Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 09:56 AM EDT

PDB ID	:	2AHC
Title	:	Chorismate lyase with inhibitor Vanilate
Authors	:	Gallagher, D.T.; Smith, N.N.
Deposited on	:	2005-07-27
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

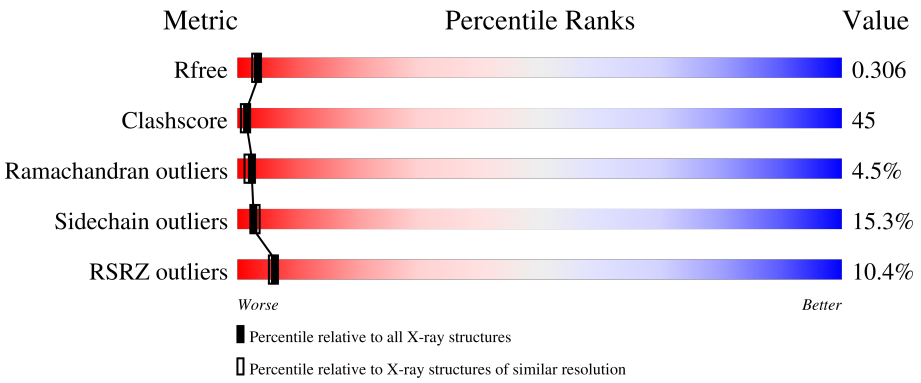
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	164	11% 43% 43% 10% •
1	B	164	6% 48% 43% 6% •
1	C	164	15% 45% 37% 14% •
1	D	164	9% 42% 43% 12% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5427 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.

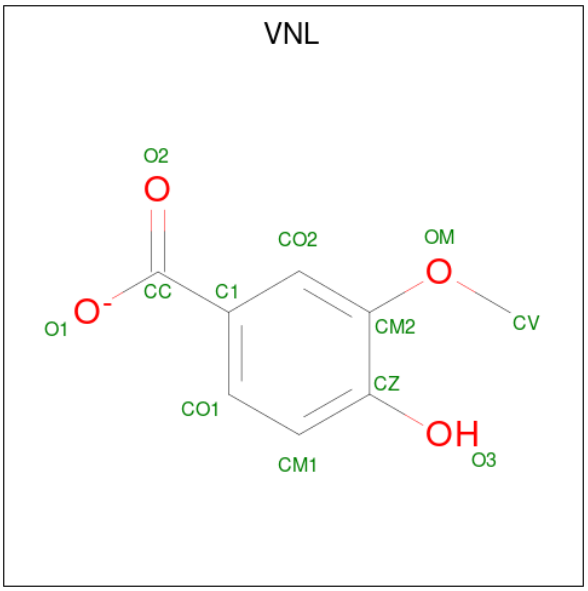
- Molecule 1 is a protein called Chorismate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	164	1315	847	226	240	2	0	0	0
1	B	164	1315	847	226	240	2	0	0	0
1	C	164	1315	847	226	240	2	0	0	0
1	D	164	1315	847	226	240	2	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	SER	CYS	engineered mutation	UNP P26602
A	81	SER	CYS	engineered mutation	UNP P26602
B	14	SER	CYS	engineered mutation	UNP P26602
B	81	SER	CYS	engineered mutation	UNP P26602
C	14	SER	CYS	engineered mutation	UNP P26602
C	81	SER	CYS	engineered mutation	UNP P26602
D	14	SER	CYS	engineered mutation	UNP P26602
D	81	SER	CYS	engineered mutation	UNP P26602

- Molecule 2 is 4-HYDROXY-3-METHOXYBENZOATE (three-letter code: VNL) (formula: $C_8H_7O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 8 4	0	0
2	B	1	Total C O 12 8 4	0	0
2	C	1	Total C O 12 8 4	0	0
2	D	1	Total C O 12 8 4	0	0

- Molecule 3 is water.

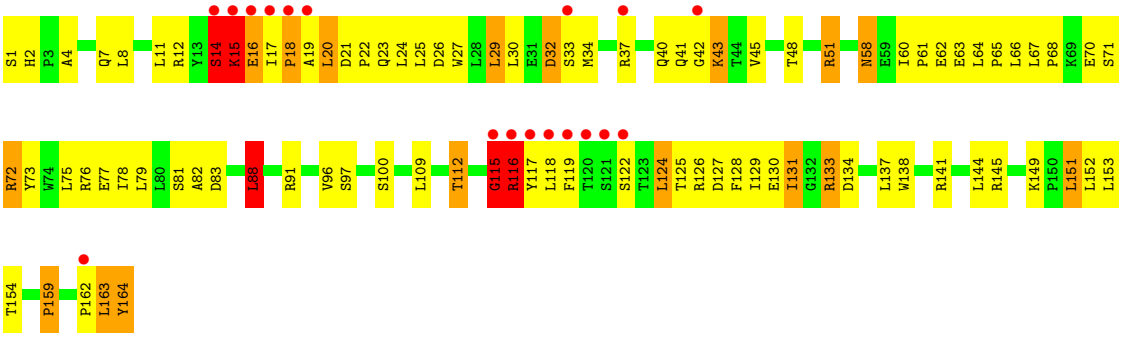
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	21	Total O 21 21	0	0
3	B	36	Total O 36 36	0	0
3	C	30	Total O 30 30	0	0
3	D	32	Total O 32 32	0	0

3 Residue-property plots (i)

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

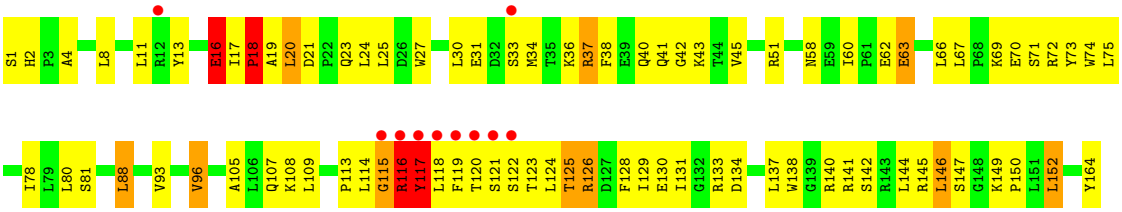
- Molecule 1: Chorismate lyase

Chain A:



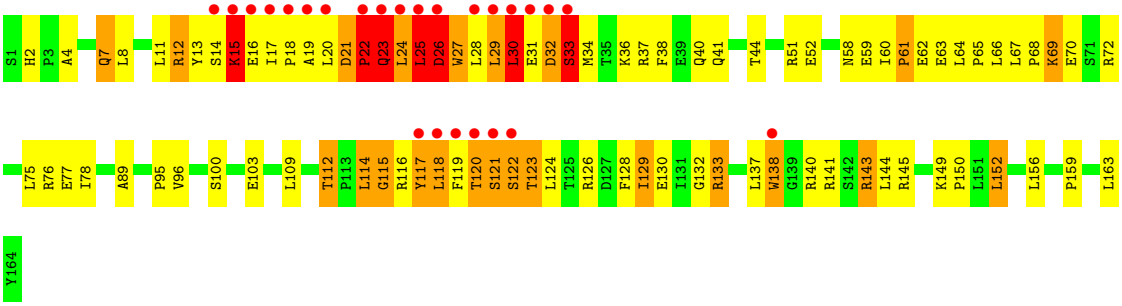
- Molecule 1: Chorismate lyase

Chain B:



