Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:28 AM GMT

PDB ID	:	2AMP
Title	:	Crystal Structure Of Porcine Transmissible Gastroenteritis Virus Mpro in Complex with an Inhibitor N1
Authors	:	Yang, H.; Xue, X.; Yang, K.; Zhao, Q.; Bartlam, M.; Rao, Z.
Deposited on	:	2005-08-10
Resolution	:	2.70 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

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

The reported resolution of this entry is 2.70 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
Rfree		0.271
Clashscore		40
Ramachandran outliers		4.7%
Sidechain outliers		9.0%
RSRZ outliers		1.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
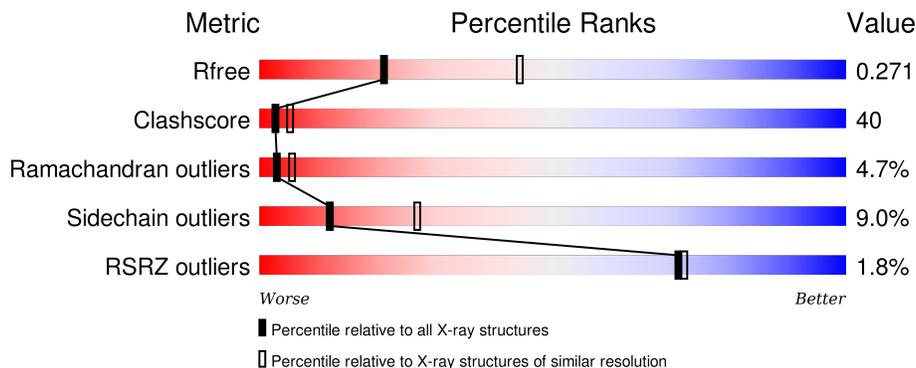
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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.

Mol	Chain	Length	Quality of chain
1	A	304	% 49% 43% 7% ·
1	B	304	2% 35% 51% 11% · ·

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	I12	A	1001	X	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4772 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 3C-like proteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2297	1448	390	443	16			
1	B	299	Total	C	N	O	S	0	0	0
			2297	1448	390	443	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP Q9IW06
A	0	SER	-	CLONING ARTIFACT	UNP Q9IW06
B	-1	GLY	-	CLONING ARTIFACT	UNP Q9IW06
B	0	SER	-	CLONING ARTIFACT	UNP Q9IW06

- Molecule 2 is N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]-L-ALANYL-L-VALYL-N 1 -((1S)-4-ETHOXY-4-OXO-1-{[(3S)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)- L-LEUCINAMIDE (three-letter code: I12) (formula: $C_{30}H_{46}N_6O_8$).
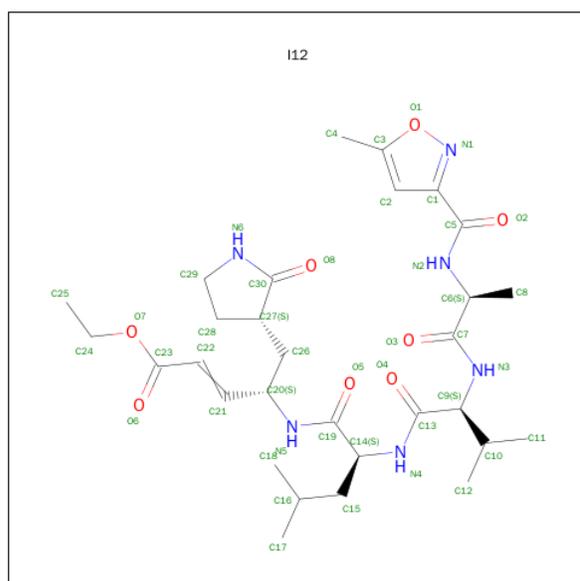
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 44	C 30	N 6	O 8	0	0
2	B	1	Total 44	C 30	N 6	O 8	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total 53	O 53	0	0
3	B	37	Total 37	O 37	0	0

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.

- Molecule 1: 3C-like proteinase
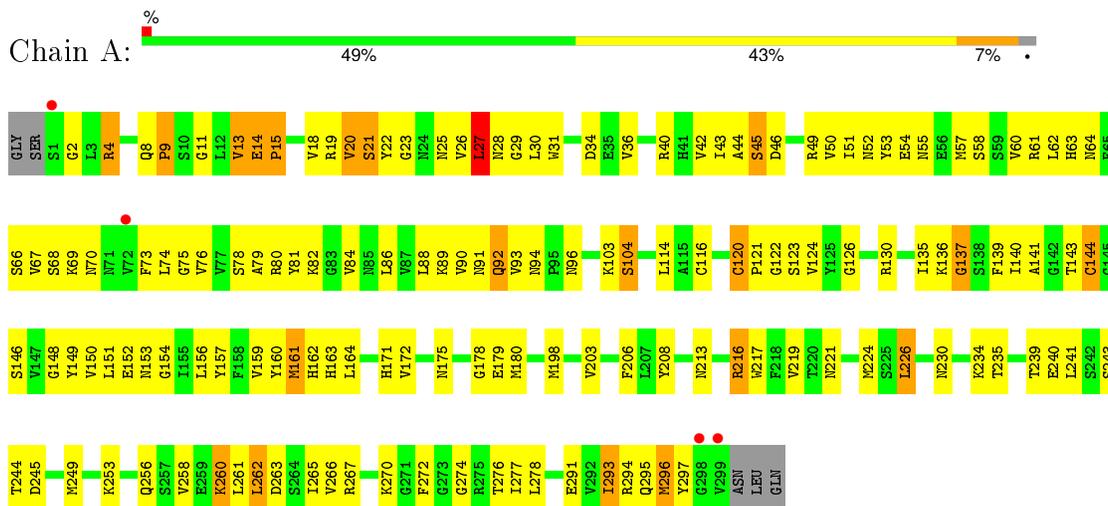
- Molecule 1: 3C-like proteinase
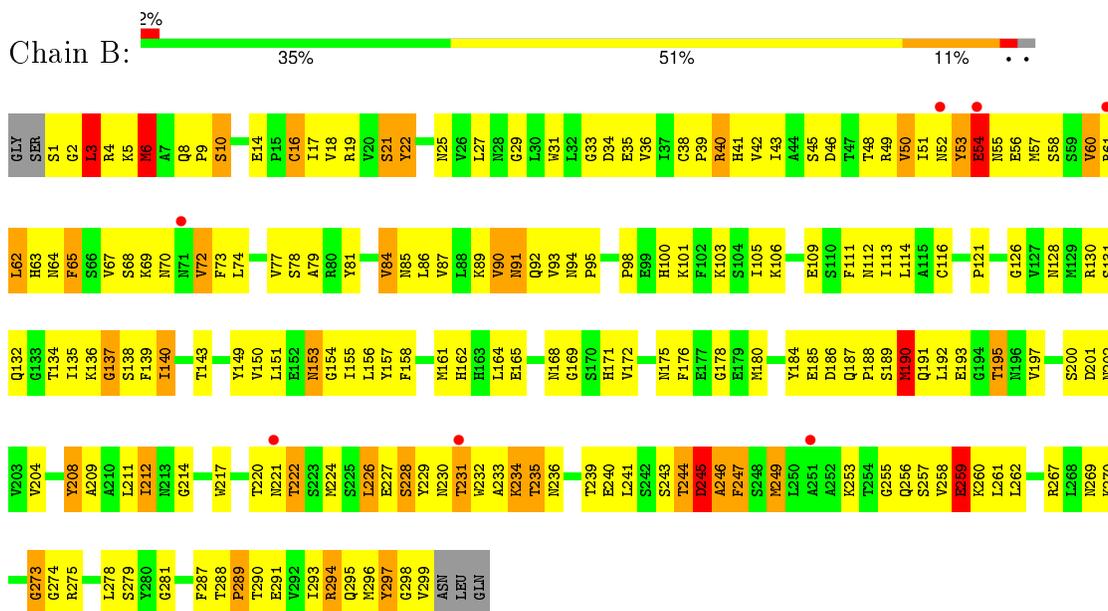
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.59Å 90.24Å 110.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 27.59 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.70) 94.6 (27.59-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.27 (at 2.68Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.271 0.233 , 0.271	Depositor DCC
R_{free} test set	868 reflections (4.86%)	DCC
Wilson B-factor (Å^2)	43.5	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.42, <L^2> = 0.24$	Xtriage
Outliers	0 of 18110 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4772	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:
I12

