Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2024 – 10:11 AM JST

PDB ID	:	8XUD
Title	:	Crystal structure of adaptor NlpI in complex with endopeptidase MepS and PDZ-protease Prc
Authors	:	Tzeng, S.R.; Wang, S.; Huang, C.H.
Deposited on	:	2024-01-12
Resolution	:	3.49 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 ⓘ 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 ⓘ) were used in the production of this report:

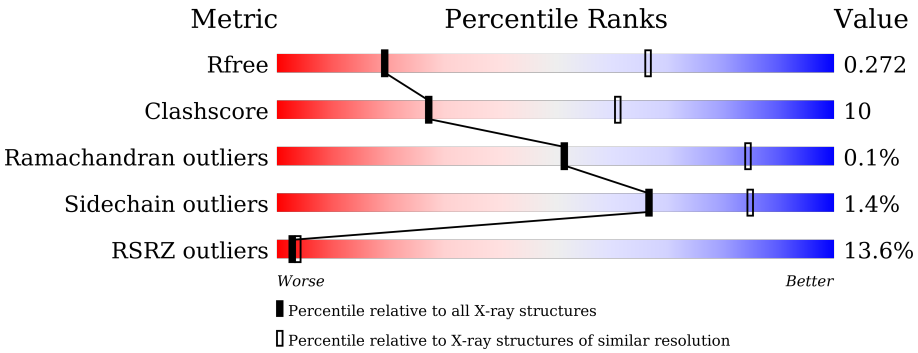
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.49 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.



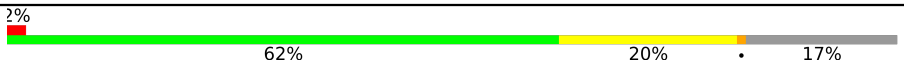
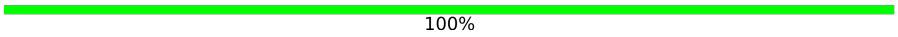
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	297	75% 13% 11%
1	B	297	% 74% 15% 11%
2	C	688	24% 66% 27% • 6%
2	D	688	20% 67% 27% • 5%
3	I	168	3% 61% 23% • 15%
3	J	168	2% 65% 21% • 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	K	168	
3	L	168	
4	M	8	
5	N	9	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 19377 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 Lipoprotein NlpI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2141	1365	356	417	3			
1	B	264	Total	C	N	O	S	0	0	0
			2141	1365	356	417	3			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP P0AFB1
A	-1	GLY	-	expression tag	UNP P0AFB1
A	0	SER	-	expression tag	UNP P0AFB1
A	1	SER	-	expression tag	UNP P0AFB1
A	2	HIS	-	expression tag	UNP P0AFB1
A	3	HIS	-	expression tag	UNP P0AFB1
A	4	HIS	-	expression tag	UNP P0AFB1
A	5	HIS	-	expression tag	UNP P0AFB1
A	6	HIS	-	expression tag	UNP P0AFB1
A	7	HIS	-	expression tag	UNP P0AFB1
A	8	SER	-	expression tag	UNP P0AFB1
A	9	SER	-	expression tag	UNP P0AFB1
A	10	GLY	-	expression tag	UNP P0AFB1
A	11	GLU	-	expression tag	UNP P0AFB1
A	12	ASN	-	expression tag	UNP P0AFB1
A	13	LEU	-	expression tag	UNP P0AFB1
A	14	TYR	-	expression tag	UNP P0AFB1
A	15	PHE	-	expression tag	UNP P0AFB1
A	16	GLN	-	expression tag	UNP P0AFB1
A	17	GLY	-	expression tag	UNP P0AFB1
A	18	HIS	-	expression tag	UNP P0AFB1
A	19	MET	-	expression tag	UNP P0AFB1
B	-2	MET	-	initiating methionine	UNP P0AFB1
B	-1	GLY	-	expression tag	UNP P0AFB1
B	0	SER	-	expression tag	UNP P0AFB1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	SER	-	expression tag	UNP P0AFB1
B	2	HIS	-	expression tag	UNP P0AFB1
B	3	HIS	-	expression tag	UNP P0AFB1
B	4	HIS	-	expression tag	UNP P0AFB1
B	5	HIS	-	expression tag	UNP P0AFB1
B	6	HIS	-	expression tag	UNP P0AFB1
B	7	HIS	-	expression tag	UNP P0AFB1
B	8	SER	-	expression tag	UNP P0AFB1
B	9	SER	-	expression tag	UNP P0AFB1
B	10	GLY	-	expression tag	UNP P0AFB1
B	11	GLU	-	expression tag	UNP P0AFB1
B	12	ASN	-	expression tag	UNP P0AFB1
B	13	LEU	-	expression tag	UNP P0AFB1
B	14	TYR	-	expression tag	UNP P0AFB1
B	15	PHE	-	expression tag	UNP P0AFB1
B	16	GLN	-	expression tag	UNP P0AFB1
B	17	GLY	-	expression tag	UNP P0AFB1
B	18	HIS	-	expression tag	UNP P0AFB1
B	19	MET	-	expression tag	UNP P0AFB1

- Molecule 2 is a protein called Tail-specific protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	647	Total	C	N	O	S	0	0	0
			5134	3230	896	996	12			
2	D	651	Total	C	N	O	S	0	0	0
			5162	3247	903	1000	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	452	ALA	SER	engineered mutation	UNP P23865
C	477	ALA	LYS	engineered mutation	UNP P23865
C	683	HIS	-	expression tag	UNP P23865
C	684	HIS	-	expression tag	UNP P23865
C	685	HIS	-	expression tag	UNP P23865
C	686	HIS	-	expression tag	UNP P23865
C	687	HIS	-	expression tag	UNP P23865
C	688	HIS	-	expression tag	UNP P23865
D	452	ALA	SER	engineered mutation	UNP P23865
D	477	ALA	LYS	engineered mutation	UNP P23865
D	683	HIS	-	expression tag	UNP P23865

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	684	HIS	-	expression tag	UNP P23865
D	685	HIS	-	expression tag	UNP P23865
D	686	HIS	-	expression tag	UNP P23865
D	687	HIS	-	expression tag	UNP P23865
D	688	HIS	-	expression tag	UNP P23865