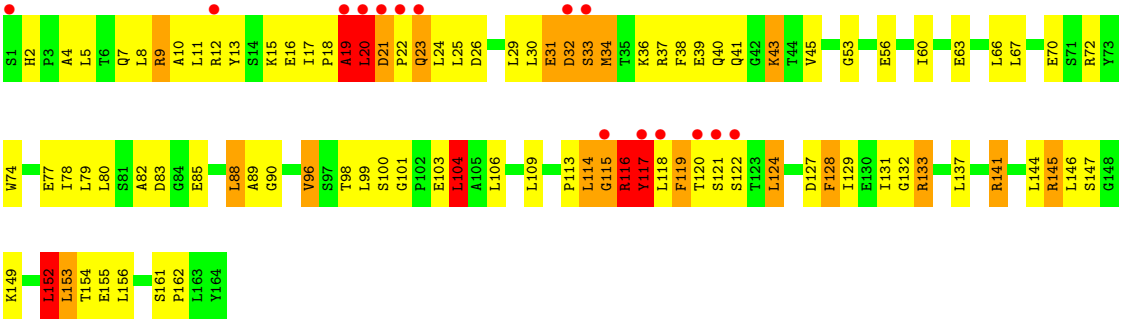
- Molecule 1: Chorismate lyase

Chain C:



• Molecule 1: Chorismate lyase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	56.17Å 58.56Å 70.65Å 70.24° 67.40° 67.17°	Depositor
Resolution (Å)	8.00 – 2.40 34.49 – 2.26	Depositor EDS
% Data completeness (in resolution range)	97.3 (8.00-2.40) 94.1 (34.49-2.26)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.05 (at 2.27Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.262 , 0.314 0.253 , 0.306	Depositor DCC
R_{free} test set	1318 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 61.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	5427	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.62	0/1345	1.00	6/1825 (0.3%)
1	B	0.74	1/1345 (0.1%)	1.05	4/1825 (0.2%)
1	C	0.72	0/1345	1.05	8/1825 (0.4%)
1	D	0.78	1/1345 (0.1%)	1.07	9/1825 (0.5%)
All	All	0.72	2/5380 (0.0%)	1.04	27/7300 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	16	GLU	CB-CG	5.16	1.61	1.52
1	D	34	MET	CG-SD	-5.13	1.67	1.81

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	115	GLY	N-CA-C	10.08	138.29	113.10
1	B	116	ARG	N-CA-C	-9.47	85.42	111.00
1	D	116	ARG	N-CA-C	-9.06	86.52	111.00
1	C	23	GLN	N-CA-C	-8.58	87.84	111.00
1	D	33	SER	N-CA-C	-7.96	89.52	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	115	GLY	N-CA-C	7.95	132.98	113.10
1	D	117	TYR	N-CA-C	-7.51	90.72	111.00
1	A	163	LEU	N-CA-C	-7.06	91.94	111.00
1	D	153	LEU	CA-CB-CG	6.96	131.32	115.30
1	D	115	GLY	N-CA-C	6.95	130.48	113.10
1	D	152	LEU	CA-CB-CG	6.91	131.19	115.30
1	D	19	ALA	N-CA-C	6.65	128.96	111.00
1	A	88	LEU	CA-CB-CG	6.50	130.25	115.30
1	A	124	LEU	CA-CB-CG	6.46	130.15	115.30
1	B	144	LEU	CA-CB-CG	6.34	129.89	115.30
1	C	15	LYS	N-CA-C	6.29	127.99	111.00
1	D	104	LEU	CA-CB-CG	6.16	129.47	115.30
1	C	118	LEU	CA-CB-CG	5.97	129.04	115.30
1	A	116	ARG	N-CA-C	5.96	127.08	111.00
1	D	20	LEU	CA-CB-CG	-5.75	102.08	115.30
1	C	144	LEU	CA-CB-CG	5.60	128.19	115.30
1	C	25	LEU	N-CA-C	-5.46	96.27	111.00
1	C	26	ASP	N-CA-C	-5.33	96.62	111.00
1	A	151	LEU	CA-CB-CG	5.25	127.39	115.30
1	B	115	GLY	C-N-CA	5.20	134.69	121.70
1	C	117	TYR	N-CA-C	-5.17	97.05	111.00
1	C	115	GLY	N-CA-C	5.09	125.83	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	117	TYR	Sidechain
1	D	13	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1315	0	1361	111	0
1	B	1315	0	1361	97	1
1	C	1315	0	1361	170	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1315	0	1361	124	1
2	A	12	0	6	2	0
2	B	12	0	6	0	0
2	C	12	0	6	0	0
2	D	12	0	6	0	0
3	A	21	0	0	3	0
3	B	36	0	0	2	0
3	C	30	0	0	4	0
3	D	32	0	0	1	0
All	All	5427	0	5468	485	1

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 45.