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	1.03	22/2343 (0.9%)	0.83	4/3171 (0.1%)
1	B	0.81	6/2343 (0.3%)	0.80	2/3171 (0.1%)
All	All	0.92	28/4686 (0.6%)	0.82	6/6342 (0.1%)

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

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	6	MET	SD-CE	-11.46	1.13	1.77
1	A	161	MET	C-N	-11.20	1.08	1.34
1	B	190	MET	SD-CE	10.94	2.39	1.77
1	A	13	VAL	CB-CG1	-9.24	1.33	1.52
1	B	6	MET	CG-SD	-9.04	1.57	1.81
1	A	20	VAL	CB-CG2	-8.86	1.34	1.52
1	A	22	TYR	CE1-CZ	-8.40	1.27	1.38
1	A	14	GLU	CD-OE1	-8.30	1.16	1.25
1	A	14	GLU	CD-OE2	-8.30	1.16	1.25
1	A	162	HIS	C-N	7.59	1.51	1.34
1	A	13	VAL	CB-CG2	-7.51	1.37	1.52
1	A	26	VAL	CB-CG1	-7.07	1.38	1.52
1	B	9	PRO	CB-CG	-6.46	1.17	1.50
1	A	262	LEU	C-N	6.20	1.48	1.34
1	A	22	TYR	CE2-CZ	-6.17	1.30	1.38
1	A	22	TYR	CD2-CE2	-6.16	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	5	LYS	CE-NZ	-6.13	1.33	1.49
1	A	15	PRO	CB-CG	-6.03	1.19	1.50
1	A	22	TYR	CG-CD2	-5.81	1.31	1.39
1	A	26	VAL	CB-CG2	-5.63	1.41	1.52
1	A	29	GLY	C-O	-5.62	1.14	1.23
1	B	5	LYS	CD-CE	-5.52	1.37	1.51
1	A	144	CYS	CB-SG	-5.40	1.73	1.81
1	A	18	VAL	CB-CG2	-5.29	1.41	1.52
1	A	27	LEU	CG-CD1	-5.29	1.32	1.51
1	A	20	VAL	CB-CG1	-5.26	1.41	1.52
1	A	15	PRO	CA-C	-5.17	1.42	1.52
1	A	4	ARG	C-N	-5.05	1.22	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	LEU	CA-CB-CG	7.35	132.20	115.30
1	A	82	LYS	N-CA-C	-6.43	93.65	111.00
1	B	190	MET	CG-SD-CE	6.32	110.31	100.20
1	A	27	LEU	CA-CB-CG	5.88	128.84	115.30
1	A	4	ARG	O-C-N	-5.17	114.42	122.70
1	A	137	GLY	N-CA-C	-5.05	100.46	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2	GLY	Peptide

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	2297	0	2245	153	1
1	B	2297	0	2246	225	0
2	A	44	0	42	2	0
2	B	44	0	41	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	53	0	0	3	0
3	B	37	0	0	6	0
All	All	4772	0	4574	374	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 40.

