Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:04 PM GMT

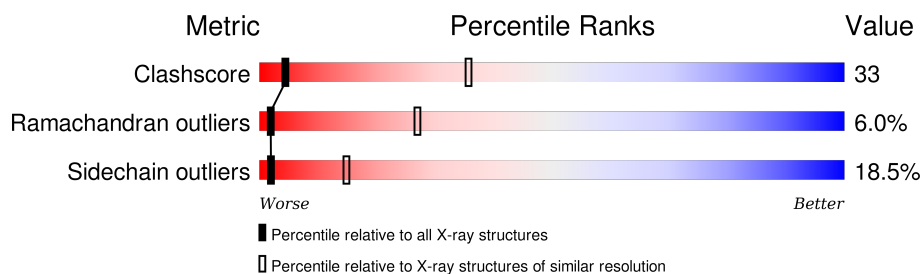|		
PDB ID	:	1NED
Title	:	CRYSTAL STRUCTURE OF HSLV (CLPQ) AT 3.8 ANGSTROMS RESOLUTION
Authors	:	Bochtler, M.; Ditzel, L.; Groll, M.; Huber, R.
Deposited on	:	1997-04-04
Resolution	:	3.80 Å(reported)

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 3.80 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	Percentile Ranks	Value
Clashscore		33
Ramachandran outliers		6.0%
Sidechain outliers		18.5%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	183	43% 42% 12% • •
1	B	183	49% 38% 11% • •
1	C	183	45% 40% 12% • •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5020 atoms, of which 896 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 HSLV.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	180	Total	C	H	N	O	S	300	0	0
			1683	869	300	249	261	4			
1	B	181	Total	C	H	N	O	S	301	0	0
			1679	864	301	250	260	4			
1	C	181	Total	C	H	N	O	S	295	0	0
			1658	855	295	244	260	4			

3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: HSLV

Chain A:

- Molecule 1: HSLV

Chain B:

- Molecule 1: HSLV

Chain C:
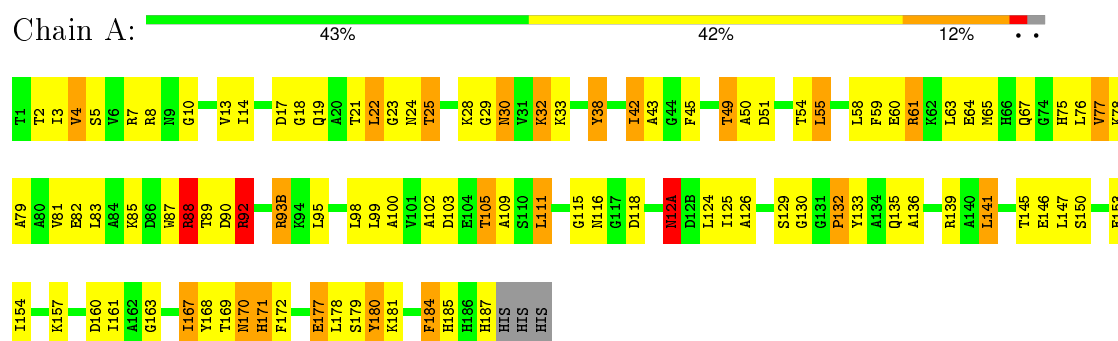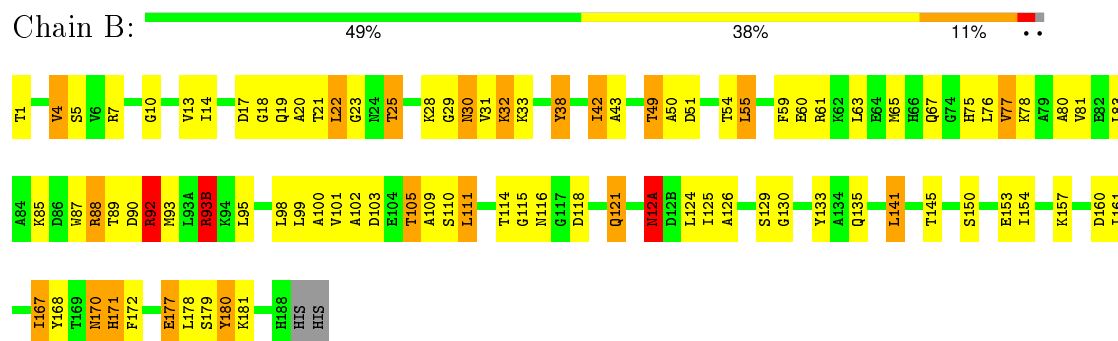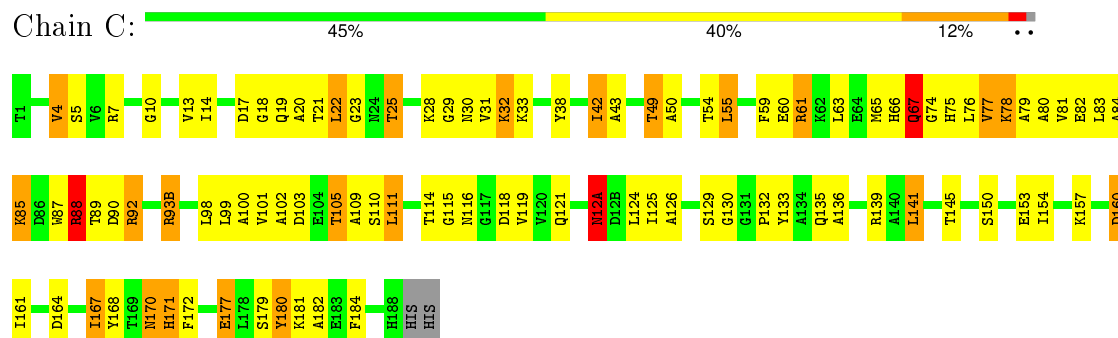
4   Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	108.40Å 108.40Å 103.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.80	Depositor
% Data completeness (in resolution range)	99.4 (15.00-3.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.842	Depositor
R, R_{free}	0.256 , 0.315	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5020	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	0.63	0/1404	0.92	5/1897 (0.3%)
1	B	0.65	0/1398	0.94	7/1890 (0.4%)
1	C	0.65	0/1380	0.92	5/1866 (0.3%)
All	All	0.64	0/4182	0.93	17/5653 (0.3%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	88	ARG	NE-CZ-NH2	7.63	124.12	120.30
1	C	92	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	C	93(B)	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	A	92	ARG	NE-CZ-NH2	7.45	124.03	120.30
1	A	93(B)	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	B	92	ARG	NE-CZ-NH2	7.11	123.85	120.30
1	B	88	ARG	NE-CZ-NH2	7.01	123.81	120.30
1	B	93(B)	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	C	88	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	B	61	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	A	61	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	B	170	ASN	N-CA-C	6.11	127.48	111.00
1	A	170	ASN	N-CA-C	6.03	127.29	111.00
1	C	170	ASN	N-CA-C	5.96	127.11	111.00
1	C	61	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	B	88	ARG	NH1-CZ-NH2	-5.77	113.06	119.40
1	B	88	ARG	NE-CZ-NH1	5.67	123.14	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1383	300	1389	86	0
1	B	1378	301	1380	90	0
1	C	1363	295	1365	94	0
All	All	4124	896	4134	270	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (270) 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:88:ARG:HG2	1:A:116:ASN:O	1.31	1.24
1:A:88:ARG:CG	1:A:116:ASN:O	1.92	1.17
1:C:88:ARG:O	1:C:88:ARG:HD2	1.43	1.13
1:C:88:ARG:C	1:C:88:ARG:HD2	1.75	1.03
1:A:88:ARG:HG2	1:A:116:ASN:C	1.79	1.02
1:C:88:ARG:O	1:C:88:ARG:CD	2.10	0.99
1:B:88:ARG:O	1:B:88:ARG:HG3	1.66	0.95
1:C:88:ARG:HG2	1:C:116:ASN:O	1.71	0.89
1:A:170:ASN:OD1	1:A:172:PHE:HB3	1.74	0.88