All (485) 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:D:115:GLY:HA3	1:D:118:LEU:HB2	1.24	1.19
1:D:116:ARG:H	1:D:118:LEU:N	1.49	1.10
1:D:116:ARG:N	1:D:118:LEU:H	1.52	1.06
1:A:65:PRO:HB3	1:C:18:PRO:HB3	1.07	1.06
1:A:141:ARG:NH2	1:C:22:PRO:HG2	1.70	1.05
1:C:29:LEU:HD13	1:C:30:LEU:H	1.16	1.04
1:D:116:ARG:CG	1:D:124:LEU:HD22	1.88	1.03
1:D:116:ARG:HG3	1:D:124:LEU:HD22	1.04	1.03
1:C:30:LEU:HD23	1:C:32:ASP:H	1.23	1.02
1:A:65:PRO:HB3	1:C:18:PRO:CB	1.94	0.97
1:C:30:LEU:HD23	1:C:31:GLU:H	1.27	0.97
1:C:51:ARG:HD3	1:C:77:GLU:OE1	1.64	0.96
1:C:15:LYS:HG2	1:C:130:GLU:HG3	1.49	0.94
1:D:2:HIS:HD2	1:D:4:ALA:H	1.11	0.91
1:B:63:GLU:HG3	1:B:152:LEU:HD13	1.53	0.91
1:D:63:GLU:O	1:D:67:LEU:HD13	1.71	0.90
1:C:23:GLN:HA	1:C:26:ASP:HB2	1.55	0.89
1:D:115:GLY:HA3	1:D:118:LEU:CB	2.03	0.89
1:C:115:GLY:HA3	1:C:117:TYR:CE2	2.08	0.88
1:C:29:LEU:HD13	1:C:30:LEU:N	1.88	0.87
1:D:17:ILE:HG22	1:D:19:ALA:H	1.36	0.87
1:D:116:ARG:HB2	1:D:124:LEU:HD13	1.54	0.87
1:C:23:GLN:CA	1:C:26:ASP:HB2	2.05	0.85
1:A:37:ARG:HA	1:A:40:GLN:HE21	1.42	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:LYS:HA	1:C:130:GLU:HG2	1.59	0.84
1:B:20:LEU:HD11	1:B:25:LEU:HD21	1.60	0.84
1:B:114:LEU:HD12	1:B:115:GLY:H	1.42	0.83
1:B:133:ARG:HG3	1:B:137:LEU:O	1.78	0.83
1:B:115:GLY:HA3	1:B:118:LEU:HB2	1.58	0.83
1:D:18:PRO:O	1:D:20:LEU:HD21	1.78	0.82
1:C:30:LEU:CD2	1:C:31:GLU:H	1.91	0.82
1:A:43:LYS:HG3	1:A:82:ALA:HB1	1.62	0.81
1:B:116:ARG:HB2	1:B:124:LEU:HD22	1.60	0.81
1:A:154:THR:HG23	3:A:678:HOH:O	1.80	0.81
1:B:36:LYS:HG2	3:B:303:HOH:O	1.78	0.81
1:C:52:GLU:OE1	1:C:76:ARG:HD2	1.80	0.80
1:D:133:ARG:HD3	1:D:137:LEU:O	1.79	0.80
1:B:33:SER:HB3	3:B:303:HOH:O	1.81	0.80
1:B:125:THR:HG23	1:B:145:ARG:HB2	1.62	0.80
1:B:70:GLU:OE2	1:B:96:VAL:HG23	1.82	0.79
1:D:116:ARG:HG3	1:D:124:LEU:CD2	2.00	0.79
1:D:2:HIS:CD2	1:D:4:ALA:H	1.99	0.79
1:A:72:ARG:HG3	1:A:72:ARG:HH11	1.46	0.79
1:A:72:ARG:O	1:A:96:VAL:HG23	1.83	0.78
1:B:66:LEU:HD12	1:B:152:LEU:HD11	1.63	0.78
1:C:27:TRP:HZ3	1:C:34:MET:HE2	1.48	0.78
1:B:120:THR:C	1:B:122:SER:H	1.84	0.78
1:C:24:LEU:HD13	1:C:28:LEU:HD11	1.63	0.78
1:D:21:ASP:OD2	1:D:23:GLN:N	2.17	0.77
1:D:23:GLN:HA	1:D:26:ASP:OD2	1.85	0.77
1:A:37:ARG:HA	1:A:40:GLN:NE2	1.98	0.77
1:D:21:ASP:HB3	1:D:24:LEU:HB2	1.66	0.77
1:B:67:LEU:HD11	1:B:152:LEU:HD12	1.66	0.76
1:D:19:ALA:C	1:D:20:LEU:HG	1.89	0.76
1:C:25:LEU:HD23	1:C:28:LEU:O	1.86	0.76
1:C:25:LEU:HA	1:C:29:LEU:HB2	1.68	0.76
1:A:17:ILE:HG23	1:A:29:LEU:HD21	1.68	0.75
1:D:43:LYS:HG2	1:D:82:ALA:HB1	1.69	0.75
1:C:29:LEU:HD23	1:C:129:ILE:HD13	1.69	0.75
1:C:133:ARG:CZ	1:C:138:TRP:CD2	2.69	0.74
1:C:16:GLU:C	1:C:18:PRO:HD3	2.08	0.74
1:B:66:LEU:C	1:B:67:LEU:HD12	2.08	0.74
1:A:116:ARG:N	1:A:119:PHE:HB2	2.03	0.73
1:C:2:HIS:CD2	1:C:4:ALA:H	2.07	0.73
1:D:60:ILE:O	1:D:60:ILE:HG13	1.87	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ARG:HH21	1:A:41:GLN:HG2	1.53	0.73
1:C:15:LYS:HA	1:C:130:GLU:CG	2.18	0.72
1:C:116:ARG:NH2	1:C:124:LEU:H	1.87	0.72
1:D:32:ASP:OD2	1:D:33:SER:O	2.08	0.72
1:B:2:HIS:HD2	1:B:4:ALA:H	1.36	0.72
1:A:109:LEU:O	1:A:112:THR:HB	1.90	0.71
1:B:63:GLU:HG3	1:B:152:LEU:CD1	2.21	0.71
1:D:101:GLY:O	1:D:104:LEU:HD23	1.91	0.71
1:C:28:LEU:HD12	1:C:28:LEU:H	1.55	0.70
1:D:37:ARG:HH21	1:D:41:GLN:HG2	1.54	0.70
1:A:141:ARG:NH2	1:C:22:PRO:CG	2.52	0.70
1:D:116:ARG:C	1:D:118:LEU:N	2.42	0.70
1:A:51:ARG:HD3	1:A:77:GLU:OE1	1.92	0.69
1:B:113:PRO:O	1:B:117:TYR:HE2	1.74	0.69
1:B:116:ARG:CB	1:B:124:LEU:HD22	2.21	0.69
1:B:115:GLY:CA	1:B:118:LEU:HB2	2.23	0.69
1:C:25:LEU:O	1:C:29:LEU:HB3	1.91	0.69
1:C:115:GLY:O	1:C:118:LEU:HB3	1.92	0.69
1:D:117:TYR:CE2	1:D:118:LEU:HG	2.28	0.69
1:C:109:LEU:O	1:C:112:THR:HB	1.93	0.69
1:D:66:LEU:C	1:D:67:LEU:HD12	2.13	0.69
1:A:37:ARG:O	1:A:37:ARG:NE	2.25	0.69
1:C:116:ARG:C	1:C:118:LEU:N	2.40	0.69
1:D:117:TYR:CD2	1:D:118:LEU:HG	2.28	0.68
1:B:115:GLY:HA3	1:B:118:LEU:N	2.09	0.68
1:C:115:GLY:HA3	1:C:117:TYR:HE2	1.58	0.68
1:A:126:ARG:HH21	1:A:128:PHE:HA	1.59	0.68
1:A:15:LYS:HD2	1:A:16:GLU:N	2.08	0.68
1:D:119:PHE:O	1:D:122:SER:HB2	1.93	0.68
1:C:29:LEU:CD1	1:C:126:ARG:HH12	2.06	0.67
1:C:32:ASP:OD1	1:C:116:ARG:HB3	1.95	0.67
1:A:130:GLU:OE1	1:C:22:PRO:HB2	1.94	0.67
1:C:27:TRP:HZ3	1:C:34:MET:CE	2.08	0.67
1:D:63:GLU:HG2	1:D:152:LEU:HD12	1.77	0.67
1:A:116:ARG:HA	1:A:119:PHE:HB2	1.75	0.67
1:A:153:LEU:HD12	2:A:166:VNL:HV3	1.76	0.67
1:D:34:MET:HB3	1:D:38:PHE:CE1	2.30	0.67
1:B:18:PRO:HA	1:D:120:THR:HG23	1.77	0.66
1:C:25:LEU:HD23	1:C:29:LEU:HB2	1.76	0.66
1:C:30:LEU:CG	1:C:31:GLU:H	2.07	0.66
1:D:106:LEU:HD11	1:D:146:LEU:HD12	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:GLY:O	1:C:138:TRP:HB2	1.96	0.66
1:D:39:GLU:HG3	1:D:45:VAL:HG23	1.76	0.66
1:D:117:TYR:O	1:D:118:LEU:HD23	1.95	0.66
1:A:25:LEU:HB3	1:A:29:LEU:HD11	1.78	0.66
1:C:37:ARG:HH22	1:C:40:GLN:HG3	1.59	0.66
1:C:19:ALA:HB3	1:C:22:PRO:HG3	1.78	0.66
1:C:63:GLU:HB3	1:C:152:LEU:HD23	1.77	0.65
1:A:66:LEU:HD23	1:C:20:LEU:HA	1.79	0.65
1:B:105:ALA:HB3	1:B:119:PHE:CE2	2.32	0.65
1:C:116:ARG:HB2	1:C:124:LEU:HD22	1.78	0.65
1:C:67:LEU:HG	1:C:152:LEU:HD22	1.77	0.65
1:D:114:LEU:O	1:D:117:TYR:CD2	2.49	0.65
1:D:103:GLU:OE1	1:D:149:LYS:HE3	1.96	0.65