All (374) 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:B:6:MET:CE	1:B:6:MET:CG	2.00	1.37
1:B:6:MET:CE	1:B:6:MET:SD	1.13	1.23
1:B:6:MET:HE1	1:B:6:MET:SD	1.72	1.13
1:B:190:MET:SD	1:B:190:MET:CE	2.39	1.11
1:B:6:MET:HE2	1:B:6:MET:SD	1.72	1.10
1:B:6:MET:HE3	1:B:6:MET:SD	1.72	1.06
1:A:140:ILE:HG22	1:A:141:ALA:H	1.18	1.03
1:B:6:MET:HE2	1:B:6:MET:HG2	1.39	1.02
1:A:140:ILE:HG22	1:A:141:ALA:N	1.74	0.99
1:B:153:ASN:O	1:B:155:ILE:N	1.96	0.99
1:A:78:SER:HB3	1:A:89:LYS:HB2	1.42	0.98
1:A:140:ILE:CG2	1:A:141:ALA:H	1.77	0.97
1:A:140:ILE:HD11	1:B:295:GLN:O	1.66	0.94
1:B:224:MET:HE2	1:B:228:SER:HB3	1.50	0.93
1:B:226:LEU:HD21	1:B:241:LEU:O	1.72	0.90
1:B:257:SER:H	1:B:260:LYS:HE3	1.34	0.90
1:B:245:ASP:O	1:B:247:PHE:N	2.09	0.86
1:B:77:VAL:CG2	1:B:78:SER:H	1.89	0.86
1:B:53:TYR:O	1:B:55:ASN:N	2.09	0.85
1:A:253:LYS:HE2	1:A:297:TYR:CB	2.06	0.85
1:A:253:LYS:HE2	1:A:297:TYR:HB2	1.56	0.84
1:A:13:VAL:O	1:A:13:VAL:HG12	1.76	0.83
1:A:253:LYS:CE	1:A:297:TYR:HB2	2.09	0.82
1:B:10:SER:OG	1:B:14:GLU:OE2	1.97	0.82
1:B:190:MET:HE2	1:B:192:LEU:HD23	1.63	0.80
1:B:40:ARG:HD3	1:B:84:VAL:HA	1.64	0.80
1:A:114:LEU:HD21	1:A:121:PRO:HB3	1.64	0.80
1:B:77:VAL:HG23	1:B:78:SER:N	1.96	0.79
1:A:296:MET:HA	1:A:296:MET:HE2	1.65	0.79
1:A:103:LYS:O	1:A:159:VAL:HG12	1.82	0.78
1:A:4:ARG:NH2	1:B:136:LYS:O	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:MET:O	1:A:239:THR:HG23	1.84	0.77
1:B:190:MET:CE	1:B:192:LEU:CD2	2.63	0.77
1:A:136:LYS:O	1:B:4:ARG:NH1	2.17	0.77
1:B:190:MET:CE	1:B:192:LEU:HD23	2.16	0.76
1:A:140:ILE:CG2	1:A:141:ALA:N	2.41	0.76
1:B:77:VAL:HG23	1:B:78:SER:H	1.51	0.75
1:B:130:ARG:HG3	1:B:134:THR:O	1.85	0.75
1:B:235:THR:HG22	1:B:236:ASN:OD1	1.87	0.74
1:B:253:LYS:NZ	1:B:297:TYR:HB2	2.04	0.73
1:B:77:VAL:CG2	1:B:78:SER:N	2.48	0.73
1:A:139:PHE:HB2	1:A:171:HIS:CD2	2.23	0.73
1:B:6:MET:HE2	1:B:6:MET:CG	1.83	0.72
1:A:75:GLY:CA	1:A:91:ASN:OD1	2.37	0.72
1:A:226:LEU:HD22	1:A:230:ASN:ND2	2.04	0.71
1:A:14:GLU:N	1:A:15:PRO:CD	2.50	0.71
1:B:101:LYS:O	1:B:157:TYR:HA	1.90	0.71
1:B:184:TYR:OH	1:B:193:GLU:HA	1.91	0.71
1:B:269:ASN:HB3	3:B:2035:HOH:O	1.90	0.70
1:B:31:TRP:CE2	1:B:94:ASN:HB2	2.26	0.70
1:A:175:ASN:HD21	1:A:179:GLU:HB2	1.57	0.69
1:B:190:MET:HE1	1:B:192:LEU:CD2	2.22	0.69
1:A:226:LEU:HD22	1:A:230:ASN:HD21	1.58	0.69
1:A:84:VAL:HG21	1:A:180:MET:HE2	1.74	0.69
1:B:296:MET:O	1:B:298:GLY:N	2.27	0.68
1:A:14:GLU:H	1:A:15:PRO:HD2	1.58	0.68
1:A:296:MET:CE	1:A:296:MET:HA	2.22	0.68
1:A:148:GLY:HA3	1:A:160:TYR:HB3	1.76	0.68
1:B:61:ARG:HB2	1:B:64:ASN:HD22	1.58	0.68
1:A:163:HIS:O	2:A:1001:I12:H20	1.94	0.68
1:A:75:GLY:N	1:A:91:ASN:OD1	2.26	0.67
1:B:151:LEU:CD2	1:B:156:LEU:HA	2.23	0.67
1:B:150:VAL:O	1:B:151:LEU:HD23	1.93	0.67
1:B:200:SER:O	1:B:204:VAL:HG23	1.93	0.67
1:A:244:THR:HB	1:A:258:VAL:HG21	1.76	0.67
1:B:8:GLN:OE1	1:B:112:ASN:ND2	2.27	0.67
1:B:91:ASN:C	1:B:91:ASN:HD22	1.97	0.67
1:A:150:VAL:HG22	1:A:157:TYR:HB2	1.77	0.67
1:A:208:TYR:CE2	1:A:261:LEU:HD11	2.30	0.67
1:B:17:ILE:HD11	1:B:114:LEU:HD23	1.76	0.66
1:B:258:VAL:O	1:B:261:LEU:N	2.20	0.66
1:A:44:ALA:CB	1:A:51:ILE:HD13	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ARG:HH11	1:A:294:ARG:HG3	1.60	0.66
1:B:151:LEU:HD21	1:B:156:LEU:HD13	1.78	0.65
1:B:287:PHE:HA	1:B:291:GLU:OE2	1.97	0.65
1:A:164:LEU:CD1	1:A:172:VAL:HB	2.26	0.65
1:A:75:GLY:HA3	1:A:91:ASN:OD1	1.95	0.65
1:A:14:GLU:N	1:A:15:PRO:HD2	2.12	0.65
1:A:31:TRP:CE2	1:A:94:ASN:HB2	2.32	0.65
1:A:34:ASP:OD2	1:A:89:LYS:HD3	1.97	0.64
1:A:208:TYR:CD2	1:A:261:LEU:HD11	2.32	0.64
1:B:16:CYS:O	1:B:31:TRP:N	2.30	0.64
2:B:2001:I12:H122	2:B:2001:I12:C7	2.28	0.64
1:B:84:VAL:HG12	1:B:186:ASP:OD1	1.98	0.63
1:A:15:PRO:HA	1:A:69:LYS:HE2	1.79	0.63
1:A:175:ASN:ND2	1:A:179:GLU:HB2	2.14	0.63
1:B:253:LYS:HZ2	1:B:297:TYR:HB2	1.63	0.63
1:B:77:VAL:HG22	1:B:89:LYS:CB	2.30	0.62
1:B:22:TYR:OH	1:B:60:VAL:HA	1.99	0.62
1:B:61:ARG:CB	1:B:64:ASN:HD22	2.13	0.62
1:B:17:ILE:HD13	1:B:116:CYS:SG	2.40	0.62
1:B:53:TYR:O	1:B:54:GLU:C	2.38	0.61
1:A:241:LEU:C	1:A:241:LEU:HD23	2.20	0.61
1:A:164:LEU:HD11	1:A:172:VAL:HB	1.82	0.61
1:B:244:THR:O	1:B:245:ASP:O	2.18	0.61
1:A:103:LYS:HG2	1:A:104:SER:N	2.15	0.61
1:A:14:GLU:H	1:A:15:PRO:CD	2.12	0.61