- Molecule 3 is a protein called Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	142	Total	C	N	O	S	0	0	0
			1137	702	215	216	4			
3	J	147	Total	C	N	O	S	0	0	0
			1190	734	232	220	4			
3	K	140	Total	C	N	O	S	0	0	0
			1120	693	210	213	4			
3	L	148	Total	C	N	O	S	0	0	0
			1197	738	233	222	4			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	MET	-	initiating methionine	UNP P0AFV4
I	163	HIS	-	expression tag	UNP P0AFV4
I	164	HIS	-	expression tag	UNP P0AFV4
I	165	HIS	-	expression tag	UNP P0AFV4
I	166	HIS	-	expression tag	UNP P0AFV4
I	167	HIS	-	expression tag	UNP P0AFV4
I	168	HIS	-	expression tag	UNP P0AFV4
J	1	MET	-	initiating methionine	UNP P0AFV4
J	163	HIS	-	expression tag	UNP P0AFV4
J	164	HIS	-	expression tag	UNP P0AFV4
J	165	HIS	-	expression tag	UNP P0AFV4
J	166	HIS	-	expression tag	UNP P0AFV4
J	167	HIS	-	expression tag	UNP P0AFV4
J	168	HIS	-	expression tag	UNP P0AFV4
K	1	MET	-	initiating methionine	UNP P0AFV4
K	163	HIS	-	expression tag	UNP P0AFV4
K	164	HIS	-	expression tag	UNP P0AFV4
K	165	HIS	-	expression tag	UNP P0AFV4
K	166	HIS	-	expression tag	UNP P0AFV4
K	167	HIS	-	expression tag	UNP P0AFV4
K	168	HIS	-	expression tag	UNP P0AFV4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	1	MET	-	initiating methionine	UNP P0AFV4
L	163	HIS	-	expression tag	UNP P0AFV4
L	164	HIS	-	expression tag	UNP P0AFV4
L	165	HIS	-	expression tag	UNP P0AFV4
L	166	HIS	-	expression tag	UNP P0AFV4
L	167	HIS	-	expression tag	UNP P0AFV4
L	168	HIS	-	expression tag	UNP P0AFV4

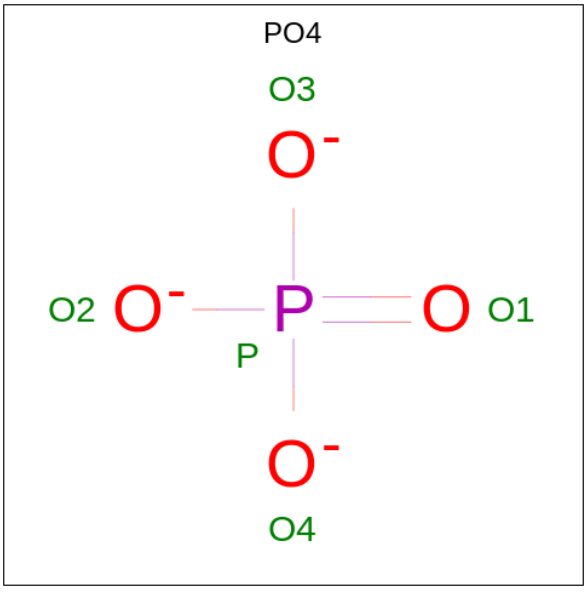
- Molecule 4 is a protein called Substrate peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	M	8	40	24	8	8	0	0	0

- Molecule 5 is a protein called Substrate peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	N	9	45	27	9	9	0	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
6	I	1	5	4	1	0	0

Continued on next page...

Continued from previous page...

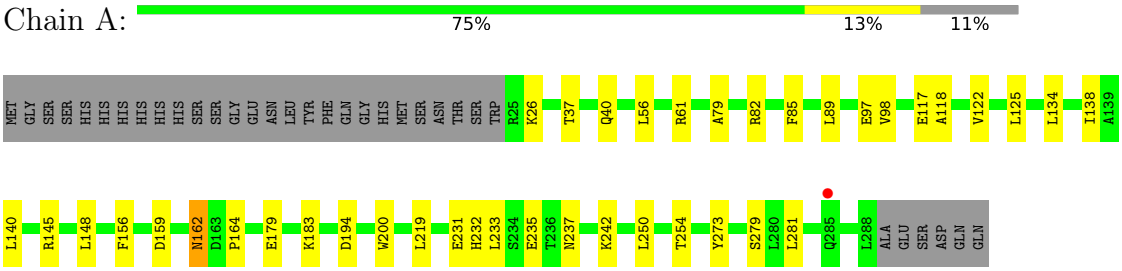
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	1	Total O P 5 4 1	0	0
6	I	1	Total O P 5 4 1	0	0
6	I	1	Total O P 5 4 1	0	0
6	J	1	Total O P 5 4 1	0	0
6	J	1	Total O P 5 4 1	0	0
6	J	1	Total O P 5 4 1	0	0
6	K	1	Total O P 5 4 1	0	0
6	K	1	Total O P 5 4 1	0	0
6	K	1	Total O P 5 4 1	0	0
6	K	1	Total O P 5 4 1	0	0
6	K	1	Total O P 5 4 1	0	0
6	L	1	Total O P 5 4 1	0	0
6	L	1	Total O P 5 4 1	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.

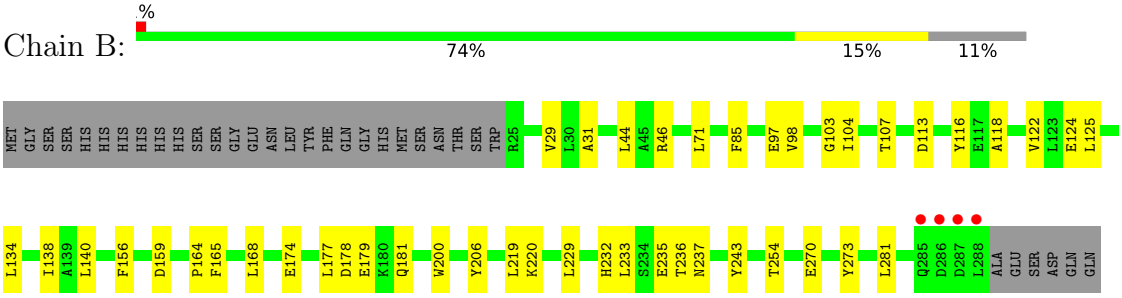
• Molecule 1: Lipoprotein NlpI

Chain A:



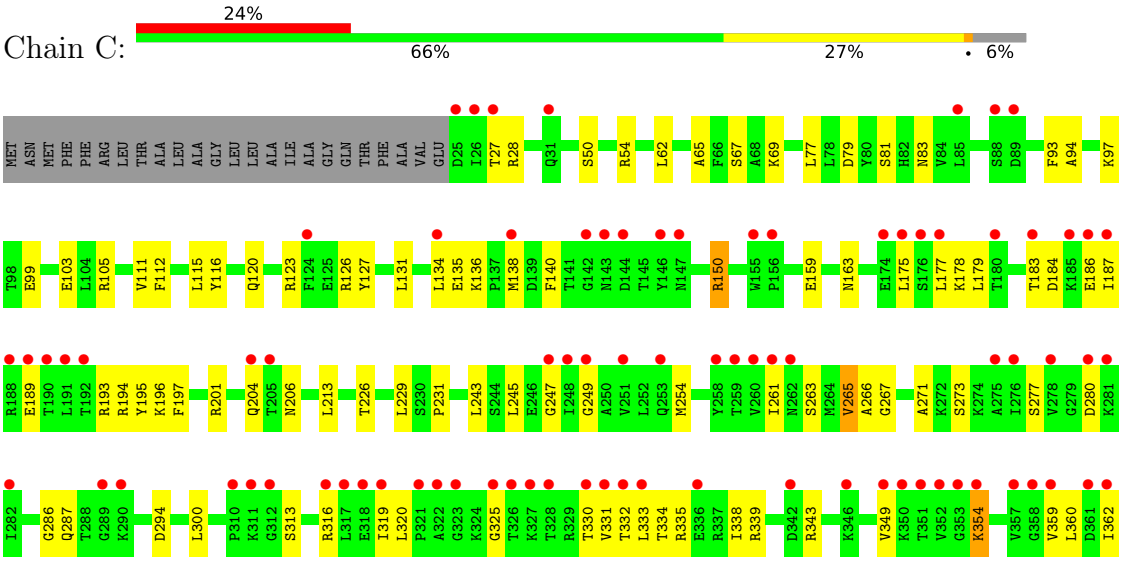
• Molecule 1: Lipoprotein NlpI

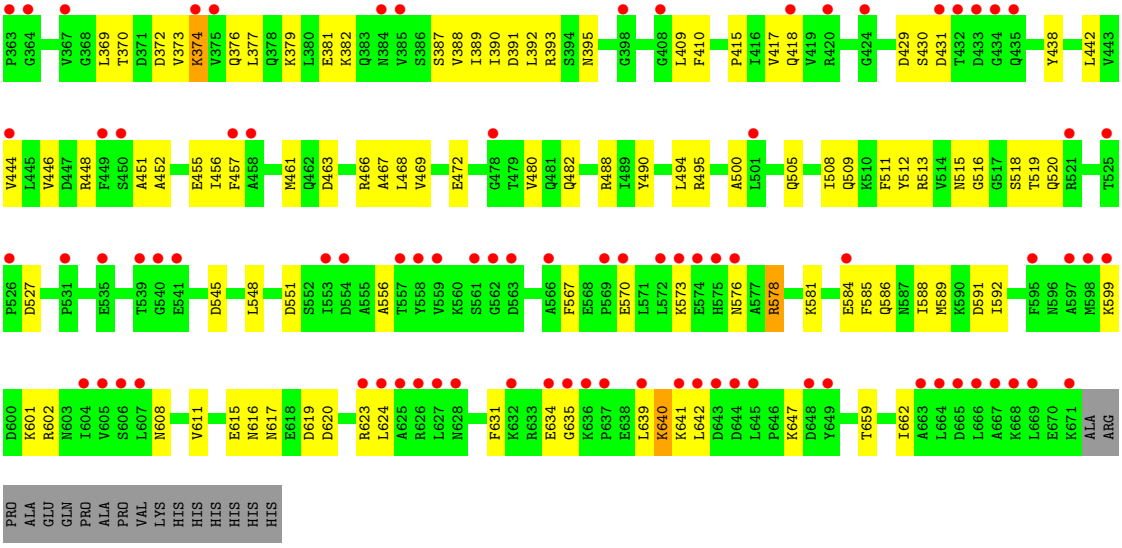
Chain B:



• Molecule 2: Tail-specific protease

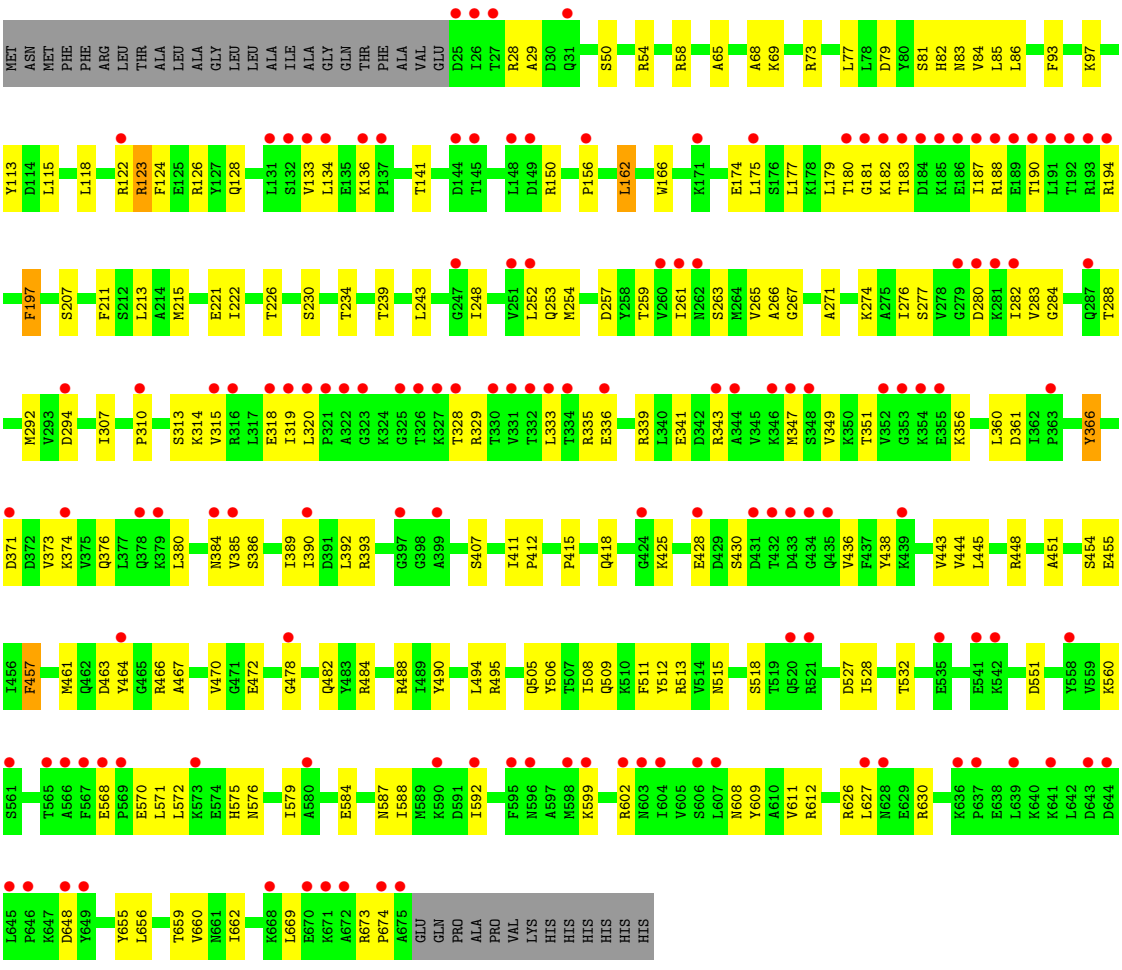
Chain C:





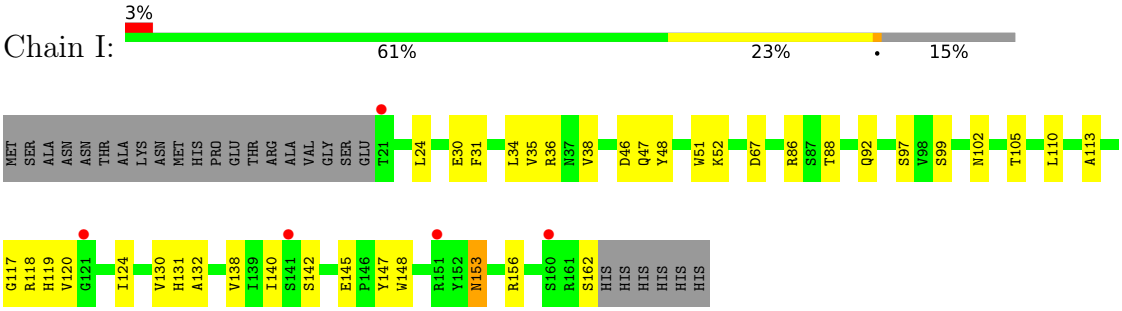
• Molecule 2: Tail-specific protease

Chain D:



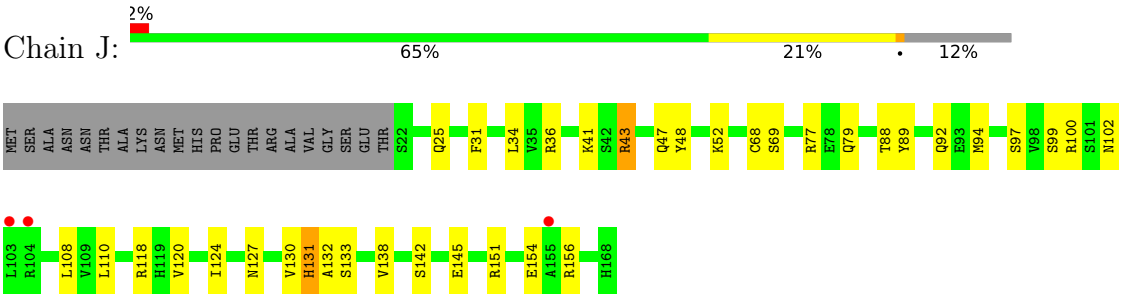
• Molecule 3: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase

Chain I:



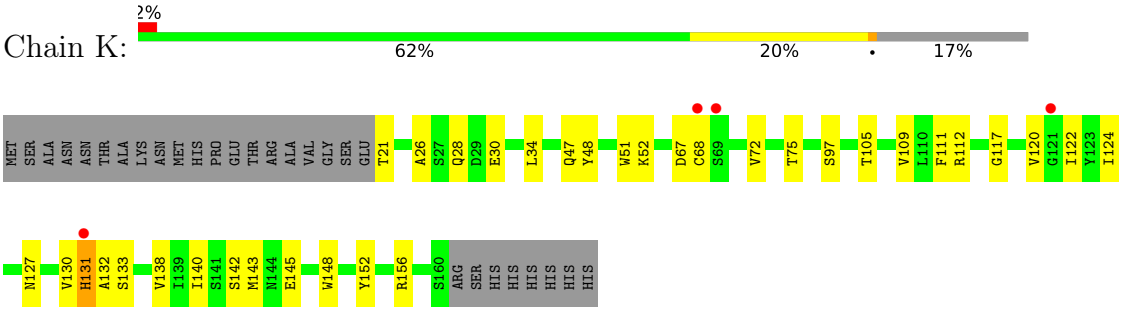
• Molecule 3: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase

Chain J:



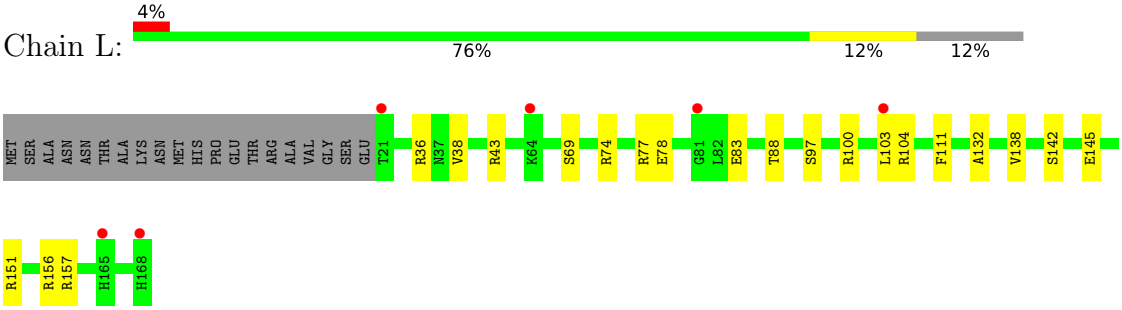
• Molecule 3: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase

Chain K:



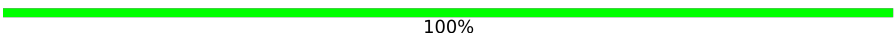
• Molecule 3: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase

Chain L:



• Molecule 4: Substrate peptide

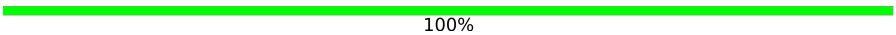
Chain M:



There are no outlier residues recorded for this chain.

• Molecule 5: Substrate peptide

Chain N:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	230.41Å 230.41Å 182.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 3.49 29.91 – 3.49	Depositor EDS
% Data completeness (in resolution range)	97.4 (29.91-3.49) 97.4 (29.91-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 3.47Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.235 , 0.272 0.238 , 0.272	Depositor DCC
R_{free} test set	1994 reflections (3.26%)	wwPDB-VP
Wilson B-factor (Å^2)	118.6	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 136.6	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	0.93	EDS
Total number of atoms	19377	wwPDB-VP
Average B, all atoms (Å^2)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2456e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.24	0/2185	0.43	0/2964
1	B	0.24	0/2185	0.43	0/2964
2	C	0.25	0/5221	0.53	0/7051
2	D	0.25	0/5250	0.51	0/7091
3	I	0.25	0/1156	0.55	0/1550
3	J	0.25	0/1215	0.55	0/1630
3	K	0.25	0/1139	0.55	0/1528
3	L	0.24	0/1222	0.57	0/1640
All	All	0.25	0/19573	0.51	0/26418

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2141	0	2072	29	0
1	B	2141	0	2072	27	0
2	C	5134	0	5146	130	0
2	D	5162	0	5176	125	0
3	I	1137	0	1118	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	1190	0	1153	25	0
3	K	1120	0	1100	25	0
3	L	1197	0	1160	15	0
4	M	40	0	13	0	0
5	N	45	0	13	0	0
6	I	20	0	0	1	0
6	J	15	0	0	1	0
6	K	25	0	0	0	0
6	L	10	0	0	0	0
All	All	19377	0	19023	386	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 10.