1:C:170:ASN:OD1	1:C:172:PHE:HB3	1.78	0.84
1:B:121:GLN:HE21	1:B:121:GLN:H	1.26	0.81
1:C:85:LYS:HB2	1:C:85:LYS:NZ	1.96	0.80
1:B:170:ASN:OD1	1:B:172:PHE:HB3	1.81	0.80
1:B:7:ARG:HH12	1:B:109:ALA:HA	1.48	0.79
1:A:59:PHE:HB2	1:A:83:LEU:HD22	1.64	0.79
1:C:67:GLN:HG3	1:C:74:GLY:N	1.95	0.79
1:B:59:PHE:HB2	1:B:83:LEU:HD22	1.65	0.78
1:A:5:SER:HA	1:A:13:VAL:O	1.84	0.77
1:A:88:ARG:HG3	1:A:116:ASN:O	1.83	0.77
1:B:17:ASP:HB2	1:B:170:ASN:HB3	1.65	0.77
1:A:7:ARG:HH12	1:A:109:ALA:HA	1.48	0.77
1:C:17:ASP:HB2	1:C:170:ASN:HB3	1.66	0.77
1:A:170:ASN:O	1:A:171:HIS:HB2	1.84	0.76
1:C:59:PHE:HB2	1:C:83:LEU:HD22	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ASN:O	1:C:171:HIS:HB2	1.85	0.75
1:B:32:LYS:HD2	1:B:32:LYS:H	1.50	0.75
1:C:7:ARG:HH12	1:C:109:ALA:HA	1.54	0.73
1:B:88:ARG:NE	1:B:116:ASN:O	2.23	0.72
1:B:88:ARG:CG	1:B:88:ARG:O	2.39	0.71
1:A:32:LYS:HD2	1:A:32:LYS:H	1.54	0.70
1:A:17:ASP:HB2	1:A:170:ASN:HB3	1.73	0.70
1:C:130:GLY:HA2	1:C:133:TYR:HD2	1.57	0.70
1:C:5:SER:HA	1:C:13:VAL:O	1.92	0.70
1:C:88:ARG:CG	1:C:88:ARG:O	2.39	0.70
1:C:82:GLU:O	1:C:85:LYS:HB3	1.91	0.70
1:B:77:VAL:O	1:B:81:VAL:HG23	1.90	0.70
1:A:130:GLY:HA2	1:A:133:TYR:HD2	1.57	0.69
1:B:5:SER:HA	1:B:13:VAL:O	1.91	0.69
1:B:170:ASN:O	1:B:171:HIS:HB2	1.92	0.68
1:C:32:LYS:HD2	1:C:32:LYS:H	1.59	0.68
1:A:77:VAL:O	1:A:81:VAL:HG23	1.94	0.67
1:A:22:LEU:HD23	1:A:25:THR:HG23	1.77	0.67
1:B:4:VAL:HA	1:B:125:ILE:O	1.96	0.66
1:B:130:GLY:HA2	1:B:133:TYR:HD2	1.59	0.66
1:A:28:LYS:HE3	1:A:30:ASN:CG	2.17	0.65
1:C:77:VAL:O	1:C:81:VAL:HG23	1.97	0.64
1:B:111:LEU:N	1:B:111:LEU:HD12	2.12	0.64
1:B:87:TRP:CD2	1:B:115:GLY:HA2	2.32	0.64
1:B:88:ARG:CD	1:B:116:ASN:O	2.46	0.63
1:C:67:GLN:HG3	1:C:74:GLY:H	1.63	0.63
1:C:98:LEU:C	1:C:99:LEU:HD12	2.18	0.63
1:B:22:LEU:HD23	1:B:25:THR:HG23	1.80	0.63
1:B:19:GLN:N	1:B:170:ASN:HB2	2.14	0.62
1:C:22:LEU:HD23	1:C:25:THR:HG23	1.82	0.62
1:C:87:TRP:CD2	1:C:115:GLY:HA2	2.34	0.61
1:A:150:SER:OG	1:A:153:GLU:HG3	1.99	0.61
1:B:150:SER:OG	1:B:153:GLU:HG3	2.01	0.61
1:A:87:TRP:CD2	1:A:115:GLY:HA2	2.35	0.61
1:C:78:LYS:NZ	1:C:82:GLU:HB2	2.15	0.61
1:A:111:LEU:N	1:A:111:LEU:HD12	2.14	0.61
1:A:89:THR:HG22	1:A:90:ASP:N	2.16	0.61
1:A:141:LEU:O	1:A:145:THR:HG22	2.00	0.61
1:C:141:LEU:O	1:C:145:THR:HG22	2.00	0.61