1:B:185:GLU:HG3	1:B:187:GLN:CG	2.30	0.60
1:A:80:ARG:O	1:A:86:LEU:HD12	2.01	0.60
1:A:203:VAL:HG12	1:A:265:ILE:HD11	1.82	0.60
1:A:140:ILE:HD12	3:B:2026:HOH:O	2.00	0.60
1:B:208:TYR:HE1	1:B:247:PHE:HB3	1.66	0.60
1:B:17:ILE:HD11	1:B:114:LEU:CD2	2.32	0.59
1:A:53:TYR:HB3	1:A:81:TYR:CZ	2.37	0.59
1:B:208:TYR:CE1	1:B:247:PHE:HB3	2.37	0.59
1:B:77:VAL:HG22	1:B:78:SER:H	1.66	0.59
1:B:38:CYS:HA	1:B:161:MET:SD	2.43	0.59
1:B:209:ALA:HA	1:B:212:ILE:HG13	1.83	0.59
1:B:61:ARG:HB2	1:B:64:ASN:ND2	2.17	0.59
1:A:13:VAL:O	1:A:13:VAL:CG1	2.43	0.59
1:A:44:ALA:HB1	1:A:51:ILE:HD13	1.85	0.59
1:B:31:TRP:HZ2	1:B:92:GLN:O	1.87	0.58
1:B:62:LEU:HD13	1:B:77:VAL:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:VAL:HG23	1:B:157:TYR:HB2	1.85	0.58
1:B:208:TYR:HA	1:B:211:LEU:HD12	1.86	0.58
1:B:243:SER:OG	1:B:245:ASP:HB2	2.04	0.58
1:A:60:VAL:C	1:A:61:ARG:HG2	2.24	0.57
1:B:151:LEU:HD23	1:B:156:LEU:HA	1.85	0.57
1:B:247:PHE:N	1:B:247:PHE:CD1	2.73	0.57
1:A:61:ARG:O	1:A:64:ASN:HB2	2.05	0.57
1:B:51:ILE:HD11	2:B:2001:I12:C18	2.35	0.56
1:B:278:LEU:O	1:B:279:SER:HB2	2.04	0.56
1:A:62:LEU:O	1:A:64:ASN:N	2.39	0.56
1:A:217:TRP:HZ2	1:A:277:ILE:HG13	1.70	0.56
1:B:190:MET:HE1	1:B:192:LEU:HD21	1.86	0.56
1:B:3:LEU:HD23	1:B:278:LEU:HD13	1.88	0.56
1:B:243:SER:C	1:B:245:ASP:H	2.08	0.56
1:B:51:ILE:HD11	2:B:2001:I12:H181	1.88	0.56
1:B:21:SER:HA	1:B:25:ASN:O	2.06	0.56
1:B:245:ASP:HB3	3:B:2030:HOH:O	2.04	0.56
1:B:204:VAL:HB	1:B:247:PHE:CE2	2.41	0.55
1:A:234:LYS:HZ2	1:A:240:GLU:HB2	1.71	0.55
1:B:220:THR:HG23	1:B:267:ARG:HH21	1.70	0.55
1:B:113:ILE:HD13	1:B:139:PHE:HZ	1.70	0.55
2:B:2001:I12:C12	2:B:2001:I12:C7	2.85	0.55
1:A:203:VAL:CG1	1:A:265:ILE:HD11	2.36	0.55
1:B:180:MET:HG2	1:B:184:TYR:O	2.06	0.55
1:A:272:PHE:CE2	1:A:277:ILE:HB	2.42	0.55
1:A:31:TRP:CD2	1:A:94:ASN:HB2	2.42	0.55
1:B:79:ALA:HA	1:B:87:VAL:O	2.07	0.55
1:A:42:VAL:HG13	1:A:43:ILE:N	2.22	0.55
1:A:94:ASN:OD1	1:A:96:ASN:N	2.37	0.55
1:A:274:GLY:HA2	1:B:273:GLY:O	2.08	0.55
1:A:19:ARG:NH1	1:A:21:SER:OG	2.40	0.54
1:A:84:VAL:HG21	1:A:180:MET:CE	2.37	0.54
1:B:8:GLN:HB2	1:B:112:ASN:ND2	2.22	0.54
1:B:288:THR:OG1	1:B:291:GLU:HG3	2.08	0.54
1:A:243:SER:OG	1:A:245:ASP:HB2	2.06	0.54
1:A:136:LYS:NZ	1:B:1:SER:O	2.40	0.54
1:B:72:VAL:O	1:B:72:VAL:HG12	2.08	0.54
1:B:185:GLU:HG3	1:B:187:GLN:HG2	1.88	0.54
1:A:20:VAL:HG22	1:A:67:VAL:HG22	1.88	0.54
1:B:31:TRP:CD2	1:B:94:ASN:HB2	2.43	0.54
1:B:49:ARG:O	1:B:50:VAL:C	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ARG:O	1:A:219:VAL:N	2.39	0.53
1:B:22:TYR:CD2	1:B:43:ILE:HA	2.43	0.53
1:A:2:GLY:HA2	1:A:213:ASN:ND2	2.23	0.53
1:A:53:TYR:HB3	1:A:81:TYR:OH	2.08	0.53
1:B:91:ASN:ND2	1:B:91:ASN:C	2.61	0.53
1:B:19:ARG:O	1:B:19:ARG:HG2	2.08	0.53
1:B:226:LEU:HD23	1:B:230:ASN:CG	2.29	0.53
1:A:42:VAL:HG13	1:A:43:ILE:HG13	1.89	0.53
1:B:208:TYR:O	1:B:212:ILE:HG13	2.08	0.53
1:B:113:ILE:HD13	1:B:139:PHE:CZ	2.44	0.53
1:B:153:ASN:C	1:B:155:ILE:H	2.11	0.53
1:B:165:GLU:OE1	1:B:171:HIS:NE2	2.42	0.53
1:B:16:CYS:SG	1:B:98:PRO:HD3	2.49	0.52
2:B:2001:I12:C7	2:B:2001:I12:N1	2.73	0.52
1:B:150:VAL:CG2	1:B:157:TYR:HB2	2.40	0.52
1:A:126:GLY:O	1:B:4:ARG:NH2	2.42	0.52
1:A:272:PHE:CZ	1:A:277:ILE:HD12	2.44	0.52
1:B:217:TRP:CZ3	1:B:275:ARG:HD2	2.45	0.52
1:A:79:ALA:HB2	1:A:88:LEU:CD2	2.39	0.52
1:B:299:VAL:HG13	3:B:2020:HOH:O	2.09	0.52
1:B:48:THR:O	1:B:49:ARG:HG3	2.09	0.52
1:B:22:TYR:CZ	1:B:60:VAL:HG23	2.45	0.52
1:B:36:VAL:HG23	1:B:90:VAL:CG2	2.40	0.52
1:B:74:LEU:CD2	1:B:92:GLN:NE2	2.73	0.52
1:A:103:LYS:NZ	1:A:152:GLU:OE1	2.42	0.52
1:B:269:ASN:O	1:B:270:LYS:HG2	2.10	0.52
1:B:74:LEU:HD22	1:B:92:GLN:HE21	1.75	0.52
1:B:235:THR:CG2	1:B:236:ASN:OD1	2.58	0.51
1:B:67:VAL:O	1:B:73:PHE:HD1	1.93	0.51
1:A:14:GLU:CB	1:A:15:PRO:HD3	2.41	0.51
1:A:30:LEU:O	1:A:36:VAL:HA	2.10	0.51
1:B:62:LEU:HD23	1:B:65:PHE:CD1	2.45	0.51
1:B:40:ARG:O	1:B:42:VAL:N	2.44	0.51
1:B:162:HIS:NE2	2:B:2001:I12:O8	2.40	0.51
1:B:77:VAL:HG22	1:B:89:LYS:O	2.11	0.51
1:B:269:ASN:C	1:B:270:LYS:HG2	2.31	0.51
1:A:62:LEU:C	1:A:64:ASN:H	2.13	0.51
1:B:86:LEU:HD12	1:B:87:VAL:N	2.26	0.51
1:B:39:PRO:HD3	1:B:161:MET:SD	2.51	0.51
1:B:257:SER:N	1:B:260:LYS:HE3	2.15	0.51
1:A:206:PHE:CZ	1:A:277:ILE:HG22	2.46	0.50