1:C:34:MET:HE3	1:C:34:MET:CA	2.16	0.65
1:D:22:PRO:HB2	1:D:23:GLN:NE2	2.11	0.64
1:A:37:ARG:CZ	1:A:40:GLN:HB2	2.27	0.64
1:C:117:TYR:CE1	1:C:118:LEU:HB2	2.32	0.64
1:A:115:GLY:HA2	1:A:119:PHE:CD1	2.33	0.64
1:C:27:TRP:HA	1:C:27:TRP:CE3	2.33	0.63
1:A:124:LEU:HD11	1:A:144:LEU:HD13	1.79	0.63
1:B:63:GLU:O	1:B:67:LEU:HD13	1.98	0.63
1:D:39:GLU:HG3	1:D:45:VAL:CG2	2.28	0.63
1:B:126:ARG:HD2	1:B:128:PHE:N	2.14	0.63
1:A:65:PRO:CB	1:C:18:PRO:HB3	2.03	0.63
1:C:19:ALA:O	1:C:22:PRO:HD3	1.98	0.63
1:A:17:ILE:CG2	1:A:25:LEU:HD22	2.29	0.63
1:A:116:ARG:CA	1:A:119:PHE:HB2	2.27	0.62
1:A:163:LEU:O	1:A:164:TYR:C	2.37	0.62
1:C:64:LEU:N	1:C:65:PRO:HD2	2.14	0.62
1:D:32:ASP:CG	1:D:33:SER:O	2.38	0.62
1:C:115:GLY:N	1:C:118:LEU:HD13	2.15	0.62
1:A:72:ARG:HG3	1:A:72:ARG:NH1	2.15	0.62
1:D:37:ARG:HH21	1:D:41:GLN:CG	2.13	0.61
1:A:75:LEU:HD11	1:A:77:GLU:HG3	1.83	0.61
1:C:37:ARG:NH2	1:C:40:GLN:HG3	2.16	0.61
1:B:126:ARG:O	1:B:126:ARG:NE	2.31	0.61
1:A:67:LEU:HB3	1:A:68:PRO:HD2	1.83	0.61
1:C:30:LEU:HD23	1:C:31:GLU:N	2.10	0.60
1:C:66:LEU:HB2	1:C:152:LEU:HD21	1.83	0.60
1:B:120:THR:C	1:B:122:SER:N	2.54	0.60
1:B:2:HIS:CD2	1:B:4:ALA:H	2.18	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ASP:N	1:C:22:PRO:HD3	2.15	0.60
1:C:29:LEU:HA	1:C:140:ARG:HH12	1.66	0.60
1:C:32:ASP:OD2	1:C:32:ASP:N	2.35	0.60
1:C:8:LEU:O	1:C:11:LEU:HB2	2.02	0.60
1:D:114:LEU:O	1:D:117:TYR:HD2	1.83	0.60
1:B:114:LEU:HD12	1:B:115:GLY:N	2.16	0.59
1:D:25:LEU:HD22	1:D:29:LEU:HD11	1.84	0.59
1:A:25:LEU:HB3	1:A:29:LEU:CD1	2.32	0.59
1:B:105:ALA:HB3	1:B:119:PHE:HE2	1.67	0.59
1:D:116:ARG:CB	1:D:124:LEU:HD13	2.31	0.59
1:A:61:PRO:HD2	1:A:62:GLU:OE1	2.01	0.59
1:C:13:TYR:HB3	1:C:130:GLU:OE2	2.03	0.59
1:D:11:LEU:HD23	1:D:132:GLY:C	2.22	0.59
1:B:60:ILE:O	1:B:60:ILE:HG13	2.03	0.59
1:D:19:ALA:C	1:D:20:LEU:CG	2.66	0.59
1:D:144:LEU:CD1	1:D:153:LEU:HG	2.33	0.59
1:B:20:LEU:CD1	1:B:25:LEU:HD21	2.33	0.59
1:A:17:ILE:HG22	1:A:25:LEU:HD22	1.83	0.58
1:C:30:LEU:HD23	1:C:32:ASP:N	2.06	0.58
1:C:15:LYS:HG2	1:C:130:GLU:CG	2.29	0.58
1:A:137:LEU:CD2	1:A:159:PRO:HD3	2.33	0.58
1:B:109:LEU:CD2	1:B:118:LEU:HD13	2.33	0.58
1:B:129:ILE:HD11	1:B:140:ARG:HD2	1.85	0.58
1:A:15:LYS:HE2	1:A:17:ILE:HG12	1.84	0.58
1:A:70:GLU:OE1	1:A:97:SER:HB2	2.04	0.58
1:B:88:LEU:C	1:B:88:LEU:HD23	2.24	0.58
1:A:126:ARG:HD2	1:A:129:ILE:HD11	1.86	0.58
1:C:17:ILE:N	1:C:18:PRO:HD3	2.15	0.58
1:A:75:LEU:HD13	1:A:76:ARG:N	2.19	0.57
1:B:129:ILE:CD1	1:B:140:ARG:HD2	2.34	0.57
1:D:145:ARG:HA	1:D:149:LYS:O	2.04	0.57
1:C:27:TRP:CZ3	1:C:34:MET:HE2	2.36	0.57
1:B:129:ILE:HD11	1:B:140:ARG:HB2	1.85	0.57
1:A:14:SER:O	1:C:23:GLN:NE2	2.37	0.57
1:A:64:LEU:HB3	1:A:65:PRO:HD3	1.87	0.57
1:C:116:ARG:NH2	1:C:123:THR:HA	2.19	0.57
1:C:115:GLY:O	1:C:118:LEU:HD22	2.04	0.57
1:A:18:PRO:O	1:A:20:LEU:N	2.38	0.57
1:C:30:LEU:HB2	3:C:609:HOH:O	2.03	0.57
1:D:21:ASP:OD2	1:D:21:ASP:C	2.42	0.57
1:D:21:ASP:CB	1:D:24:LEU:HB2	2.34	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ARG:NH2	1:A:128:PHE:HA	2.20	0.56
1:B:78:ILE:C	1:B:78:ILE:HD12	2.25	0.56
1:D:77:GLU:HA	1:D:90:GLY:O	2.06	0.56
1:A:37:ARG:NH2	1:A:40:GLN:HB2	2.19	0.56
1:C:30:LEU:HD22	1:C:32:ASP:O	2.05	0.56
1:C:2:HIS:HD2	1:C:4:ALA:H	1.51	0.56
1:A:130:GLU:OE2	1:C:22:PRO:HD2	2.06	0.56
1:A:130:GLU:OE2	1:C:22:PRO:HB2	2.05	0.56
1:C:103:GLU:HA	1:C:119:PHE:CZ	2.40	0.56
1:C:116:ARG:HH22	1:C:123:THR:HA	1.69	0.56
1:B:109:LEU:HD22	1:B:118:LEU:HD13	1.87	0.56
1:B:117:TYR:CG	1:B:117:TYR:O	2.58	0.56
1:C:31:GLU:HA	3:C:704:HOH:O	2.06	0.56
1:C:20:LEU:H	1:C:20:LEU:HD12	1.70	0.55
1:C:37:ARG:HH22	1:C:40:GLN:CG	2.19	0.55
1:B:45:VAL:HA	1:B:81:SER:O	2.07	0.55
1:D:17:ILE:HG12	1:D:131:ILE:HG13	1.88	0.55
1:C:30:LEU:CD2	1:C:32:ASP:H	2.09	0.54
1:C:66:LEU:HD13	1:C:128:PHE:HZ	1.72	0.54
1:A:71:SER:O	1:A:72:ARG:HG3	2.08	0.54
1:C:60:ILE:N	1:C:61:PRO:HD3	2.23	0.54
1:A:130:GLU:CD	1:C:22:PRO:HB2	2.26	0.54
1:C:70:GLU:OE1	1:C:95:PRO:HB2	2.07	0.54
1:C:114:LEU:HG	1:C:115:GLY:N	2.22	0.54
1:D:116:ARG:N	1:D:118:LEU:O	2.41	0.54
1:C:30:LEU:CG	1:C:31:GLU:N	2.69	0.54
1:C:37:ARG:HA	1:C:37:ARG:NE	2.22	0.54
1:C:32:ASP:O	1:C:33:SER:O	2.25	0.54
1:C:16:GLU:C	1:C:17:ILE:HD12	2.29	0.54
1:C:25:LEU:CA	1:C:29:LEU:HB2	2.36	0.53
1:B:36:LYS:O	1:B:40:GLN:HG3	2.08	0.53
1:A:116:ARG:H	1:A:119:PHE:HB2	1.73	0.53
1:A:37:ARG:HD2	1:A:40:GLN:NE2	2.24	0.53
1:B:120:THR:O	1:B:122:SER:N	2.42	0.53
1:D:45:VAL:CG1	1:D:80:LEU:HD11	2.38	0.53
1:D:88:LEU:HD11	1:D:155:GLU:HB3	1.91	0.53
1:B:109:LEU:HD22	1:B:118:LEU:CD1	2.39	0.53
1:B:114:LEU:O	1:B:117:TYR:HD2	1.91	0.53
1:D:116:ARG:HB2	1:D:124:LEU:CD1	2.30	0.53
1:A:125:THR:OG1	1:A:145:ARG:HB2	2.08	0.53
1:C:30:LEU:CD2	1:C:32:ASP:O	2.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLN:C	1:C:26:ASP:HB2	2.28	0.53
1:C:120:THR:O	1:C:122:SER:O	2.26	0.53
1:A:33:SER:HB3	3:A:203:HOH:O	2.08	0.53
1:A:127:ASP:O	1:A:128:PHE:HB3	2.09	0.52
1:D:7:GLN:O	1:D:10:ALA:HB3	2.09	0.52
1:A:153:LEU:HD12	2:A:166:VNL:CV	2.38	0.52
1:D:21:ASP:HB3	1:D:24:LEU:CB	2.38	0.52
1:A:137:LEU:HD21	1:A:159:PRO:HD3	1.91	0.52
1:C:29:LEU:CD1	1:C:30:LEU:H	2.05	0.52
1:D:22:PRO:O	1:D:26:ASP:OD2	2.28	0.52
1:B:20:LEU:HD12	1:B:20:LEU:H	1.75	0.52
1:C:27:TRP:CZ3	1:C:34:MET:CE	2.91	0.52