All (386) 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)
2:D:282:ILE:HD13	2:D:318:GLU:HB2	1.66	0.78
2:D:243:LEU:HG	2:D:366:TYR:CZ	2.22	0.73
3:J:69:SER:OG	3:J:88:THR:OG1	2.06	0.73
2:C:265:VAL:HG23	2:C:271:ALA:HB2	1.70	0.73
2:C:131:LEU:HD21	2:C:195:TYR:HB3	1.69	0.72
2:C:178:LYS:NZ	2:C:184:ASP:OD1	2.22	0.72
3:J:88:THR:HG23	3:J:120:VAL:HG13	1.71	0.71
1:A:56:LEU:HD21	1:A:61:ARG:HH11	1.55	0.70
2:D:79:ASP:OD2	2:D:83:ASN:N	2.24	0.70
2:D:73:ARG:NH1	2:D:221:GLU:OE1	2.25	0.69
2:D:669:LEU:O	2:D:673:ARG:N	2.26	0.69
3:L:100:ARG:HD2	3:L:103:LEU:HD21	1.75	0.68
2:C:389:ILE:HG22	2:C:659:THR:HG21	1.75	0.68
1:A:82:ARG:NH1	3:K:26:ALA:O	2.23	0.67
1:A:85:PHE:HB3	1:A:98:VAL:HG13	1.75	0.67
2:D:418:GLN:HG2	2:D:428:GLU:HG3	1.77	0.67
2:D:288:THR:HG23	2:D:314:LYS:HB2	1.77	0.66
1:A:279:SER:HG	3:K:21:THR:N	1.94	0.66
3:J:100:ARG:NH2	3:J:127:ASN:OD1	2.27	0.66
1:A:145:ARG:HB3	1:A:148:LEU:HD13	1.79	0.65
2:D:182:LYS:HB2	2:D:187:ILE:HD13	1.79	0.64
3:I:147:TYR:OH	6:I:201:PO4:O4	2.15	0.64
3:I:92:GLN:HG3	3:I:110:LEU:HD13	1.80	0.64
2:C:140:PHE:HZ	2:C:175:LEU:HB2	1.63	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:130:VAL:HG22	3:K:140:ILE:HG12	1.80	0.64
2:C:415:PRO:HA	2:C:430:SER:HB3	1.79	0.63
2:D:243:LEU:HD13	2:D:341:GLU:HG2	1.80	0.63
3:I:145:GLU:OE2	3:J:77:ARG:NH1	2.32	0.63
2:C:77:LEU:HB3	2:C:213:LEU:HD11	1.79	0.63
1:B:44:LEU:HD13	1:B:71:LEU:HD23	1.79	0.63
3:K:97:SER:HA	3:K:156:ARG:HD2	1.80	0.63
2:C:624:LEU:HD11	2:C:639:LEU:HD22	1.81	0.63
2:D:448:ARG:NH1	2:D:472:GLU:OE2	2.32	0.63
2:D:226:THR:HA	2:D:505:GLN:O	1.99	0.62
3:J:41:LYS:NZ	3:J:124:ILE:O	2.33	0.62
2:C:461:MET:HB3	2:C:467:ALA:HB3	1.82	0.62
2:D:243:LEU:N	2:D:366:TYR:OH	2.33	0.62
2:D:283:VAL:HG23	2:D:284:GLY:H	1.65	0.62
2:C:417:VAL:HG13	2:C:429:ASP:HB3	1.82	0.61
2:C:261:ILE:HG22	2:C:263:SER:HB2	1.83	0.61
3:K:105:THR:HG23	3:K:124:ILE:HA	1.81	0.61
3:K:145:GLU:OE2	3:L:77:ARG:NH1	2.33	0.61
1:A:162:ASN:ND2	1:A:194:ASP:OD2	2.33	0.60
2:D:113:TYR:HH	2:D:207:SER:HG	1.48	0.60
2:D:307:ILE:O	2:D:335:ARG:NH1	2.34	0.60
2:C:243:LEU:HB2	2:C:339:ARG:HE	1.67	0.60
2:D:386:SER:O	2:D:438:TYR:OH	2.19	0.60
2:D:50:SER:OG	2:D:54:ARG:NH1	2.34	0.60
2:D:81:SER:HB2	2:D:83:ASN:HD21	1.67	0.60
3:L:69:SER:HB3	3:L:88:THR:HG23	1.84	0.60
1:B:29:VAL:HG22	1:B:220:LYS:HE3	1.83	0.59
3:I:46:ASP:OD1	3:J:36:ARG:NH2	2.35	0.59
2:D:124:PHE:O	2:D:128:GLN:NE2	2.35	0.59
2:D:461:MET:HB3	2:D:467:ALA:HB3	1.83	0.59
2:D:488:ARG:NH1	2:D:490:TYR:OH	2.35	0.59
2:D:211:PHE:O	2:D:215:MET:HG2	2.02	0.59
2:C:417:VAL:HG23	2:C:511:PHE:CD1	2.38	0.58
2:D:371:ASP:O	2:D:374:LYS:NZ	2.34	0.58
2:D:571:LEU:HD13	2:D:662:ILE:HG23	1.85	0.58
2:C:134:LEU:HD21	2:C:195:TYR:HE2	1.68	0.58
2:C:226:THR:HA	2:C:505:GLN:O	2.04	0.58
2:D:175:LEU:HG	2:D:612:ARG:HH22	1.67	0.58
1:B:85:PHE:HB3	1:B:98:VAL:HG13	1.84	0.58
2:C:589:MET:HA	2:C:592:ILE:HG12	1.84	0.58
2:D:349:VAL:HG21	2:D:380:LEU:HD12	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:67:SER:OG	2:C:97:LYS:O	2.19	0.58
3:L:36:ARG:HG2	3:L:38:VAL:HG13	1.85	0.58
3:L:132:ALA:HA	3:L:138:VAL:HA	1.85	0.58
2:C:482:GLN:HB2	2:C:508:ILE:HD13	1.86	0.57
2:D:608:ASN:HB3	2:D:611:VAL:HG12	1.87	0.57
3:J:151:ARG:NH1	6:J:201:PO4:O4	2.38	0.57
2:C:578:ARG:HA	2:C:581:LYS:HE2	1.85	0.57
2:C:591:ASP:OD1	2:C:623:ARG:NH1	2.37	0.57
2:D:134:LEU:HD23	2:D:188:ARG:HD2	1.87	0.57
2:C:372:ASP:O	2:C:376:GLN:NE2	2.29	0.57
1:A:79:ALA:O	1:A:82:ARG:HG2	2.05	0.57
2:C:390:ILE:HB	2:C:444:VAL:HG12	1.86	0.57
3:I:97:SER:HA	3:I:156:ARG:HD3	1.85	0.57
3:L:77:ARG:NH2	3:L:83:GLU:OE2	2.37	0.57
3:L:142:SER:HB3	3:L:145:GLU:HG3	1.87	0.57
2:D:133:VAL:HG13	2:D:136:LYS:HG3	1.86	0.57
2:C:183:THR:HB	2:C:186:GLU:HB3	1.86	0.56