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:SER:HB3	1:A:73:PHE:HA	1.94	0.50
1:B:40:ARG:HG3	1:B:53:TYR:CE2	2.46	0.50
1:B:105:ILE:HG22	1:B:106:LYS:O	2.12	0.50
1:B:3:LEU:HG	1:B:287:PHE:CE2	2.46	0.50
1:A:43:ILE:HD11	1:A:86:LEU:HD21	1.93	0.50
1:A:49:ARG:HG2	1:A:49:ARG:HH11	1.76	0.50
1:B:77:VAL:HG22	1:B:89:LYS:HB2	1.94	0.49
1:B:60:VAL:HG22	1:B:60:VAL:O	2.12	0.49
1:A:53:TYR:HB3	1:A:81:TYR:CE1	2.46	0.49
1:B:273:GLY:HA3	1:B:275:ARG:HH21	1.76	0.49
1:B:230:ASN:O	1:B:233:ALA:HB3	2.12	0.49
1:A:31:TRP:CZ2	1:A:94:ASN:HA	2.48	0.49
1:A:103:LYS:CG	1:A:104:SER:N	2.76	0.49
1:B:289:PRO:O	1:B:293:ILE:HG13	2.12	0.49
1:A:69:LYS:O	1:A:70:ASN:HB2	2.12	0.49
1:A:79:ALA:HB2	1:A:88:LEU:HD23	1.95	0.49
1:A:230:ASN:O	1:A:234:LYS:HG3	2.12	0.49
1:A:258:VAL:O	1:A:262:LEU:HG	2.12	0.49
1:A:216:ARG:O	1:A:217:TRP:C	2.51	0.49
1:A:76:VAL:CG1	1:A:88:LEU:HD22	2.42	0.49
1:B:226:LEU:HD23	1:B:230:ASN:OD1	2.13	0.49
1:B:241:LEU:HD11	1:B:262:LEU:HD21	1.95	0.49
1:B:151:LEU:HA	1:B:155:ILE:O	2.13	0.48
1:A:234:LYS:NZ	1:A:240:GLU:HB2	2.27	0.48
1:A:164:LEU:HD12	1:A:172:VAL:HB	1.94	0.48
1:B:217:TRP:CH2	1:B:275:ARG:HB2	2.49	0.48
1:B:158:PHE:HB3	1:B:176:PHE:CE1	2.48	0.48
1:B:226:LEU:HD23	1:B:230:ASN:ND2	2.28	0.48
1:B:77:VAL:HG22	1:B:89:LYS:HB3	1.95	0.48
1:B:234:LYS:HE2	1:B:240:GLU:OE1	2.14	0.48
1:B:52:ASN:O	1:B:56:GLU:HG2	2.14	0.48
1:B:228:SER:O	1:B:229:TYR:C	2.52	0.48
1:B:134:THR:HG22	1:B:172:VAL:HG22	1.95	0.48
1:B:294:ARG:HG3	1:B:299:VAL:HG23	1.95	0.48
1:A:263:ASP:OD1	1:A:267:ARG:NH1	2.47	0.48
1:A:40:ARG:HA	1:A:86:LEU:HB2	1.96	0.48
1:A:164:LEU:C	1:A:164:LEU:HD12	2.34	0.48
1:A:216:ARG:NH2	1:A:256:GLN:HE21	2.12	0.48
1:A:122:GLY:O	1:A:123:SER:HB3	2.13	0.47
1:B:209:ALA:CA	1:B:212:ILE:HG13	2.44	0.47
1:B:188:PRO:HA	2:B:2001:I12:O3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LYS:HD2	1:B:157:TYR:CD2	2.50	0.47
1:A:224:MET:SD	1:A:266:VAL:HG21	2.54	0.47
1:A:291:GLU:O	1:A:295:GLN:HB2	2.14	0.47
1:A:9:PRO:HB3	1:B:14:GLU:CD	2.35	0.47
1:B:73:PHE:O	1:B:74:LEU:HD23	2.14	0.47
1:B:168:ASN:OD1	1:B:169:GLY:N	2.47	0.47
1:B:100:HIS:O	1:B:101:LYS:HG3	2.15	0.47
1:B:77:VAL:CG2	1:B:89:LYS:HB3	2.44	0.47
1:B:296:MET:HA	1:B:296:MET:HE2	1.96	0.47
1:B:140:ILE:HA	2:B:2001:I12:H292	1.96	0.47
1:B:114:LEU:HD11	1:B:121:PRO:HB3	1.97	0.47
1:A:45:SER:OG	1:A:46:ASP:N	2.45	0.47
1:B:291:GLU:O	1:B:295:GLN:HB2	2.15	0.47
1:A:90:VAL:HG23	1:A:92:GLN:H	1.80	0.47
1:B:6:MET:CE	1:B:6:MET:HG2	2.00	0.47
1:A:73:PHE:O	1:A:74:LEU:HD23	2.15	0.47
1:B:151:LEU:HD22	1:B:156:LEU:HA	1.94	0.46
1:B:53:TYR:O	1:B:56:GLU:N	2.47	0.46
1:B:253:LYS:HZ1	1:B:297:TYR:HB2	1.78	0.46
1:B:175:ASN:OD1	1:B:175:ASN:C	2.52	0.46
1:A:62:LEU:HD23	1:A:62:LEU:N	2.30	0.46
1:B:132:GLN:HG2	3:B:2002:HOH:O	2.15	0.46
1:B:224:MET:HG2	1:B:229:TYR:H	1.81	0.46
1:B:296:MET:HA	1:B:296:MET:CE	2.45	0.46
1:A:40:ARG:HG2	1:A:84:VAL:O	2.15	0.46
1:A:62:LEU:C	1:A:64:ASN:N	2.68	0.46
1:B:294:ARG:CZ	1:B:299:VAL:HG21	2.46	0.46
1:A:42:VAL:CG1	1:A:43:ILE:N	2.79	0.46
1:B:112:ASN:HA	1:B:126:GLY:HA2	1.98	0.46
1:A:51:ILE:HG22	1:A:52:ASN:N	2.29	0.46
1:A:216:ARG:NH2	1:A:256:GLN:NE2	2.64	0.46
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.76	0.46
1:A:76:VAL:HG13	1:A:88:LEU:HD22	1.98	0.46
1:B:149:TYR:N	1:B:149:TYR:CD2	2.84	0.46
1:B:31:TRP:CD1	1:B:36:VAL:HG22	2.52	0.45
1:B:51:ILE:CD1	2:B:2001:I12:H181	2.46	0.45
1:B:243:SER:C	1:B:245:ASP:N	2.69	0.45
1:B:57:MET:O	1:B:60:VAL:HG12	2.17	0.45
1:A:55:ASN:O	1:A:58:SER:HB2	2.17	0.45
1:A:226:LEU:CD2	1:A:230:ASN:HD21	2.28	0.45
1:B:184:TYR:HE2	1:B:192:LEU:O	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:VAL:CG2	1:B:89:LYS:CB	2.95	0.45
1:A:294:ARG:CG	1:A:294:ARG:HH11	2.29	0.45
1:A:57:MET:CE	1:A:80:ARG:HA	2.47	0.45
1:B:211:LEU:O	1:B:214:GLY:N	2.49	0.45
1:B:61:ARG:O	1:B:63:HIS:N	2.49	0.45
1:A:152:GLU:C	1:A:154:GLY:H	2.20	0.45
1:A:135:ILE:HD11	1:A:160:TYR:CZ	2.51	0.45
1:A:217:TRP:CZ2	1:A:277:ILE:HG13	2.50	0.45
1:B:231:THR:O	1:B:234:LYS:N	2.50	0.45
1:B:296:MET:O	1:B:297:TYR:C	2.55	0.44