1:C:130:GLU:OE1	1:C:141:ARG:NH2	2.42	0.52
1:B:21:ASP:O	1:B:24:LEU:HB2	2.09	0.52
1:C:27:TRP:HZ2	1:C:41:GLN:HE21	1.58	0.52
1:C:133:ARG:CZ	1:C:138:TRP:CE3	2.92	0.52
1:A:37:ARG:NH2	1:A:41:GLN:OE1	2.42	0.52
1:B:74:TRP:CD2	1:B:107:GLN:HG3	2.46	0.51
1:B:30:LEU:HD13	1:B:37:ARG:HD3	1.90	0.51
1:B:51:ARG:HD3	1:B:75:LEU:CD2	2.41	0.51
1:C:133:ARG:NH2	1:C:138:TRP:CE2	2.78	0.51
1:B:42:GLY:O	1:B:43:LYS:HD2	2.10	0.51
1:A:34:MET:HG3	1:A:88:LEU:CD1	2.41	0.51
1:A:41:GLN:O	1:A:43:LYS:HD2	2.11	0.51
1:B:125:THR:CG2	1:B:145:ARG:HB2	2.36	0.51
1:C:29:LEU:HA	1:C:140:ARG:NH1	2.25	0.51
1:C:63:GLU:C	1:C:65:PRO:HD2	2.31	0.51
1:C:115:GLY:C	1:C:118:LEU:HB3	2.30	0.51
1:A:75:LEU:CD1	1:A:77:GLU:HG3	2.40	0.51
1:C:25:LEU:HD22	1:C:29:LEU:HG	1.92	0.51
1:C:116:ARG:NH2	1:C:122:SER:O	2.44	0.51
1:A:8:LEU:HD23	1:A:8:LEU:C	2.32	0.51
1:C:25:LEU:C	1:C:29:LEU:HB3	2.31	0.51
1:A:58:ASN:C	1:A:58:ASN:HD22	2.15	0.51
1:B:117:TYR:O	1:B:117:TYR:CD1	2.64	0.51
1:D:36:LYS:HD3	1:D:39:GLU:OE2	2.11	0.51
1:D:127:ASP:O	1:D:128:PHE:HB3	2.10	0.51
1:A:24:LEU:HD11	1:A:163:LEU:HD23	1.93	0.50
1:D:116:ARG:HD3	1:D:117:TYR:N	2.24	0.50
1:B:27:TRP:CD2	1:B:37:ARG:NH2	2.79	0.50
1:C:17:ILE:N	1:C:17:ILE:HD12	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:HIS:HD2	1:D:4:ALA:N	1.93	0.50
1:D:113:PRO:O	1:D:117:TYR:HE2	1.93	0.50
1:A:17:ILE:HG22	1:A:25:LEU:CD2	2.40	0.50
1:C:72:ARG:O	1:C:96:VAL:HG23	2.10	0.50
1:C:20:LEU:HD12	1:C:20:LEU:N	2.26	0.50
1:C:133:ARG:NH2	1:C:138:TRP:CD2	2.80	0.50
1:D:78:ILE:C	1:D:78:ILE:HD12	2.30	0.50
1:A:117:TYR:CE2	1:A:118:LEU:HD22	2.47	0.50
1:D:114:LEU:HD12	1:D:115:GLY:H	1.76	0.50
1:A:18:PRO:C	1:A:20:LEU:N	2.65	0.50
1:A:128:PHE:CD1	1:A:128:PHE:C	2.85	0.50
1:C:34:MET:HE3	1:C:34:MET:HA	1.93	0.50
1:C:78:ILE:C	1:C:78:ILE:HD12	2.31	0.50
1:B:20:LEU:HD12	1:B:20:LEU:N	2.27	0.50
1:C:37:ARG:NH2	1:C:40:GLN:HB2	2.27	0.50
1:D:22:PRO:HB2	1:D:23:GLN:HE21	1.75	0.50
1:D:128:PHE:CD1	1:D:128:PHE:C	2.85	0.50
1:B:130:GLU:OE1	1:B:141:ARG:NH2	2.41	0.50
1:A:78:ILE:C	1:A:78:ILE:HD12	2.31	0.49
1:D:37:ARG:NH2	1:D:41:GLN:OE1	2.45	0.49
1:A:62:GLU:HG2	1:A:63:GLU:OE1	2.12	0.49
1:B:8:LEU:O	1:B:11:LEU:HD12	2.13	0.49
1:B:18:PRO:O	1:B:19:ALA:C	2.51	0.49
1:C:29:LEU:CD2	1:C:129:ILE:HG21	2.42	0.49
1:C:116:ARG:HG3	1:C:116:ARG:O	2.11	0.49
1:C:58:ASN:OD1	1:C:59:GLU:HG3	2.12	0.49
1:D:116:ARG:C	1:D:116:ARG:HD3	2.33	0.49
1:A:48:THR:HB	1:A:79:LEU:HB2	1.94	0.49
1:B:16:GLU:OE2	1:D:118:LEU:HA	2.12	0.49
1:C:116:ARG:O	1:C:117:TYR:C	2.51	0.49
1:D:99:LEU:O	1:D:104:LEU:HB3	2.12	0.49
1:C:133:ARG:NE	1:C:138:TRP:HB3	2.27	0.49
1:A:133:ARG:O	1:A:134:ASP:HB2	2.11	0.49
1:A:141:ARG:HH22	1:C:22:PRO:HG2	1.71	0.49
1:D:53:GLY:HA2	1:D:74:TRP:CZ3	2.48	0.48
1:C:21:ASP:HB3	1:C:24:LEU:HG	1.95	0.48
3:A:622:HOH:O	1:D:104:LEU:HD22	2.12	0.48
1:B:36:LYS:N	1:B:36:LYS:HE2	2.28	0.48
1:B:8:LEU:C	1:B:8:LEU:HD23	2.33	0.48
1:B:63:GLU:HG2	1:B:93:VAL:HG21	1.94	0.48
1:B:34:MET:HG3	1:B:38:PHE:CE1	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLY:N	1:B:118:LEU:HB2	2.29	0.48
1:D:116:ARG:C	1:D:116:ARG:CD	2.82	0.48
1:A:2:HIS:CD2	1:A:4:ALA:H	2.31	0.48
1:C:38:PHE:O	1:C:41:GLN:HB2	2.14	0.48
1:C:64:LEU:HG	1:C:69:LYS:HE2	1.96	0.48
1:D:45:VAL:HG12	1:D:80:LEU:HD11	1.96	0.48
1:D:133:ARG:HG3	3:D:643:HOH:O	2.13	0.48
1:B:27:TRP:CE2	1:B:37:ARG:NH2	2.82	0.48
1:C:24:LEU:HD13	1:C:28:LEU:CD1	2.39	0.48
1:B:116:ARG:N	1:B:118:LEU:H	2.12	0.47
1:C:29:LEU:CD1	1:C:30:LEU:N	2.70	0.47
1:B:16:GLU:CD	1:D:117:TYR:O	2.52	0.47
1:C:23:GLN:O	1:C:26:ASP:C	2.52	0.47
1:C:133:ARG:NH1	1:C:138:TRP:CE3	2.82	0.47
1:A:17:ILE:CG2	1:A:29:LEU:HD21	2.41	0.47
1:B:115:GLY:HA3	1:B:118:LEU:CB	2.37	0.47
1:D:20:LEU:O	1:D:21:ASP:HB3	2.14	0.47
1:B:19:ALA:CB	1:D:121:SER:HB3	2.44	0.47
1:A:75:LEU:HD21	1:A:91:ARG:CZ	2.45	0.47
1:C:19:ALA:HB2	1:C:25:LEU:HD12	1.96	0.47
1:C:29:LEU:HD13	1:C:126:ARG:HH12	1.76	0.47
1:D:115:GLY:CA	1:D:118:LEU:HB2	2.17	0.47
1:A:17:ILE:HD12	1:A:29:LEU:CD2	2.44	0.47
1:C:21:ASP:OD1	1:C:21:ASP:O	2.32	0.47
1:A:30:LEU:HD11	1:A:32:ASP:OD2	2.15	0.47
1:A:118:LEU:HG	1:A:119:PHE:CD1	2.50	0.47
1:A:17:ILE:HA	1:A:18:PRO:HD2	1.68	0.46
1:A:37:ARG:HH21	1:A:41:GLN:CG	2.23	0.46
1:D:109:LEU:HD13	1:D:114:LEU:HA	1.97	0.46
1:D:122:SER:CB	1:D:146:LEU:HD22	2.45	0.46
1:A:20:LEU:O	1:A:21:ASP:C	2.54	0.46
1:A:100:SER:OG	1:A:149:LYS:NZ	2.35	0.46
1:B:118:LEU:C	1:B:119:PHE:CD1	2.89	0.46
1:C:25:LEU:CD2	1:C:29:LEU:HB2	2.44	0.46
1:C:60:ILE:N	1:C:61:PRO:CD	2.79	0.46
1:C:36:LYS:HD2	1:C:36:LYS:N	2.30	0.46
1:B:116:ARG:NH1	1:B:124:LEU:HD23	2.30	0.46
1:C:24:LEU:HA	1:C:27:TRP:HB2	1.97	0.46
1:B:107:GLN:O	1:B:107:GLN:HG2	2.16	0.46
1:A:37:ARG:HD2	1:A:40:GLN:HE22	1.79	0.46
1:A:73:TYR:N	1:A:73:TYR:CD1	2.84	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:VAL:HA	1:A:81:SER:O	2.16	0.45
1:A:124:LEU:HA	1:A:145:ARG:O	2.16	0.45
1:C:16:GLU:HG2	1:C:17:ILE:N	2.31	0.45
1:A:37:ARG:NH1	1:A:40:GLN:NE2	2.64	0.45
1:B:1:SER:OG	1:B:2:HIS:N	2.48	0.45
1:C:128:PHE:CE2	1:C:143:ARG:HB2	2.52	0.45
1:A:118:LEU:N	1:A:118:LEU:HD23	2.31	0.45
1:D:117:TYR:CE1	1:D:118:LEU:HD21	2.51	0.45
1:B:67:LEU:HD12	1:B:67:LEU:N	2.29	0.45
1:C:17:ILE:O	1:C:17:ILE:HG22	2.16	0.45
1:D:114:LEU:O	1:D:117:TYR:CE2	2.69	0.45