2:C:631:PHE:HA	2:C:634:GLU:HG2	1.87	0.56
3:I:130:VAL:HG22	3:I:140:ILE:HG12	1.87	0.56
1:A:140:LEU:HD21	2:C:54:ARG:HD3	1.87	0.56
2:C:379:LYS:HG3	2:C:382:LYS:HD2	1.87	0.56
2:D:177:LEU:HD12	2:D:181:GLY:HA3	1.86	0.56
1:B:124:GLU:OE1	2:D:488:ARG:NH1	2.38	0.56
2:C:254:MET:HB2	2:C:300:LEU:HD21	1.87	0.56
2:C:480:VAL:HB	2:C:509:GLN:HB2	1.87	0.56
2:D:418:GLN:NE2	2:D:513:ARG:O	2.38	0.56
2:D:230:SER:O	2:D:234:THR:N	2.35	0.56
2:D:361:ASP:OD2	2:D:393:ARG:NH2	2.38	0.56
2:D:494:LEU:HD12	2:D:495:ARG:HG2	1.88	0.56
2:C:247:GLY:HA2	2:C:335:ARG:HD2	1.88	0.56
2:C:388:VAL:O	2:C:442:LEU:HA	2.04	0.56
3:I:117:GLY:O	3:I:118:ARG:HD3	2.05	0.56
1:A:37:THR:HG23	1:A:40:GLN:H	1.69	0.56
2:D:277:SER:H	2:D:280:ASP:HB3	1.70	0.56
3:L:97:SER:HA	3:L:156:ARG:HG2	1.88	0.56
2:C:140:PHE:CE2	2:C:175:LEU:HD13	2.41	0.55
2:D:239:THR:O	2:D:366:TYR:OH	2.24	0.55
2:D:351:THR:HA	2:D:356:LYS:HG2	1.86	0.55
2:C:516:GLY:HA2	2:C:556:ALA:H	1.71	0.55
2:D:313:SER:HB3	2:D:335:ARG:HD2	1.88	0.55
2:D:599:LYS:HA	2:D:602:ARG:HB2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:99:SER:OG	3:I:102:ASN:OD1	2.21	0.55
3:I:142:SER:HB3	3:I:145:GLU:HG3	1.88	0.55
2:C:135:GLU:HG3	2:C:135:GLU:O	2.06	0.55
2:C:313:SER:OG	2:C:335:ARG:NH2	2.40	0.55
2:D:248:ILE:HD11	2:D:315:VAL:HG11	1.89	0.55
1:A:56:LEU:HG	1:A:61:ARG:HG2	1.88	0.55
1:A:254:THR:HG22	1:A:281:LEU:HD13	1.90	0.54
2:D:392:LEU:HD13	2:D:454:SER:HB3	1.88	0.54
2:C:193:ARG:HH21	2:C:194:ARG:HH22	1.55	0.54
2:C:599:LYS:HB3	2:C:602:ARG:HD3	1.89	0.54
2:D:81:SER:HA	2:D:150:ARG:HG3	1.89	0.54
2:C:331:VAL:HG22	2:C:332:THR:H	1.73	0.54
2:C:573:LYS:HA	2:C:576:ASN:HB2	1.90	0.54
2:D:373:VAL:HA	2:D:376:GLN:HG2	1.90	0.54
2:C:417:VAL:HG23	2:C:511:PHE:HD1	1.73	0.54
2:D:253:GLN:NE2	2:D:254:MET:O	2.41	0.53
2:C:468:LEU:HD22	2:C:662:ILE:HD11	1.90	0.53
2:D:584:GLU:HA	2:D:587:ASN:ND2	2.24	0.53
3:K:109:VAL:HG23	3:K:152:TYR:HE1	1.73	0.53
2:D:81:SER:HB2	2:D:83:ASN:ND2	2.23	0.53
2:D:318:GLU:HA	2:D:329:ARG:O	2.07	0.53
2:C:127:TYR:O	2:C:131:LEU:HD23	2.08	0.53
3:J:47:GLN:OE1	3:J:79:GLN:NE2	2.25	0.53
2:D:197:PHE:CE2	2:D:257:ASP:HB3	2.44	0.53
2:D:86:LEU:HD11	2:D:122:ARG:HG3	1.90	0.53
2:D:81:SER:OG	2:D:150:ARG:NE	2.41	0.53
2:D:436:VAL:HG21	2:D:466:ARG:HH12	1.74	0.53
2:C:359:VAL:HG13	2:C:389:ILE:HD11	1.90	0.52
2:C:431:ASP:OD1	2:C:431:ASP:N	2.42	0.52
3:K:48:TYR:O	3:K:52:LYS:N	2.42	0.52
2:C:520:GLN:NE2	2:C:548:LEU:O	2.42	0.52
2:D:271:ALA:O	2:D:274:LYS:HG2	2.10	0.52
1:B:219:LEU:HD12	1:B:236:THR:HG21	1.91	0.52
2:D:478:GLY:HA2	2:D:511:PHE:CE2	2.44	0.52
3:I:113:ALA:HB2	3:I:119:HIS:HB2	1.90	0.52
1:A:134:LEU:HB2	1:A:156:PHE:CD2	2.45	0.52
3:I:48:TYR:O	3:I:52:LYS:N	2.43	0.52
2:C:631:PHE:O	2:C:635:GLY:N	2.40	0.52
2:D:412:PRO:HB3	2:D:436:VAL:HG12	1.92	0.52
2:C:201:ARG:HA	2:C:204:GLN:HG2	1.92	0.51
2:C:584:GLU:HB2	2:C:588:ILE:HD12	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:360:LEU:HB2	2:D:390:ILE:HD12	1.91	0.51
2:D:451:ALA:O	2:D:455:GLU:HG3	2.10	0.51
2:C:585:PHE:CZ	2:C:586:GLN:HG3	2.46	0.51
2:D:79:ASP:HB3	2:D:85:LEU:HD11	1.91	0.51
2:D:93:PHE:HD2	2:D:115:LEU:HG	1.76	0.51
1:A:117:GLU:OE2	2:C:488:ARG:NH1	2.43	0.51
1:B:164:PRO:HG3	1:B:200:TRP:CD1	2.45	0.51
3:J:94:MET:O	3:J:156:ARG:HD3	2.11	0.51
2:C:62:LEU:HB3	2:C:105:ARG:HH21	1.76	0.51
2:D:252:LEU:HB3	2:D:259:THR:CG2	2.40	0.51
3:I:132:ALA:HA	3:I:138:VAL:HA	1.92	0.51
2:C:245:LEU:HD13	2:C:249:GLY:HA2	1.92	0.51
2:C:387:SER:HB2	2:C:659:THR:HB	1.93	0.51
2:C:452:ALA:HA	2:C:455:GLU:HG2	1.93	0.50
3:I:47:GLN:O	3:I:51:TRP:HB2	2.12	0.50
1:B:140:LEU:HD21	2:D:54:ARG:HD3	1.93	0.50
2:C:103:GLU:OE2	2:C:111:VAL:N	2.37	0.50
2:C:349:VAL:HG11	2:C:377:LEU:HB2	1.94	0.50