1:B:8:GLN:HB2	1:B:112:ASN:HD21	1.82	0.44
1:B:256:GLN:HA	1:B:256:GLN:NE2	2.32	0.44
1:A:149:TYR:HA	1:A:159:VAL:HG22	1.98	0.44
1:B:67:VAL:CG1	1:B:74:LEU:HD12	2.46	0.44
1:A:262:LEU:O	1:A:265:ILE:HB	2.18	0.44
1:B:36:VAL:HG23	1:B:90:VAL:HG21	1.99	0.44
1:B:202:ASN:OD1	1:B:288:THR:HG22	2.17	0.44
1:A:253:LYS:HE3	1:A:297:TYR:HB2	1.93	0.44
1:A:267:ARG:HG3	1:A:267:ARG:HH11	1.82	0.44
1:A:272:PHE:CE1	1:A:277:ILE:HD12	2.53	0.44
1:A:84:VAL:HG22	1:A:178:GLY:O	2.18	0.44
1:B:155:ILE:HG21	1:B:157:TYR:CZ	2.53	0.44
1:B:249:MET:O	1:B:249:MET:HE3	2.18	0.44
1:B:232:TRP:HZ2	3:B:2035:HOH:O	2.00	0.43
1:A:8:GLN:NE2	1:A:151:LEU:HB2	2.32	0.43
1:A:116:CYS:SG	1:A:121:PRO:HA	2.58	0.43
1:B:16:CYS:SG	1:B:98:PRO:CD	3.07	0.43
1:B:52:ASN:O	1:B:53:TYR:O	2.36	0.43
1:A:152:GLU:O	1:A:153:ASN:HB2	2.19	0.43
1:A:150:VAL:CG2	1:A:157:TYR:HB2	2.47	0.43
1:A:66:SER:OG	1:A:73:PHE:HE1	2.01	0.43
1:A:34:ASP:HB3	1:A:93:VAL:HG22	2.00	0.43
1:B:258:VAL:O	1:B:259:GLU:C	2.57	0.43
1:B:69:LYS:O	1:B:70:ASN:HB2	2.18	0.43
2:A:1001:I12:H122	2:A:1001:I12:C7	2.48	0.43
1:A:23:GLY:C	1:A:25:ASN:H	2.21	0.43
1:B:62:LEU:HD23	1:B:65:PHE:HD1	1.84	0.43
1:B:153:ASN:C	1:B:155:ILE:N	2.70	0.43
1:B:57:MET:HB2	1:B:81:TYR:CZ	2.54	0.42
1:B:46:ASP:OD1	1:B:49:ARG:HD3	2.18	0.42
1:B:61:ARG:O	1:B:62:LEU:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ILE:O	1:A:294:ARG:C	2.56	0.42
1:B:105:ILE:CG2	1:B:109:GLU:HB2	2.50	0.42
3:A:1031:HOH:O	1:B:3:LEU:HA	2.19	0.42
1:B:247:PHE:HD1	1:B:247:PHE:H	1.62	0.42
1:B:86:LEU:HD12	1:B:87:VAL:H	1.83	0.42
1:B:55:ASN:O	1:B:58:SER:HB2	2.18	0.42
1:A:80:ARG:HG2	3:A:1027:HOH:O	2.20	0.42
1:B:111:PHE:HB2	1:B:150:VAL:HG13	2.00	0.42
1:B:243:SER:O	1:B:245:ASP:N	2.53	0.42
1:B:68:SER:HB3	1:B:73:PHE:CD1	2.55	0.42
1:A:203:VAL:CG1	1:A:265:ILE:CD1	2.97	0.42
1:A:73:PHE:C	1:A:74:LEU:HD23	2.40	0.42
1:B:290:THR:O	1:B:294:ARG:HB2	2.20	0.42
1:B:158:PHE:HB3	1:B:176:PHE:CD1	2.54	0.42
1:A:27:LEU:HB2	1:A:28:ASN:H	1.35	0.42
1:B:85:ASN:ND2	1:B:178:GLY:HA2	2.35	0.42
2:B:2001:I12:O3	2:B:2001:I12:N1	2.53	0.42
1:A:274:GLY:CA	1:B:273:GLY:O	2.67	0.42
1:A:234:LYS:HZ1	1:A:240:GLU:CD	2.22	0.42
1:B:227:GLU:O	1:B:230:ASN:HB2	2.20	0.41
1:B:61:ARG:CB	1:B:64:ASN:ND2	2.78	0.41
1:A:146:SER:O	1:A:161:MET:HA	2.20	0.41
1:B:228:SER:O	1:B:231:THR:N	2.51	0.41
1:A:103:LYS:C	1:A:159:VAL:HG12	2.39	0.41
1:A:241:LEU:CD2	1:A:241:LEU:C	2.88	0.41
1:B:151:LEU:HD21	1:B:156:LEU:CD1	2.50	0.41
1:A:137:GLY:O	1:A:171:HIS:CE1	2.74	0.41
1:B:116:CYS:O	1:B:143:THR:HA	2.20	0.41
1:B:164:LEU:HB3	2:B:2001:I12:H14	2.03	0.41
1:A:253:LYS:HE2	1:A:297:TYR:CG	2.56	0.41
1:B:226:LEU:HD12	1:B:244:THR:HG23	2.03	0.41
1:A:60:VAL:CG1	1:A:61:ARG:N	2.84	0.41
1:A:151:LEU:HD21	1:A:156:LEU:HD13	2.02	0.41
1:B:221:ASN:O	1:B:222:THR:CB	2.69	0.41
1:B:34:ASP:HB3	1:B:93:VAL:HG22	2.03	0.41
1:B:18:VAL:HG22	1:B:29:GLY:O	2.21	0.41
1:B:40:ARG:HG3	1:B:53:TYR:HE2	1.86	0.41
1:A:164:LEU:O	1:A:164:LEU:HD12	2.21	0.41
1:A:60:VAL:O	1:A:61:ARG:HG2	2.21	0.41
1:B:135:ILE:HD11	1:B:139:PHE:HE1	1.86	0.41
1:B:33:GLY:C	1:B:35:GLU:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:THR:HG22	1:B:281:GLY:HA3	2.03	0.41
1:A:21:SER:OG	1:A:66:SER:HB3	2.20	0.40
1:A:249:MET:HB3	3:A:1052:HOH:O	2.21	0.40
1:B:287:PHE:CD1	1:B:287:PHE:N	2.89	0.40
1:B:224:MET:HE1	1:B:229:TYR:HA	2.03	0.40
1:B:229:TYR:CG	1:B:262:LEU:HB3	2.56	0.40
1:A:143:THR:O	1:A:144:CYS:C	2.58	0.40
1:B:189:SER:O	1:B:191:GLN:HG3	2.22	0.40
1:B:297:TYR:CD1	1:B:297:TYR:N	2.88	0.40
1:B:16:CYS:HB3	1:B:31:TRP:O	2.20	0.40
1:B:94:ASN:HA	1:B:95:PRO:HD2	1.92	0.40
1:B:131:SER:CB	1:B:197:VAL:HB	2.51	0.40
1:B:246:ALA:HB3	1:B:247:PHE:CD1	2.57	0.40
1:A:120:CYS:HA	1:A:121:PRO:HD3	1.88	0.40
1:B:136:LYS:O	1:B:137:GLY:O	2.39	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:A:54:GLU:OE1	1:A:260:LYS:NZ[2_455]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/304 (98%)	250 (84%)	43 (14%)	4 (1%)	15	37
1	B	297/304 (98%)	234 (79%)	39 (13%)	24 (8%)	1	1
All	All	594/608 (98%)	484 (82%)	82 (14%)	28 (5%)	3	5