1:A:40:GLN:C	1:A:42:GLY:H	2.19	0.45
1:C:23:GLN:HA	1:C:26:ASP:CB	2.35	0.45
1:B:146:LEU:O	1:B:147:SER:HB2	2.15	0.45
1:D:118:LEU:C	1:D:119:PHE:CG	2.90	0.45
1:A:118:LEU:CD2	1:A:119:PHE:HD1	2.30	0.45
1:B:37:ARG:O	1:B:41:GLN:HG2	2.17	0.45
1:C:128:PHE:CD1	1:C:128:PHE:C	2.90	0.45
1:B:51:ARG:HD3	1:B:75:LEU:HD21	1.99	0.44
1:A:23:GLN:NE2	1:A:26:ASP:OD2	2.44	0.44
1:B:45:VAL:CG1	1:B:80:LEU:HD11	2.48	0.44
1:B:60:ILE:O	1:B:60:ILE:CG1	2.64	0.44
1:D:30:LEU:HD21	1:D:32:ASP:HB3	1.98	0.44
1:D:116:ARG:H	1:D:118:LEU:H	0.68	0.44
1:A:137:LEU:HD22	1:A:159:PRO:HD3	1.99	0.44
1:A:18:PRO:HG2	1:A:25:LEU:CD2	2.47	0.44
1:D:118:LEU:O	1:D:119:PHE:CG	2.70	0.44
1:A:2:HIS:HD2	1:A:4:ALA:HB3	1.82	0.44
1:A:7:GLN:HE22	1:A:137:LEU:HD13	1.83	0.44
1:D:32:ASP:CG	1:D:33:SER:H	2.21	0.44
1:B:114:LEU:HA	1:B:118:LEU:HD12	1.99	0.44
1:C:19:ALA:HB2	1:C:25:LEU:CD1	2.48	0.44
1:C:19:ALA:C	1:C:21:ASP:H	2.21	0.43
1:C:52:GLU:HA	1:C:75:LEU:O	2.18	0.43
1:D:31:GLU:O	1:D:32:ASP:HB2	2.18	0.43
1:D:114:LEU:HG	1:D:115:GLY:N	2.33	0.43
1:A:17:ILE:HD12	1:A:29:LEU:HD21	1.99	0.43
1:B:17:ILE:H	1:D:118:LEU:HD22	1.83	0.43
1:C:51:ARG:CD	1:C:77:GLU:OE1	2.50	0.43
1:C:89:ALA:HB3	1:C:156:LEU:HB3	2.00	0.43
1:D:2:HIS:CE1	1:D:79:LEU:HD11	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:VAL:O	1:D:99:LEU:HB2	2.17	0.43
1:D:118:LEU:O	1:D:119:PHE:CD1	2.72	0.43
1:B:146:LEU:HD23	1:B:146:LEU:HA	1.90	0.43
1:B:73:TYR:N	1:B:73:TYR:CD1	2.86	0.43
1:C:19:ALA:HB2	1:C:25:LEU:HG	1.98	0.43
1:C:145:ARG:HA	1:C:149:LYS:O	2.17	0.43
1:D:23:GLN:HG3	1:D:26:ASP:OD2	2.19	0.43
1:D:98:THR:HG23	1:D:149:LYS:CB	2.49	0.43
1:A:18:PRO:C	1:A:20:LEU:H	2.22	0.43
1:D:32:ASP:CG	1:D:33:SER:N	2.72	0.43
1:D:23:GLN:N	1:D:23:GLN:HE21	2.16	0.43
1:C:100:SER:O	1:C:103:GLU:HB2	2.19	0.43
1:D:24:LEU:C	1:D:26:ASP:N	2.72	0.43
1:D:66:LEU:O	1:D:67:LEU:HD12	2.18	0.43
1:B:72:ARG:C	1:B:73:TYR:CD1	2.92	0.43
1:D:21:ASP:O	1:D:22:PRO:C	2.56	0.43
1:A:17:ILE:HA	1:A:131:ILE:HG13	2.01	0.43
1:B:145:ARG:HA	1:B:149:LYS:O	2.18	0.43
1:C:24:LEU:HB3	1:C:28:LEU:HD13	2.01	0.43
1:C:133:ARG:NH2	1:C:138:TRP:CG	2.87	0.43
1:D:43:LYS:HG3	1:D:83:ASP:OD2	2.19	0.43
1:A:18:PRO:HG2	1:A:25:LEU:HD21	2.01	0.42
1:D:141:ARG:HG2	1:D:154:THR:OG1	2.19	0.42
1:A:137:LEU:HD23	1:A:164:TYR:CZ	2.54	0.42
1:B:118:LEU:O	1:B:119:PHE:CD1	2.72	0.42
1:B:119:PHE:CD1	1:B:146:LEU:HD11	2.54	0.42
1:C:126:ARG:HD3	3:C:704:HOH:O	2.19	0.42
1:D:161:SER:HA	1:D:162:PRO:HD3	1.85	0.42
1:B:109:LEU:HD21	1:B:118:LEU:HD22	2.01	0.42
1:A:27:TRP:CH2	1:A:162:PRO:HG2	2.53	0.42
1:A:23:GLN:NE2	1:A:26:ASP:CG	2.73	0.42
1:B:13:TYR:HB3	1:B:130:GLU:HG3	2.02	0.42
1:D:36:LYS:HE3	1:D:117:TYR:CE1	2.55	0.42
1:D:146:LEU:O	1:D:147:SER:HB2	2.19	0.42
1:A:70:GLU:OE1	1:A:97:SER:CB	2.67	0.42
1:C:76:ARG:NH1	1:C:109:LEU:HB2	2.34	0.42
1:C:133:ARG:NH1	1:C:138:TRP:CZ3	2.88	0.42
1:D:122:SER:HB3	1:D:146:LEU:HD22	2.00	0.42
1:D:11:LEU:HD23	1:D:132:GLY:HA3	2.02	0.42
1:A:24:LEU:CD1	1:A:163:LEU:HD23	2.49	0.42
1:B:108:LYS:HB2	1:B:108:LYS:HE3	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:PRO:O	1:B:117:TYR:CE2	2.64	0.42
1:B:118:LEU:O	1:B:119:PHE:CG	2.72	0.42
1:C:29:LEU:HD11	1:C:126:ARG:HH12	1.80	0.42
1:C:116:ARG:O	1:C:120:THR:N	2.52	0.42
1:D:21:ASP:CG	1:D:24:LEU:HB2	2.40	0.42
1:C:37:ARG:NH2	1:C:40:GLN:CG	2.79	0.42
1:C:51:ARG:HG2	1:C:77:GLU:HB2	2.02	0.42
1:D:37:ARG:NH2	1:D:41:GLN:HG2	2.27	0.42
1:D:37:ARG:HH12	1:D:40:GLN:HB3	1.84	0.42
1:A:30:LEU:HD23	1:A:34:MET:HE2	2.02	0.41
1:A:60:ILE:O	1:A:60:ILE:HG13	2.18	0.41
1:B:13:TYR:HA	1:B:131:ILE:O	2.20	0.41
1:B:133:ARG:HA	1:B:137:LEU:O	2.20	0.41
1:C:117:TYR:CD2	1:C:117:TYR:N	2.88	0.41
1:C:116:ARG:C	1:C:118:LEU:H	2.16	0.41
1:D:89:ALA:HB3	1:D:156:LEU:HB3	2.02	0.41
1:A:18:PRO:HD2	1:A:131:ILE:HG13	2.01	0.41
1:B:114:LEU:C	1:B:118:LEU:HD12	2.41	0.41
1:C:120:THR:O	1:C:122:SER:N	2.53	0.41
1:D:18:PRO:O	1:D:20:LEU:CD2	2.59	0.41
1:D:117:TYR:CE2	1:D:118:LEU:CG	3.02	0.41
1:A:37:ARG:NH2	1:A:40:GLN:CB	2.82	0.41
1:B:72:ARG:O	1:B:96:VAL:HG22	2.19	0.41
1:C:21:ASP:H	1:C:22:PRO:HD3	1.84	0.41
1:C:37:ARG:NH2	1:C:40:GLN:CB	2.83	0.41
1:C:64:LEU:N	1:C:65:PRO:CD	2.81	0.41
1:C:120:THR:O	1:C:121:SER:C	2.57	0.41
1:C:137:LEU:HD21	1:C:159:PRO:HG3	2.01	0.41
1:B:109:LEU:HD23	1:B:109:LEU:HA	1.85	0.41
1:D:15:LYS:HB2	1:D:15:LYS:HE3	1.87	0.41
1:A:15:LYS:HG2	1:A:130:GLU:HB2	2.03	0.41
1:C:2:HIS:HD2	1:C:4:ALA:N	2.17	0.41
1:C:133:ARG:HE	1:C:138:TRP:HB3	1.84	0.41
1:C:150:PRO:HD2	3:C:705:HOH:O	2.20	0.41
1:C:163:LEU:HD12	1:C:163:LEU:N	2.35	0.41
1:D:56:GLU:HG2	1:D:72:ARG:CZ	2.51	0.41
1:D:37:ARG:NH1	1:D:40:GLN:HB2	2.35	0.41
1:C:7:GLN:O	1:C:7:GLN:NE2	2.54	0.40
1:C:30:LEU:O	1:C:126:ARG:NH1	2.54	0.40
1:C:149:LYS:HA	1:C:150:PRO:HD3	1.96	0.40
1:A:24:LEU:HD21	1:A:138:TRP:NE1	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:LEU:O	1:D:9:ARG:HG2	2.21	0.40
1:D:20:LEU:O	1:D:24:LEU:HB3	2.22	0.40
1:D:117:TYR:O	1:D:117:TYR:CD1	2.75	0.40
1:C:24:LEU:O	1:C:25:LEU:HG	2.21	0.40
1:D:37:ARG:NH1	1:D:40:GLN:CB	2.84	0.40
1:B:133:ARG:NH1	1:B:138:TRP:CZ2	2.90	0.40
1:D:8:LEU:HD23	1:D:8:LEU:C	2.42	0.40
1:D:70:GLU:OE2	1:D:96:VAL:HG23	2.21	0.40
1:C:12:ARG:HH11	1:C:12:ARG:HG2	1.86	0.40
1:C:67:LEU:HB3	1:C:68:PRO:HD2	2.03	0.40