2:D:284:GLY:HA3	2:D:294:ASP:HA	1.93	0.50
2:C:494:LEU:HD12	2:C:495:ARG:HG2	1.93	0.50
2:D:463:ASP:OD1	2:D:515:ASN:ND2	2.45	0.50
2:D:627:LEU:HD23	2:D:630:ARG:HH11	1.77	0.50
2:D:183:THR:O	2:D:187:ILE:HG12	2.12	0.50
2:D:315:VAL:HG13	2:D:333:LEU:HB3	1.94	0.50
3:J:43:ARG:HD3	3:J:79:GLN:O	2.11	0.50
2:C:545:ASP:OD1	2:C:545:ASP:N	2.45	0.49
3:L:104:ARG:HB3	3:L:157:ARG:HH12	1.78	0.49
2:D:484:ARG:NH2	2:D:506:TYR:OH	2.45	0.49
3:K:145:GLU:HB2	3:K:148:TRP:HD1	1.78	0.49
3:L:77:ARG:HG3	3:L:78:GLU:HG3	1.94	0.49
3:J:110:LEU:HD12	3:J:154:GLU:HG3	1.95	0.49
3:K:111:PHE:CE1	3:K:148:TRP:HB3	2.48	0.49
1:B:174:GLU:HA	1:B:177:LEU:HD13	1.94	0.49
2:C:448:ARG:NH1	2:C:472:GLU:OE2	2.45	0.49
2:C:624:LEU:HD22	2:C:642:LEU:HD13	1.94	0.49
2:D:673:ARG:N	2:D:674:PRO:HD3	2.28	0.49
1:B:138:ILE:HG21	1:B:273:TYR:CE2	2.48	0.49
1:B:178:ASP:HB3	1:B:181:GLN:HB3	1.95	0.49
2:C:286:GLY:HA3	2:C:316:ARG:HB2	1.95	0.49
2:C:320:LEU:HD21	2:C:325:GLY:HA2	1.95	0.49
3:K:132:ALA:HA	3:K:138:VAL:HA	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:PRO:HB3	1:A:200:TRP:CD2	2.47	0.48
2:C:50:SER:OG	2:C:54:ARG:NH1	2.46	0.48
3:K:127:ASN:HB3	3:K:143:MET:HB2	1.95	0.48
2:C:27:THR:OG1	2:C:28:ARG:N	2.46	0.48
2:C:65:ALA:O	2:C:69:LYS:HG2	2.13	0.48
2:C:135:GLU:O	2:C:136:LYS:HD3	2.13	0.48
2:D:390:ILE:HG23	2:D:444:VAL:HG13	1.95	0.48
1:B:134:LEU:HB2	1:B:156:PHE:CD2	2.47	0.48
2:C:551:ASP:OD1	2:C:551:ASP:N	2.44	0.48
2:D:82:HIS:HA	2:D:85:LEU:HD13	1.95	0.48
2:D:265:VAL:HG23	2:D:271:ALA:HB2	1.95	0.48
3:K:124:ILE:HD13	3:K:130:VAL:HG23	1.96	0.48
2:C:463:ASP:OD1	2:C:515:ASN:ND2	2.47	0.48
2:D:551:ASP:OD1	2:D:551:ASP:N	2.43	0.48
2:C:273:SER:HB2	2:C:333:LEU:HD13	1.96	0.48
3:J:89:TYR:O	3:J:92:GLN:HG2	2.13	0.48
2:C:277:SER:HB3	2:C:319:ILE:HD12	1.95	0.48
1:B:235:GLU:HA	1:B:270:GLU:HG2	1.96	0.48
2:D:243:LEU:O	2:D:339:ARG:HA	2.14	0.47
2:C:94:ALA:HB1	2:C:97:LYS:HE3	1.95	0.47
2:C:451:ALA:O	2:C:455:GLU:HG2	2.13	0.47
2:C:469:VAL:HG23	2:C:527:ASP:H	1.78	0.47
3:J:43:ARG:HG2	3:J:79:GLN:HB3	1.96	0.47
3:J:131:HIS:CE1	3:J:133:SER:HB3	2.49	0.47
1:A:138:ILE:HG21	1:A:273:TYR:CE2	2.49	0.47
3:K:30:GLU:O	3:K:34:LEU:HG	2.15	0.47
1:B:125:LEU:HD21	2:D:490:TYR:CG	2.50	0.47
2:C:615:GLU:HA	2:C:619:ASP:OD2	2.14	0.47
2:D:77:LEU:HB3	2:D:213:LEU:HD11	1.97	0.47
2:D:85:LEU:O	2:D:156:PRO:HG2	2.15	0.47
2:D:512:TYR:CD2	2:D:518:SER:HB3	2.49	0.47
2:C:277:SER:HB3	2:C:319:ILE:CD1	2.45	0.47
1:B:104:ILE:O	1:B:107:THR:OG1	2.27	0.47
3:J:97:SER:HA	3:J:156:ARG:HG2	1.96	0.46
3:J:142:SER:HB3	3:J:145:GLU:HG3	1.96	0.46
1:B:219:LEU:HG	1:B:232:HIS:HB3	1.97	0.46
2:D:380:LEU:HD22	2:D:385:VAL:HG12	1.97	0.46
3:J:108:LEU:HD23	3:J:156:ARG:O	2.15	0.46
3:K:112:ARG:HA	3:K:117:GLY:O	2.16	0.46
2:D:179:LEU:HG	2:D:180:THR:HG23	1.97	0.46
3:K:67:ASP:OD1	3:K:68:CYS:N	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:370:THR:HG23	2:C:409:LEU:HD11	1.97	0.46
2:D:282:ILE:CD1	2:D:318:GLU:HB2	2.41	0.46
2:D:292:MET:SD	2:D:292:MET:N	2.88	0.46
3:I:30:GLU:O	3:I:34:LEU:HG	2.15	0.46
1:A:148:LEU:HD12	1:A:148:LEU:H	1.81	0.46
2:C:93:PHE:CG	2:C:115:LEU:HD13	2.51	0.46
2:C:374:LYS:HB3	2:C:374:LYS:HE3	1.75	0.46
2:C:410:PHE:O	2:C:466:ARG:NH1	2.49	0.46
2:C:482:GLN:O	2:C:505:GLN:HA	2.16	0.46
2:D:175:LEU:HG	2:D:612:ARG:NH2	2.31	0.46
2:D:655:TYR:O	2:D:659:THR:HG23	2.15	0.46
2:C:392:LEU:HB2	2:C:446:VAL:HG12	1.97	0.46
2:D:118:LEU:O	2:D:122:ARG:HG2	2.15	0.45
3:K:47:GLN:O	3:K:51:TRP:HB2	2.16	0.45
3:L:111:PHE:HB3	3:L:151:ARG:O	2.16	0.45
2:C:391:ASP:OD2	2:C:393:ARG:NH1	2.50	0.45
2:D:65:ALA:O	2:D:69:LYS:HG3	2.16	0.45
2:D:276:ILE:HB	2:D:280:ASP:O	2.17	0.45
3:J:124:ILE:HD13	3:J:130:VAL:HG13	1.99	0.45
2:C:511:PHE:HE2	2:C:519:THR:HG22	1.80	0.45
