	1.45	1.39
2	B	505	JHM	O1-C1	2.59	1.45	1.39
2	C	503	JHM	O1-C1	2.59	1.45	1.39
2	E	521	JHM	O1-C1	2.60	1.45	1.39
2	E	517	JHM	O1-C1	2.60	1.45	1.39
2	A	507	JHM	O1-C1	2.61	1.45	1.39
2	D	511	JHM	O1-C1	2.61	1.45	1.39
2	C	501	JHM	O1-C1	2.62	1.45	1.39

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	509	JHM	C3-C4-C5	-3.28	106.62	109.93
2	C	503	JHM	C3-C4-C5	-3.23	106.68	109.93
2	D	515	JHM	C3-C4-C5	-3.22	106.68	109.93
2	D	511	JHM	C3-C4-C5	-3.22	106.69	109.93
2	A	507	JHM	C3-C4-C5	-3.22	106.69	109.93
2	E	523	JHM	C3-C4-C5	-3.22	106.69	109.93
2	A	519	JHM	C3-C4-C5	-3.20	106.71	109.93
2	B	505	JHM	C3-C4-C5	-3.20	106.71	109.93
2	E	517	JHM	C3-C4-C5	-3.20	106.71	109.93
2	E	521	JHM	C3-C4-C5	-3.18	106.73	109.93
2	C	501	JHM	C3-C4-C5	-3.18	106.73	109.93
2	E	527	JHM	C3-C4-C5	-3.17	106.73	109.93
2	E	525	JHM	C3-C4-C5	-3.17	106.74	109.93
2	E	513	JHM	C3-C4-C5	-3.15	106.76	109.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	519	JHM	C2-C3-C4	-2.51	107.14	110.56
2	C	503	JHM	C2-C3-C4	-2.50	107.16	110.56
2	E	513	JHM	C2-C3-C4	-2.49	107.17	110.56
2	C	501	JHM	C2-C3-C4	-2.49	107.17	110.56
2	E	523	JHM	C2-C3-C4	-2.49	107.17	110.56
2	D	511	JHM	C2-C3-C4	-2.49	107.17	110.56
2	D	515	JHM	C2-C3-C4	-2.48	107.18	110.56
2	E	521	JHM	C2-C3-C4	-2.48	107.19	110.56
2	B	505	JHM	C1-C2-C3	-2.47	106.99	111.23
2	A	507	JHM	C1-C2-C3	-2.47	106.99	111.23
2	E	517	JHM	C2-C3-C4	-2.47	107.20	110.56
2	C	501	JHM	C1-C2-C3	-2.47	107.00	111.23
2	E	517	JHM	C1-C2-C3	-2.47	107.00	111.23
2	E	513	JHM	C1-C2-C3	-2.46	107.00	111.23
2	A	519	JHM	C1-C2-C3	-2.46	107.01	111.23
2	E	527	JHM	C2-C3-C4	-2.46	107.21	110.56
2	B	505	JHM	C2-C3-C4	-2.45	107.22	110.56
2	E	527	JHM	C1-C2-C3	-2.45	107.02	111.23
2	A	507	JHM	C2-C3-C4	-2.45	107.22	110.56
2	E	525	JHM	C2-C3-C4	-2.45	107.22	110.56
2	D	511	JHM	C1-C2-C3	-2.45	107.03	111.23
2	C	509	JHM	C1-C2-C3	-2.45	107.04	111.23
2	C	509	JHM	C2-C3-C4	-2.45	107.23	110.56
2	E	521	JHM	C1-C2-C3	-2.44	107.05	111.23
2	C	503	JHM	C1-C2-C3	-2.44	107.05	111.23
2	E	525	JHM	C1-C2-C3	-2.43	107.06	111.23
2	E	523	JHM	C1-C2-C3	-2.43	107.07	111.23
2	D	515	JHM	C1-C2-C3	-2.43	107.07	111.23
3	D	510	IDS	C1-C2-C3	2.76	113.66	109.89
3	B	506	IDS	C1-C2-C3	2.76	113.67	109.89
3	C	502	IDS	C1-C2-C3	2.78	113.69	109.89
3	C	504	IDS	C1-C2-C3	2.79	113.71	109.89
3	B	508	IDS	C1-C2-C3	2.81	113.74	109.89
3	D	512	IDS	C1-C2-C3	2.81	113.74	109.89
3	E	518	IDS	C1-C2-C3	2.82	113.75	109.89
3	D	516	IDS	C1-C2-C3	2.83	113.75	109.89
3	E	522	IDS	C1-C2-C3	2.83	113.76	109.89
3	E	514	IDS	C1-C2-C3	2.84	113.77	109.89
3	E	526	IDS	C1-C2-C3	2.85	113.78	109.89
3	A	520	IDS	C1-C2-C3	2.85	113.78	109.89
3	E	524	IDS	C1-C2-C3	2.87	113.81	109.89
3	E	528	IDS	C1-C2-C3	2.88	113.82	109.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 95 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	507	JHM	18	0
2	A	519	JHM	2	0
3	A	520	IDS	1	0
2	C	501	JHM	12	0
3	C	502	IDS	8	0
2	C	503	JHM	5	0
3	C	504	IDS	16	0
2	C	509	JHM	8	2
3	D	510	IDS	2	3
2	D	511	JHM	2	0
3	D	516	IDS	8	0
2	E	513	JHM	6	0
2	E	517	JHM	1	0
2	E	521	JHM	3	0
3	E	522	IDS	1	0
2	E	523	JHM	2	1
2	E	525	JHM	4	0
3	E	526	IDS	2	2
2	E	527	JHM	7	0
3	E	528	IDS	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	421/428 (98%)	0.06	13 (3%) 52 40	22, 41, 84, 126	0