1:C:19:GLN:N	1:C:170:ASN:HB2	2.15	0.61
1:A:141:LEU:HD23	1:A:154:ILE:HG23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:GLN:NE2	1:B:121:GLN:H	1.99	0.61
1:B:10:GLY:O	1:B:179:SER:HA	2.00	0.61
1:C:121:GLN:HG3	1:C:121:GLN:O	2.01	0.60
1:C:10:GLY:O	1:C:179:SER:HA	2.00	0.60
1:C:89:THR:HG22	1:C:90:ASP:N	2.16	0.60
1:B:102:ALA:HA	1:B:109:ALA:O	2.01	0.60
1:B:180:TYR:N	1:B:180:TYR:CD1	2.70	0.60
1:C:87:TRP:CE2	1:C:115:GLY:HA2	2.36	0.59
1:C:150:SER:OG	1:C:153:GLU:HG3	2.02	0.59
1:A:87:TRP:CE2	1:A:115:GLY:HA2	2.38	0.59
1:C:78:LYS:HE2	1:C:78:LYS:HA	1.85	0.59
1:B:141:LEU:O	1:B:145:THR:HG22	2.03	0.59
1:B:87:TRP:CE2	1:B:115:GLY:HA2	2.38	0.58
1:A:19:GLN:N	1:A:170:ASN:HB2	2.18	0.58
1:C:85:LYS:HB2	1:C:85:LYS:HZ3	1.66	0.58
1:B:141:LEU:HD23	1:B:154:ILE:HG23	1.85	0.58
1:B:98:LEU:C	1:B:99:LEU:HD12	2.23	0.58
1:B:59:PHE:CA	1:B:83:LEU:HD13	2.34	0.58
1:B:59:PHE:HA	1:B:83:LEU:HD13	1.85	0.58
1:C:130:GLY:HA2	1:C:133:TYR:CD2	2.38	0.58
1:B:55:LEU:HD21	1:B:87:TRP:CD2	2.39	0.58
1:B:167:ILE:HD12	1:B:168:TYR:H	1.68	0.58
1:A:167:ILE:HD12	1:A:168:TYR:H	1.68	0.58
1:A:65:MET:O	1:A:65:MET:HG2	2.04	0.57
1:B:13:VAL:HG13	1:B:177:GLU:HB3	1.86	0.57
1:C:18:GLY:H	1:C:170:ASN:HB3	1.68	0.57
1:A:130:GLY:HA2	1:A:133:TYR:CD2	2.38	0.57
1:A:98:LEU:C	1:A:99:LEU:HD12	2.25	0.57
1:A:10:GLY:O	1:A:179:SER:HA	2.05	0.57
1:C:4:VAL:HA	1:C:125:ILE:O	2.04	0.56
1:B:89:THR:HG22	1:B:90:ASP:N	2.20	0.56
1:C:141:LEU:HD23	1:C:154:ILE:HG23	1.87	0.56
1:B:65:MET:O	1:B:65:MET:HG2	2.05	0.56
1:C:55:LEU:HD21	1:C:87:TRP:CD2	2.41	0.56
1:C:28:LYS:HE3	1:C:30:ASN:CG	2.25	0.56
1:C:59:PHE:HA	1:C:83:LEU:HD13	1.87	0.56
1:C:102:ALA:HA	1:C:109:ALA:O	2.06	0.56
1:A:19:GLN:HB2	1:A:170:ASN:HB2	1.87	0.56
1:B:180:TYR:HD1	1:B:180:TYR:N	2.03	0.56
1:A:4:VAL:HA	1:A:125:ILE:O	2.06	0.56
1:B:121:GLN:N	1:B:121:GLN:HE21	2.01	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PHE:HA	1:A:83:LEU:HD13	1.88	0.56
1:A:55:LEU:HD21	1:A:87:TRP:CD2	2.42	0.55
1:C:59:PHE:CA	1:C:83:LEU:HD13	2.36	0.55
1:A:93(B):ARG:O	1:A:93(B):ARG:CG	2.55	0.55
1:A:180:TYR:N	1:A:180:TYR:CD1	2.74	0.55
1:B:130:GLY:HA2	1:B:133:TYR:CD2	2.41	0.55
1:A:132:PRO:O	1:A:135:GLN:HB3	2.07	0.55
1:B:43:ALA:HA	1:B:100:ALA:O	2.07	0.55
1:A:59:PHE:HB2	1:A:83:LEU:CD2	2.36	0.54