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	SER
1	B	53	TYR
1	B	54	GLU
1	B	154	GLY
1	B	222	THR
1	B	245	ASP
1	B	246	ALA
1	B	297	TYR
1	B	41	HIS
1	B	50	VAL
1	B	62	LEU
1	B	137	GLY
1	B	138	SER
1	A	63	HIS
1	B	228	SER
1	B	244	THR
1	B	259	GLU
1	B	274	GLY
1	B	22	TYR
1	B	153	ASN
1	B	195	THR
1	B	249	MET
1	B	231	THR
1	A	293	ILE
1	B	273	GLY
1	B	140	ILE
1	B	255	GLY
1	A	11	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	255/259 (98%)	239 (94%)	16 (6%)	22	48
1	B	255/259 (98%)	225 (88%)	30 (12%)	6	15
All	All	510/518 (98%)	464 (91%)	46 (9%)	12	27

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	21	SER
1	A	27	LEU
1	A	50	VAL
1	A	92	GLN
1	A	104	SER
1	A	120	CYS
1	A	124	VAL
1	A	130	ARG
1	A	216	ARG
1	A	221	ASN
1	A	226	LEU
1	A	235	THR
1	A	260	LYS
1	A	270	LYS
1	A	296	MET
1	B	3	LEU
1	B	6	MET
1	B	10	SER
1	B	16	CYS
1	B	21	SER
1	B	27	LEU
1	B	40	ARG
1	B	45	SER
1	B	54	GLU
1	B	60	VAL
1	B	65	PHE
1	B	72	VAL
1	B	84	VAL
1	B	90	VAL
1	B	91	ASN
1	B	128	ASN
1	B	190	MET
1	B	195	THR
1	B	201	ASP
1	B	208	TYR
1	B	212	ILE
1	B	226	LEU
1	B	234	LYS
1	B	235	THR
1	B	239	THR
1	B	245	ASP