All (1) 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:B:108:LYS:NZ	1:D:21:ASP:O[1_655]	2.10	0.10

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	162/164 (99%)	133 (82%)	21 (13%)	8 (5%)	2 1
1	B	162/164 (99%)	150 (93%)	8 (5%)	4 (2%)	5 6
1	C	162/164 (99%)	134 (83%)	18 (11%)	10 (6%)	1 0
1	D	162/164 (99%)	147 (91%)	8 (5%)	7 (4%)	2 2
All	All	648/656 (99%)	564 (87%)	55 (8%)	29 (4%)	2 2

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	C	15	LYS
1	C	25	LEU
1	C	30	LEU
1	C	33	SER
1	D	19	ALA
1	D	119	PHE
1	A	16	GLU
1	A	19	ALA
1	A	115	GLY
1	B	18	PRO
1	B	116	ARG
1	B	121	SER
1	C	22	PRO
1	C	23	GLN
1	C	122	SER
1	D	116	ARG
1	A	18	PRO
1	C	14	SER
1	D	32	ASP
1	D	114	LEU
1	A	15	LYS
1	C	121	SER
1	D	21	ASP
1	A	116	ARG
1	C	21	ASP
1	D	128	PHE
1	B	134	ASP
1	A	22	PRO

5.3.2 Protein sidechains (i)

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	145/145 (100%)	122 (84%)	23 (16%)	2 3
1	B	145/145 (100%)	123 (85%)	22 (15%)	3 3
1	C	145/145 (100%)	121 (83%)	24 (17%)	2 2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	145/145 (100%)	125 (86%)	20 (14%)	3 4
All	All	580/580 (100%)	491 (85%)	89 (15%)	2 3