1:B:59:PHE:HB2	1:B:83:LEU:CD2	2.36	0.54
1:A:59:PHE:CA	1:A:83:LEU:HD13	2.37	0.54
1:C:78:LYS:HZ2	1:C:82:GLU:HB2	1.73	0.54
1:B:51:ASP:HA	1:B:95:LEU:HD23	1.91	0.53
1:B:18:GLY:H	1:B:170:ASN:HB3	1.72	0.53
1:A:180:TYR:N	1:A:180:TYR:HD1	2.07	0.53
1:A:30:ASN:HA	1:A:172:PHE:CD2	2.45	0.52
1:A:82:GLU:O	1:A:85:LYS:HB3	2.09	0.52
1:C:180:TYR:N	1:C:180:TYR:CD1	2.76	0.52
1:A:88:ARG:HD2	1:A:88:ARG:O	2.10	0.52
1:C:38:TYR:CD2	1:C:63:LEU:HG	2.45	0.52
1:C:65:MET:O	1:C:65:MET:HG2	2.09	0.52
1:B:19:GLN:HB2	1:B:170:ASN:HB2	1.91	0.52
1:A:7:ARG:NH1	1:A:109:ALA:HA	2.23	0.52
1:C:59:PHE:HB2	1:C:83:LEU:CD2	2.39	0.52
1:B:157:LYS:O	1:B:161:ILE:HG13	2.10	0.52
1:A:18:GLY:H	1:A:170:ASN:HB3	1.74	0.51
1:C:19:GLN:HB2	1:C:170:ASN:HB2	1.92	0.51
1:C:98:LEU:HD23	1:C:114:THR:HA	1.92	0.51
1:C:43:ALA:HA	1:C:100:ALA:O	2.10	0.51
1:C:13:VAL:HG13	1:C:177:GLU:HB3	1.92	0.51
1:B:28:LYS:HE3	1:B:30:ASN:CG	2.31	0.51
1:A:146:GLU:O	1:A:147:LEU:HB2	2.11	0.50
1:A:178:LEU:O	1:A:178:LEU:HD12	2.12	0.50
1:B:38:TYR:HB2	1:B:63:LEU:HD23	1.94	0.50
1:A:167:ILE:HD13	1:A:168:TYR:CD1	2.46	0.50
1:A:38:TYR:HB2	1:A:63:LEU:HD23	1.94	0.50
1:A:28:LYS:HE3	1:A:30:ASN:ND2	2.26	0.49
1:B:1:THR:HA	1:B:33:LYS:HZ3	1.77	0.49
1:C:38:TYR:HB2	1:C:63:LEU:HD23	1.94	0.49
1:A:17:ASP:O	1:A:33:LYS:HD2	2.13	0.49
1:B:7:ARG:NH1	1:B:109:ALA:HA	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PHE:CD1	1:A:83:LEU:HD22	2.47	0.49
1:B:92:ARG:O	1:B:93(B):ARG:HB3	2.12	0.49
1:C:111:LEU:N	1:C:111:LEU:HD12	2.27	0.49
1:C:85:LYS:HB2	1:C:85:LYS:HZ2	1.74	0.48
1:B:18:GLY:O	1:B:29:GLY:HA2	2.13	0.48
1:C:180:TYR:N	1:C:180:TYR:HD1	2.11	0.48
1:B:126:ALA:CB	1:B:135:GLN:HB2	2.43	0.48
1:A:76:LEU:HD21	1:A:111:LEU:HD11	1.96	0.48
1:A:43:ALA:HA	1:A:100:ALA:O	2.13	0.48
1:A:102:ALA:HA	1:A:109:ALA:O	2.13	0.48
1:C:14:ILE:HD12	1:C:42:ILE:HB	1.95	0.48
1:B:76:LEU:HD22	1:B:103:ASP:OD1	2.14	0.48
1:A:19:GLN:CB	1:A:170:ASN:HB2	2.44	0.48
1:A:13:VAL:HG13	1:A:177:GLU:HB3	1.94	0.48
1:C:38:TYR:HD2	1:C:63:LEU:HG	1.78	0.48
1:A:136:ALA:O	1:A:139:ARG:HB3	2.14	0.48
1:C:18:GLY:H	1:C:170:ASN:CB	2.27	0.48
1:B:59:PHE:HE1	1:B:80:ALA:N	2.12	0.48
1:B:5:SER:HB3	1:B:125:ILE:HB	1.95	0.48
1:B:38:TYR:CD2	1:B:63:LEU:HG	2.48	0.48
1:B:178:LEU:HD12	1:B:178:LEU:O	2.14	0.48