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Mol	Chain	Res	Type
1	B	247	PHE
1	B	259	GLU
1	B	289	PRO
1	B	294	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	92	GLN
1	A	132	GLN
1	A	153	ASN
1	A	213	ASN
1	A	221	ASN
1	A	256	GLN
1	A	295	GLN
1	B	41	HIS
1	B	63	HIS
1	B	64	ASN
1	B	70	ASN
1	B	85	ASN
1	B	91	ASN
1	B	92	GLN
1	B	128	ASN
1	B	132	GLN

5.3.3　RNA (i)

There are no RNA molecules in this entry.

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

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

5.5　Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	I12	A	1001	1	42,45,45	3.46	21 (50%)	50,61,61	4.82	22 (44%)
2	I12	B	2001	1	42,45,45	4.08	21 (50%)	50,61,61	5.19	27 (54%)

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	I12	A	1001	1	1/1/13/20	1/49/62/62	0/1/2/2
2	I12	B	2001	1	-	1/49/62/62	0/1/2/2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	I12	C6-N2	-12.53	1.20	1.46
2	B	2001	I12	C9-C13	-11.86	1.23	1.52
2	B	2001	I12	C5-N2	-7.11	1.18	1.34
2	A	1001	I12	C6-N2	-6.99	1.31	1.46
2	B	2001	I12	C13-N4	-4.51	1.23	1.34
2	A	1001	I12	C13-N4	-4.31	1.24	1.34
2	B	2001	I12	C4-C3	-4.30	1.43	1.48
2	A	1001	I12	C19-N5	-4.16	1.24	1.34
2	B	2001	I12	C19-N5	-3.95	1.24	1.34
2	A	1001	I12	O8-C30	-3.94	1.15	1.23
2	B	2001	I12	C20-N5	-3.81	1.40	1.46
2	A	1001	I12	C4-C3	-3.44	1.44	1.48
2	A	1001	I12	C27-C30	-3.44	1.47	1.52
2	B	2001	I12	C27-C30	-3.39	1.47	1.52
2	A	1001	I12	O7-C24	-3.06	1.36	1.46
2	A	1001	I12	C26-C27	-2.97	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	I12	C26-C27	-2.80	1.46	1.53
2	B	2001	I12	C7-N3	-2.76	1.27	1.34
2	B	2001	I12	O8-C30	-2.74	1.18	1.23
2	A	1001	I12	O3-C7	-2.08	1.19	1.23
2	B	2001	I12	C6-C7	-2.06	1.47	1.52
2	A	1001	I12	C30-N6	-2.05	1.31	1.33
2	A	1001	I12	C10-C9	2.26	1.61	1.54
2	A	1001	I12	C2-C1	2.31	1.44	1.40
2	B	2001	I12	C10-C9	2.36	1.61	1.54
2	A	1001	I12	O6-C23	2.42	1.26	1.21
2	B	2001	I12	C1-N1	2.66	1.38	1.33
2	B	2001	I12	O4-C13	2.97	1.29	1.23
2	A	1001	I12	O4-C13	3.31	1.29	1.23
2	B	2001	I12	O5-C19	3.58	1.30	1.23
2	B	2001	I12	C2-C1	3.78	1.46	1.40
2	A	1001	I12	O5-C19	3.96	1.31	1.23
2	A	1001	I12	C1-C5	5.03	1.62	1.50
2	A	1001	I12	O2-C5	5.14	1.33	1.23
2	B	2001	I12	O2-C5	5.41	1.34	1.23
2	B	2001	I12	C1-C5	5.53	1.63	1.50
2	A	1001	I12	C14-N4	5.99	1.59	1.45
2	A	1001	I12	C14-C19	6.92	1.71	1.52
2	B	2001	I12	C14-N4	7.27	1.62	1.45
2	B	2001	I12	C22-C21	7.27	1.51	1.32
2	A	1001	I12	C22-C21	7.33	1.51	1.32
2	A	1001	I12	C5-N2	10.01	1.56	1.34

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	I12	O3-C7-N3	-12.38	98.69	122.93
2	B	2001	I12	O2-C5-N2	-12.32	100.18	122.44
2	B	2001	I12	C26-C20-C21	-11.80	91.84	111.09
2	B	2001	I12	O3-C7-N3	-11.01	101.37	122.93
2	A	1001	I12	C26-C20-C21	-8.79	96.75	111.09
2	B	2001	I12	O4-C13-C9	-8.04	104.14	120.68
2	A	1001	I12	C1-C5-N2	-7.13	99.26	115.10
2	B	2001	I12	C19-C14-N4	-4.73	97.93	111.26
2	B	2001	I12	C7-C6-N2	-4.72	99.89	111.67
2	B	2001	I12	C2-C1-N1	-4.60	102.66	110.06
2	A	1001	I12	O5-C19-N5	-4.55	114.02	122.93
2	B	2001	I12	O5-C19-N5	-4.42	114.28	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	I12	C9-N3-C7	-3.74	112.01	121.85
2	A	1001	I12	C2-C1-N1	-3.71	104.09	110.06
2	A	1001	I12	O7-C24-C25	-3.19	96.41	108.42
2	A	1001	I12	C20-C21-C22	-2.85	111.44	126.58
2	A	1001	I12	C26-C20-N5	-2.80	103.50	110.48
2	B	2001	I12	C20-C21-C22	-2.37	113.99	126.58
2	A	1001	I12	O8-C30-N6	-2.28	123.45	125.96
2	A	1001	I12	C8-C6-C7	-2.14	105.97	110.19
2	B	2001	I12	C1-C5-N2	-2.06	110.51	115.10
2	A	1001	I12	O6-C23-C22	-2.06	115.97	123.46
2	A	1001	I12	C7-C6-N2	-2.04	106.58	111.67
2	B	2001	I12	C20-N5-C19	-2.04	117.06	121.63
2	A	1001	I12	C13-C9-N3	-2.02	105.11	110.59
2	A	1001	I12	O7-C23-C22	2.03	118.34	111.64
2	B	2001	I12	O4-C13-N4	2.13	127.11	122.93
2	B	2001	I12	C6-C7-N3	2.14	121.88	116.83
2	A	1001	I12	O4-C13-N4	2.30	127.42	122.93
2	A	1001	I12	C6-C7-N3	2.80	123.42	116.83
2	B	2001	I12	C24-O7-C23	2.91	122.22	116.31
2	B	2001	I12	C21-C22-C23	2.93	129.96	122.71
2	B	2001	I12	C13-C9-N3	3.14	119.14	110.59
2	B	2001	I12	C15-C14-N4	3.25	118.59	110.49
2	B	2001	I12	O7-C23-O6	3.48	131.98	122.89
2	B	2001	I12	C9-N3-C7	4.14	132.74	121.85
2	B	2001	I12	C14-N4-C13	4.80	132.38	121.62
2	B	2001	I12	C14-C19-N5	4.82	127.88	116.78
2	B	2001	I12	C10-C9-C13	5.34	125.33	111.31
2	B	2001	I12	C9-C13-N4	5.58	128.75	116.44
2	B	2001	I12	C1-C2-C3	6.83	109.57	106.08
2	A	1001	I12	C1-C2-C3	8.51	110.42	106.08
2	A	1001	I12	O2-C5-C1	9.03	140.46	121.23
2	A	1001	I12	C21-C22-C23	10.22	148.01	122.71
2	B	2001	I12	O2-C5-C1	11.68	146.09	121.23
2	B	2001	I12	C26-C20-N5	13.04	143.01	110.48
2	A	1001	I12	C6-N2-C5	13.67	153.71	121.64
2	B	2001	I12	C6-N2-C5	14.76	156.27	121.64
2	A	1001	I12	C20-N5-C19	17.10	159.91	121.63

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1001	I12	C20

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	I12	C20-C21-C22-C23
2	B	2001	I12	C20-C21-C22-C23

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	I12	2	0
2	B	2001	I12	11	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	299/304 (98%)	-0.10	4 (1%)	79	79	15, 33, 47, 63	0
1	B	299/304 (98%)	0.18	7 (2%)	64	64	18, 45, 63, 70	0
All	All	598/608 (98%)	0.04	11 (1%)	71	72	15, 37, 60, 70	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	GLY	5.5
1	A	1	SER	5.0
1	B	251	ALA	3.1
1	B	221	ASN	2.8
1	B	61	ARG	2.8
1	B	52	ASN	2.5
1	B	71	ASN	2.5
1	A	299	VAL	2.4
1	A	72	VAL	2.3
1	B	231	THR	2.1
1	B	54	GLU	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 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
2	I12	A	1001	44/44	0.82	0.27	2.20	26,47,63,64	0
2	I12	B	2001	44/44	0.87	0.24	1.83	33,50,67,69	0

6.5 Other polymers (i)

There are no such residues in this entry.