1	B	421/428 (98%)	0.10	19 (4%) 37 26	22, 41, 88, 127	0
1	C	421/428 (98%)	0.11	12 (2%) 55 43	22, 41, 87, 125	0
1	D	421/428 (98%)	0.17	21 (4%) 32 21	23, 42, 89, 126	0
1	E	421/428 (98%)	0.07	12 (2%) 55 43	21, 40, 82, 130	0
All	All	2105/2140 (98%)	0.10	77 (3%) 45 33	21, 41, 88, 130	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	474	LEU	9.7
1	E	474	LEU	7.9
1	A	474	LEU	5.8
1	C	438	GLU	5.6
1	E	56	ASN	5.4
1	B	474	LEU	4.8
1	D	55	PRO	4.7
1	B	136	ALA	4.6
1	B	175	CYS	4.5
1	D	474	LEU	4.4
1	E	403	ASN	4.1
1	B	56	ASN	4.1
1	B	174	PRO	4.0
1	B	403	ASN	3.9
1	D	56	ASN	3.8
1	D	95	THR	3.7
1	A	56	ASN	3.7
1	D	438	GLU	3.6
1	D	90	PHE	3.6
1	E	141	VAL	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	353	THR	3.5
1	D	283	THR	3.5
1	D	88	THR	3.5
1	E	175	CYS	3.2
1	D	89	SER	3.2
1	B	178	VAL	3.2
1	C	472	LEU	3.1
1	A	138	ASN	3.1
1	D	396	SER	3.1
1	A	176	THR	3.1
1	A	348	ILE	3.0
1	E	54	LYS	3.0
1	D	443	LYS	3.0
1	E	55	PRO	3.0
1	C	56	ASN	2.9
1	B	472	LEU	2.8
1	C	139	ALA	2.7
1	C	175	CYS	2.7
1	C	142	ASP	2.7
1	D	85	PHE	2.7
1	A	139	ALA	2.6
1	B	352	GLU	2.6
1	D	87	ASP	2.6
1	D	403	ASN	2.6
1	D	282	SER	2.6
1	B	40	SER	2.5
1	D	40	SER	2.5
1	D	353	THR	2.5
1	E	139	ALA	2.5
1	D	472	LEU	2.4
1	A	403	ASN	2.4
1	B	54	LYS	2.4
1	B	179	ALA	2.4
1	B	176	THR	2.4
1	A	61	LEU	2.3
1	B	177	GLN	2.3
1	C	137	ALA	2.3
1	C	99	VAL	2.3
1	D	383	LEU	2.3
1	E	472	LEU	2.2
1	A	179	ALA	2.2
1	A	353	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	390	TYR	2.2
1	A	55	PRO	2.2
1	C	473	GLY	2.2
1	B	351	SER	2.2
1	C	390	TYR	2.2
1	A	82	LYS	2.2
1	D	177	GLN	2.2
1	B	353	THR	2.2
1	B	141	VAL	2.1
1	E	438	GLU	2.1
1	E	442	LYS	2.1
1	B	360	PHE	2.1
1	A	445	THR	2.1
1	C	57	ASN	2.1
1	B	355	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	IDS	C	502	15/17	0.57	0.74	19.13	29,30,37,41	0
2	JHM	D	511	15/15	0.55	0.76	14.98	45,65,87,88	0
3	IDS	D	512	15/17	0.63	0.77	10.84	29,30,37,41	0
3	IDS	D	510	15/17	0.49	0.89	10.32	29,30,37,41	0
2	JHM	C	509	15/15	0.26	1.02	9.02	45,65,87,88	0
2	JHM	A	519	15/15	0.64	0.72	6.54	45,65,87,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	JHM	A	507	15/15	0.57	0.74	5.88	45,65,87,88	0
2	JHM	E	521	15/15	0.38	0.73	-	45,65,87,88	0
2	JHM	C	501	15/15	0.39	0.70	-	45,65,87,88	0
3	IDS	D	516	15/17	0.81	0.72	-	29,30,37,41	0
2	JHM	B	505	15/15	0.41	0.88	-	45,65,87,88	0
3	IDS	C	504	15/17	0.65	0.71	-	29,30,37,41	0
3	IDS	E	514	15/17	0.75	0.67	-	29,30,37,41	0
2	JHM	E	523	15/15	0.47	0.42	-	45,65,87,88	0
3	IDS	E	518	15/17	0.70	0.70	-	29,30,37,41	0
2	JHM	C	503	15/15	0.44	0.76	-	45,65,87,88	0
3	IDS	B	506	15/17	0.67	0.85	-	29,30,37,41	0
3	IDS	E	528	15/17	0.62	0.51	-	29,30,37,41	0
2	JHM	E	517	15/15	0.35	0.57	-	45,65,87,88	0
3	IDS	E	524	15/17	0.71	0.58	-	29,30,37,41	0
3	IDS	B	508	15/17	0.65	0.71	-	29,30,37,41	0
2	JHM	E	527	15/15	0.49	0.47	-	45,65,87,88	0
3	IDS	E	522	15/17	0.48	0.70	-	29,30,37,41	0
2	JHM	E	513	15/15	0.62	0.53	-	45,65,87,88	0
3	IDS	E	526	15/17	0.52	0.52	-	29,30,37,41	0
2	JHM	E	525	15/15	0.45	0.40	-	45,65,87,88	0
3	IDS	A	520	15/17	0.78	0.67	-	29,30,37,41	0
2	JHM	D	515	15/15	0.51	0.81	-	45,65,87,88	0

6.5 Other polymers

There are no such residues in this entry.