1:A:51:ASP:HA	1:A:95:LEU:HD23	1.96	0.48
1:A:103:ASP:OD1	1:A:105:THR:HB	2.14	0.48
1:B:111:LEU:H	1:B:111:LEU:HD12	1.79	0.47
1:C:167:ILE:N	1:C:167:ILE:HD12	2.30	0.47
1:B:20:ALA:HB3	1:B:28:LYS:O	2.14	0.47
1:C:59:PHE:CD1	1:C:83:LEU:HD22	2.50	0.47
1:B:98:LEU:HD23	1:B:114:THR:HA	1.96	0.47
1:A:93(B):ARG:O	1:A:93(B):ARG:HG3	2.14	0.47
1:B:93(B):ARG:O	1:B:93(B):ARG:HD3	2.14	0.47
1:C:126:ALA:CB	1:C:135:GLN:HB2	2.44	0.47
1:C:157:LYS:O	1:C:160:ASP:HB2	2.15	0.47
1:C:60:GLU:HA	1:C:63:LEU:HB2	1.96	0.47
1:C:161:ILE:O	1:C:164:ASP:HB2	2.15	0.47
1:B:59:PHE:CD1	1:B:83:LEU:HD22	2.50	0.46
1:A:60:GLU:HA	1:A:63:LEU:HB2	1.98	0.46
1:C:167:ILE:HD12	1:C:168:TYR:H	1.81	0.46
1:B:1:THR:HA	1:B:33:LYS:NZ	2.29	0.46
1:A:28:LYS:HE3	1:A:30:ASN:OD1	2.16	0.46
1:A:2:THR:C	1:A:3:ILE:HG13	2.36	0.46
1:A:58:LEU:O	1:A:61:ARG:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ALA:HB3	1:C:28:LYS:O	2.17	0.45
1:C:28:LYS:HE2	1:C:31:VAL:HG12	1.96	0.45
1:B:60:GLU:HA	1:B:63:LEU:HB2	1.96	0.45
1:C:38:TYR:HB2	1:C:63:LEU:CD2	2.47	0.45
1:B:167:ILE:HD12	1:B:167:ILE:N	2.31	0.45
1:B:55:LEU:HD21	1:B:87:TRP:CE2	2.51	0.45
1:A:167:ILE:N	1:A:167:ILE:HD12	2.31	0.45
1:B:103:ASP:OD1	1:B:105:THR:HB	2.17	0.45
1:A:157:LYS:O	1:A:161:ILE:HG13	2.17	0.45
1:A:87:TRP:C	1:A:89:THR:H	2.21	0.45
1:C:5:SER:HB3	1:C:125:ILE:HB	1.98	0.45
1:C:85:LYS:NZ	1:C:85:LYS:CB	2.75	0.45
1:A:78:LYS:O	1:A:79:ALA:C	2.55	0.45
1:C:12(A):ASN:C	1:C:124:LEU:N	2.71	0.45
1:C:31:VAL:CG2	1:C:33:LYS:HE3	2.47	0.44
1:B:38:TYR:HD2	1:B:63:LEU:HG	1.82	0.44
1:B:17:ASP:HA	1:B:172:PHE:O	2.16	0.44
1:B:19:GLN:CB	1:B:170:ASN:HB2	2.47	0.44
1:B:167:ILE:HD13	1:B:168:TYR:CD1	2.53	0.44
1:B:101:VAL:O	1:B:110:SER:HA	2.17	0.44
1:C:84:ALA:HB2	1:C:119:VAL:HG22	2.00	0.44
1:B:14:ILE:HD12	1:B:42:ILE:HB	1.99	0.44
1:A:33:LYS:HA	1:A:45:PHE:CE1	2.52	0.44
1:B:10:GLY:HA3	1:B:181:LYS:HG2	1.98	0.44
1:B:93(B):ARG:C	1:B:93(B):ARG:HD3	2.38	0.44
1:B:59:PHE:HE1	1:B:80:ALA:CA	2.31	0.44
1:C:133:TYR:O	1:C:136:ALA:HB3	2.17	0.44
1:A:184:PHE:N	1:A:184:PHE:CD1	2.82	0.44
1:A:51:ASP:O	1:A:55:LEU:HD12	2.17	0.43
1:A:42:ILE:HD11	1:A:178:LEU:HG	2.00	0.43
1:C:59:PHE:CB	1:C:83:LEU:HD22	2.45	0.43
1:A:181:LYS:HE3	1:A:181:LYS:HB2	1.69	0.43
1:A:7:ARG:HH22	1:A:109:ALA:C	2.22	0.43
1:A:38:TYR:CD2	1:A:63:LEU:HG	2.54	0.43