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	11	LEU
1	A	12	ARG
1	A	14	SER
1	A	15	LYS
1	A	20	LEU
1	A	29	LEU
1	A	32	ASP
1	A	43	LYS
1	A	51	ARG
1	A	58	ASN
1	A	72	ARG
1	A	83	ASP
1	A	88	LEU
1	A	112	THR
1	A	116	ARG
1	A	122	SER
1	A	131	ILE
1	A	133	ARG
1	A	151	LEU
1	A	152	LEU
1	A	159	PRO
1	A	164	TYR
1	B	16	GLU
1	B	18	PRO
1	B	20	LEU
1	B	23	GLN
1	B	31	GLU
1	B	37	ARG
1	B	58	ASN
1	B	62	GLU
1	B	63	GLU
1	B	69	LYS
1	B	71	SER
1	B	88	LEU
1	B	96	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	117	TYR
1	B	123	THR
1	B	125	THR
1	B	126	ARG
1	B	142	SER
1	B	146	LEU
1	B	150	PRO
1	B	152	LEU
1	B	164	TYR
1	C	7	GLN
1	C	12	ARG
1	C	15	LYS
1	C	22	PRO
1	C	24	LEU
1	C	26	ASP
1	C	27	TRP
1	C	29	LEU
1	C	30	LEU
1	C	32	ASP
1	C	33	SER
1	C	44	THR
1	C	61	PRO
1	C	62	GLU
1	C	69	LYS
1	C	112	THR
1	C	114	LEU
1	C	120	THR
1	C	123	THR
1	C	129	ILE
1	C	133	ARG
1	C	138	TRP
1	C	143	ARG
1	C	152	LEU
1	D	9	ARG
1	D	12	ARG
1	D	16	GLU
1	D	20	LEU
1	D	23	GLN
1	D	31	GLU
1	D	43	LYS
1	D	85	GLU
1	D	88	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	96	VAL
1	D	100	SER
1	D	104	LEU
1	D	116	ARG
1	D	117	TYR
1	D	124	LEU
1	D	129	ILE
1	D	133	ARG
1	D	141	ARG
1	D	145	ARG
1	D	152	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	7	GLN
1	A	40	GLN
1	A	58	ASN
1	B	2	HIS
1	C	2	HIS
1	C	7	GLN
1	D	2	HIS
1	D	23	GLN
1	D	57	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	VNL	D	466	-	12,12,12	2.13	5 (41%)	16,16,16	1.50	2 (12%)
2	VNL	B	266	-	12,12,12	2.18	5 (41%)	16,16,16	1.44	2 (12%)
2	VNL	A	166	-	12,12,12	1.92	5 (41%)	16,16,16	1.57	3 (18%)
2	VNL	C	366	-	12,12,12	1.90	4 (33%)	16,16,16	1.31	3 (18%)

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	VNL	D	466	-	-	0/6/6/6	0/1/1/1
2	VNL	B	266	-	-	0/6/6/6	0/1/1/1
2	VNL	A	166	-	-	0/6/6/6	0/1/1/1
2	VNL	C	366	-	-	1/6/6/6	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	466	VNL	CO2-CM2	4.12	1.46	1.38
2	A	166	VNL	C1-CC	-3.81	1.41	1.49
2	B	266	VNL	CO2-CM2	3.62	1.45	1.38
2	B	266	VNL	CO2-C1	3.47	1.44	1.39
2	A	166	VNL	OM-CV	-3.29	1.32	1.42
2	C	366	VNL	CO2-CM2	3.27	1.44	1.38
2	B	266	VNL	C1-CC	-3.10	1.42	1.49
2	C	366	VNL	C1-CC	-3.09	1.42	1.49
2	B	266	VNL	OM-CV	-3.08	1.33	1.42
2	D	466	VNL	OM-CV	-3.06	1.33	1.42
2	C	366	VNL	OM-CV	-2.88	1.34	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	466	VNL	C1-CC	-2.82	1.43	1.49
2	A	166	VNL	O1-CC	-2.64	1.22	1.30
2	D	466	VNL	CO1-C1	2.52	1.43	1.39
2	D	466	VNL	O1-CC	-2.32	1.23	1.30
2	A	166	VNL	OM-CM2	-2.22	1.33	1.37
2	B	266	VNL	O1-CC	-2.12	1.24	1.30
2	A	166	VNL	CZ-CM2	2.10	1.44	1.40
2	C	366	VNL	O1-CC	-2.07	1.24	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	266	VNL	CV-OM-CM2	3.75	123.19	117.53
2	D	466	VNL	CV-OM-CM2	3.68	123.08	117.53
2	A	166	VNL	OM-CM2-CZ	3.59	119.77	114.57
2	D	466	VNL	OM-CM2-CZ	3.56	119.72	114.57
2	A	166	VNL	CV-OM-CM2	3.55	122.89	117.53
2	C	366	VNL	OM-CM2-CO2	-2.93	119.08	124.12
2	B	266	VNL	OM-CM2-CZ	2.84	118.68	114.57
2	A	166	VNL	OM-CM2-CO2	-2.43	119.94	124.12
2	C	366	VNL	CO2-CM2-CZ	-2.25	117.63	120.06
2	C	366	VNL	OM-CM2-CZ	2.03	117.50	114.57

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	366	VNL	CO2-CM2-OM-CV

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	166	VNL	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	164/164 (100%)	0.48	18 (10%)	5	5	5, 22, 50, 56	0
1	B	164/164 (100%)	0.01	10 (6%)	21	20	9, 20, 35, 51	0
1	C	164/164 (100%)	0.77	25 (15%)	2	1	11, 23, 49, 55	0
1	D	164/164 (100%)	0.18	15 (9%)	9	8	7, 19, 41, 48	0
All	All	656/656 (100%)	0.36	68 (10%)	6	6	5, 21, 47, 56	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	18	PRO	14.4
1	D	19	ALA	14.3
1	C	22	PRO	11.9
1	B	121	SER	9.2
1	D	121	SER	9.0
1	D	22	PRO	8.7
1	A	117	TYR	8.7
1	A	17	ILE	7.5
1	A	120	THR	7.0
1	C	119	PHE	6.7
1	A	18	PRO	6.6
1	C	118	LEU	6.5
1	A	16	GLU	6.1
1	B	118	LEU	6.0
1	B	117	TYR	5.8
1	C	121	SER	5.8
1	C	117	TYR	5.8
1	A	118	LEU	5.7
1	D	23	GLN	5.6
1	C	120	THR	5.5
1	C	26	ASP	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	121	SER	5.4
1	C	19	ALA	5.2
1	B	119	PHE	4.9
1	A	115	GLY	4.8
1	C	138	TRP	4.8
1	A	116	ARG	4.8
1	D	120	THR	4.7
1	C	14	SER	4.7
1	C	31	GLU	4.6
1	D	117	TYR	4.6
1	A	19	ALA	4.5
1	A	33	SER	4.4
1	C	17	ILE	4.2
1	C	25	LEU	4.1
1	B	120	THR	4.1
1	D	21	ASP	4.0
1	C	15	LYS	4.0
1	C	20	LEU	3.9
1	A	122	SER	3.8
1	C	32	ASP	3.7
1	A	162	PRO	3.1
1	B	122	SER	3.0
1	C	33	SER	3.0
1	D	33	SER	3.0
1	D	115	GLY	3.0
1	A	15	LYS	3.0
1	C	24	LEU	3.0
1	D	122	SER	3.0
1	A	119	PHE	2.8
1	C	122	SER	2.8
1	B	116	ARG	2.7
1	D	118	LEU	2.7
1	C	28	LEU	2.7
1	D	1	SER	2.7
1	A	37	ARG	2.7
1	C	23	GLN	2.6
1	B	115	GLY	2.6
1	C	16	GLU	2.5
1	B	33	SER	2.4
1	A	42	GLY	2.3
1	C	29	LEU	2.3
1	D	20	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	14	SER	2.2
1	C	30	LEU	2.2
1	B	12	ARG	2.2
1	D	12	ARG	2.1
1	D	32	ASP	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	VNL	A	166	12/12	0.84	0.18	22,26,28,29	0
2	VNL	C	366	12/12	0.87	0.16	24,25,27,27	0
2	VNL	B	266	12/12	0.91	0.19	18,20,22,22	0
2	VNL	D	466	12/12	0.91	0.18	15,23,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.