1:B:19:GLN:H	1:B:170:ASN:HB2	1.84	0.43
1:A:12(A):ASN:C	1:A:124:LEU:N	2.72	0.43
1:C:170:ASN:O	1:C:171:HIS:CB	2.62	0.43
1:C:18:GLY:O	1:C:29:GLY:HA2	2.19	0.43
1:C:67:GLN:CG	1:C:74:GLY:N	2.70	0.43
1:C:7:ARG:NH1	1:C:109:ALA:HA	2.29	0.43
1:C:136:ALA:O	1:C:139:ARG:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ASP:O	1:B:55:LEU:HD12	2.18	0.43
1:C:101:VAL:O	1:C:110:SER:HA	2.18	0.42
1:C:59:PHE:HE1	1:C:80:ALA:CA	2.32	0.42
1:A:76:LEU:HD22	1:A:103:ASP:OD1	2.20	0.42
1:C:78:LYS:O	1:C:79:ALA:C	2.57	0.42
1:B:30:ASN:HA	1:B:172:PHE:CD2	2.54	0.42
1:A:59:PHE:CB	1:A:83:LEU:HD22	2.42	0.42
1:C:84:ALA:CB	1:C:119:VAL:HG22	2.50	0.42
1:C:59:PHE:HE1	1:C:80:ALA:HA	1.85	0.42
1:B:87:TRP:C	1:B:89:THR:H	2.22	0.42
1:C:19:GLN:CB	1:C:170:ASN:HB2	2.50	0.41
1:C:59:PHE:CE1	1:C:80:ALA:HA	2.54	0.41
1:A:163:GLY:HA2	1:A:169:THR:HB	2.01	0.41
1:C:59:PHE:HE1	1:C:80:ALA:N	2.18	0.41
1:C:141:LEU:C	1:C:145:THR:HG22	2.41	0.41
1:C:76:LEU:O	1:C:77:VAL:C	2.59	0.41
1:A:4:VAL:O	1:A:14:ILE:HA	2.20	0.41
1:A:146:GLU:O	1:A:147:LEU:CB	2.67	0.41
1:B:18:GLY:H	1:B:170:ASN:CB	2.33	0.41
1:C:66:HIS:O	1:C:67:GLN:HB3	2.20	0.41
1:A:22:LEU:O	1:A:24:ASN:N	2.53	0.41
1:B:59:PHE:CE1	1:B:80:ALA:HA	2.55	0.41
1:B:88:ARG:CG	1:B:116:ASN:O	2.68	0.41
1:A:28:LYS:CG	1:A:29:GLY:N	2.83	0.41
1:B:28:LYS:CG	1:B:29:GLY:N	2.83	0.41
1:C:157:LYS:O	1:C:161:ILE:HG13	2.20	0.41
1:B:31:VAL:HG23	1:B:33:LYS:HG3	2.02	0.41
1:A:92:ARG:O	1:A:93(B):ARG:HB3	2.21	0.41
1:A:126:ALA:CB	1:A:135:GLN:HB2	2.50	0.41
1:B:20:ALA:HB3	1:B:28:LYS:H	1.86	0.41
1:B:90:ASP:OD1	1:B:93:MET:HB3	2.21	0.41
1:C:31:VAL:HG23	1:C:33:LYS:HG3	2.02	0.41
1:A:38:TYR:HD1	1:A:38:TYR:O	2.04	0.41
1:C:103:ASP:OD1	1:C:105:THR:HB	2.21	0.41
1:B:38:TYR:HB2	1:B:63:LEU:CD2	2.50	0.41
1:A:177:GLU:O	1:A:177:GLU:HG3	2.21	0.40
1:B:177:GLU:HG3	1:B:177:GLU:O	2.21	0.40
1:B:28:LYS:HE2	1:B:31:VAL:HG12	2.02	0.40
1:C:4:VAL:O	1:C:14:ILE:HA	2.21	0.40
1:C:99:LEU:HD12	1:C:99:LEU:N	2.36	0.40
1:B:12(A):ASN:C	1:B:124:LEU:N	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	178/183 (97%)	123 (69%)	45 (25%)	10 (6%)	2	29
1	B	179/183 (98%)	123 (69%)	46 (26%)	10 (6%)	2	29
1	C	179/183 (98%)	123 (69%)	44 (25%)	12 (7%)	1	25
All	All	536/549 (98%)	369 (69%)	135 (25%)	32 (6%)	2	27

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	49	THR
1	C	181	LYS
1	A	49	THR
1	A	105	THR
1	A	171	HIS
1	B	105	THR
1	C	49	THR
1	C	105	THR
1	C	171	HIS
1	A	50	ALA
1	A	12(A)	ASN
1	B	12(A)	ASN
1	B	171	HIS
1	C	50	ALA
1	C	12(A)	ASN
1	A	30	ASN
1	A	67	GLN
1	B	30	ASN
1	B	67	GLN
1	C	67	GLN
1	C	77	VAL

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Mol	Chain	Res	Type
1	C	85	LYS
1	B	50	ALA
1	C	182	ALA
1	C	184	PHE
1	A	38	TYR
1	A	77	VAL
1	B	38	TYR
1	B	77	VAL
1	B	23	GLY
1	A	23	GLY
1	C	23	GLY

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	141/144 (98%)	114 (81%)	27 (19%)	2	13
1	B	139/144 (96%)	115 (83%)	24 (17%)	2	18
1	C	136/144 (94%)	110 (81%)	26 (19%)	2	13
All	All	416/432 (96%)	339 (82%)	77 (18%)	2	15

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	8	ARG
1	A	21	THR
1	A	22	LEU
1	A	25	THR
1	A	32	LYS
1	A	42	ILE
1	A	49	THR
1	A	54	THR
1	A	55	LEU
1	A	64	GLU

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Mol	Chain	Res	Type
1	A	75	HIS
1	A	88	ARG
1	A	92	ARG
1	A	111	LEU
1	A	118	ASP
1	A	12(A)	ASN
1	A	129	SER
1	A	132	PRO
1	A	141	LEU
1	A	160	ASP
1	A	167	ILE
1	A	177	GLU
1	A	180	TYR
1	A	184	PHE
1	A	185	HIS
1	A	187	HIS
1	B	4	VAL
1	B	21	THR
1	B	22	LEU
1	B	25	THR
1	B	32	LYS
1	B	42	ILE
1	B	49	THR
1	B	54	THR
1	B	55	LEU
1	B	75	HIS
1	B	78	LYS
1	B	85	LYS
1	B	92	ARG
1	B	93(B)	ARG
1	B	111	LEU
1	B	118	ASP
1	B	121	GLN
1	B	12(A)	ASN
1	B	129	SER
1	B	141	LEU
1	B	160	ASP
1	B	167	ILE
1	B	177	GLU
1	B	180	TYR
1	C	4	VAL
1	C	21	THR

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Mol	Chain	Res	Type
1	C	22	LEU
1	C	25	THR
1	C	32	LYS
1	C	42	ILE
1	C	49	THR
1	C	54	THR
1	C	55	LEU
1	C	61	ARG
1	C	67	GLN
1	C	75	HIS
1	C	78	LYS
1	C	88	ARG
1	C	92	ARG
1	C	93(B)	ARG
1	C	111	LEU
1	C	118	ASP
1	C	12(A)	ASN
1	C	129	SER
1	C	132	PRO
1	C	141	LEU
1	C	160	ASP
1	C	167	ILE
1	C	177	GLU
1	C	180	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	12(A)	ASN
1	B	116	ASN
1	B	121	GLN
1	B	12(A)	ASN
1	B	185	HIS
1	C	67	GLN
1	C	116	ASN
1	C	12(A)	ASN

5.3.3　RNA (i)

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.