1:B:233:LEU:O	1:B:237:ASN:ND2	2.40	0.45
2:C:193:ARG:HA	2:C:196:LYS:HG2	1.99	0.45
2:D:407:SER:HA	2:D:457:PHE:CE1	2.52	0.45
1:B:165:PHE:HA	1:B:168:LEU:HD12	1.99	0.45
2:C:116:TYR:O	2:C:120:GLN:HG2	2.17	0.45
2:C:417:VAL:CG1	2:C:429:ASP:HB3	2.46	0.45
1:B:31:ALA:HB2	1:B:229:LEU:HG	1.99	0.44
1:B:97:GLU:H	1:B:97:GLU:CD	2.20	0.44
2:D:315:VAL:HB	2:D:335:ARG:CZ	2.47	0.44
2:C:354:LYS:HA	2:C:354:LYS:HD3	1.83	0.44
2:D:508:ILE:HG12	2:D:509:GLN:HG3	1.99	0.44
3:K:48:TYR:CZ	3:K:140:ILE:HG13	2.52	0.44
1:B:29:VAL:HB	1:B:233:LEU:HD21	1.99	0.44
3:K:51:TRP:O	3:K:138:VAL:HG11	2.17	0.44
2:C:567:PHE:HB3	2:C:570:GLU:HB3	1.99	0.44
1:B:254:THR:HG22	1:B:281:LEU:HD13	2.00	0.44
2:C:79:ASP:OD2	2:C:83:ASN:N	2.51	0.44
2:C:508:ILE:HG13	2:C:509:GLN:HG3	2.00	0.44
2:D:380:LEU:HD21	2:D:384:ASN:O	2.17	0.44
2:D:482:GLN:O	2:D:505:GLN:HA	2.18	0.44
3:K:131:HIS:CE1	3:K:133:SER:HB2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:74:ARG:HA	3:L:77:ARG:HG2	2.00	0.44
3:I:118:ARG:NH1	3:I:153:ASN:OD1	2.51	0.44
3:J:31:PHE:O	3:J:34:LEU:HG	2.18	0.44
2:C:343:ARG:HD3	2:C:343:ARG:HA	1.81	0.43
1:A:179:GLU:HG2	1:A:183:LYS:HE3	2.00	0.43
2:C:177:LEU:HD23	2:C:187:ILE:HG23	1.99	0.43
2:D:411:ILE:HG12	2:D:464:TYR:CD2	2.53	0.43
3:J:99:SER:OG	3:J:102:ASN:OD1	2.36	0.43
2:D:532:THR:HG22	2:D:592:ILE:HD11	2.00	0.43
3:J:48:TYR:O	3:J:52:LYS:N	2.50	0.43
2:C:103:GLU:HG2	2:C:112:PHE:CE2	2.54	0.43
2:D:113:TYR:OH	2:D:207:SER:OG	2.22	0.43
2:D:122:ARG:HA	2:D:122:ARG:HD2	1.79	0.43
2:D:347:MET:SD	2:D:376:GLN:HA	2.58	0.43
2:D:415:PRO:HA	2:D:430:SER:HB3	1.99	0.43
2:C:123:ARG:HA	2:C:123:ARG:HD2	1.88	0.43
2:C:140:PHE:CZ	2:C:175:LEU:HD13	2.54	0.43
1:A:233:LEU:O	1:A:237:ASN:ND2	2.38	0.43
2:D:68:ALA:HB1	2:D:97:LYS:HE2	1.99	0.43
2:C:511:PHE:CE2	2:C:519:THR:HG22	2.54	0.43
2:C:617:ASN:HA	2:C:620:ASP:OD2	2.18	0.43
3:J:132:ALA:HA	3:J:138:VAL:HA	1.99	0.43
1:B:46:ARG:HA	1:B:46:ARG:HD2	1.72	0.43
2:D:319:ILE:HB	2:D:329:ARG:HB3	2.01	0.43
1:A:125:LEU:HD21	2:C:490:TYR:CG	2.54	0.43
1:A:82:ARG:HG3	3:K:28:GLN:OE1	2.19	0.42
2:D:83:ASN:HB3	2:D:166:TRP:CZ2	2.54	0.42
2:D:570:GLU:CD	2:D:669:LEU:HD11	2.39	0.42
2:D:576:ASN:HA	2:D:579:ILE:HG12	2.01	0.42
3:I:124:ILE:HD13	3:I:130:VAL:HG23	2.01	0.42
3:K:52:LYS:HE2	3:L:43:ARG:CD	2.49	0.42
2:C:193:ARG:HA	2:C:196:LYS:HE3	2.00	0.42
2:D:587:ASN:OD1	2:D:588:ILE:N	2.53	0.42
3:L:69:SER:HB3	3:L:88:THR:CG2	2.49	0.42
2:C:280:ASP:HB3	2:C:320:LEU:H	1.84	0.42
2:C:179:LEU:HD21	2:C:616:ASN:OD1	2.19	0.42
3:I:31:PHE:O	3:I:35:VAL:HG23	2.20	0.42
2:C:103:GLU:HG2	2:C:112:PHE:HE2	1.85	0.42
2:D:84:VAL:HB	2:D:123:ARG:NH2	2.33	0.42
1:A:89:LEU:HG	1:A:98:VAL:HG11	2.01	0.42
2:C:512:TYR:CD2	2:C:518:SER:HB3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:68:CYS:HA	3:J:132:ALA:HB3	2.00	0.42
3:L:100:ARG:O	3:L:103:LEU:HG	2.20	0.42
2:D:134:LEU:HG	2:D:174:GLU:OE2	2.19	0.42
2:D:343:ARG:HD2	2:D:343:ARG:HA	1.88	0.42
2:D:445:LEU:HD22	2:D:659:THR:HG21	2.02	0.42
3:I:105:THR:HG23	3:J:25:GLN:HE22	1.84	0.42
1:A:118:ALA:O	1:A:122:VAL:HG23	2.20	0.42
2:C:273:SER:O	2:C:277:SER:OG	2.37	0.42
1:A:89:LEU:HD23	1:A:89:LEU:HA	1.86	0.42
2:C:360:LEU:HD11	2:C:373:VAL:HG22	2.02	0.42
2:C:231:PRO:HB3	2:C:500:ALA:HB3	2.02	0.42
2:C:456:ILE:HG12	2:C:511:PHE:CE1	2.55	0.42
2:C:647:LYS:HE3	2:C:647:LYS:HB3	1.88	0.42
2:D:58:ARG:NH1	2:D:222:ILE:O	2.41	0.42
1:A:219:LEU:HG	1:A:232:HIS:HB3	2.02	0.41
1:B:206:TYR:CE1	1:B:243:TYR:HB2	2.55	0.41
2:D:28:ARG:HB3	2:D:29:ALA:H	1.74	0.41
2:D:389:ILE:HA	2:D:443:VAL:O	2.20	0.41
3:K:142:SER:HB3	3:K:145:GLU:HG3	2.01	0.41
1:A:231:GLU:O	1:A:235:GLU:HG2	2.19	0.41
1:B:118:ALA:O	1:B:122:VAL:HG23	2.20	0.41
1:A:97:GLU:H	1:A:97:GLU:CD	2.24	0.41
1:A:162:ASN:OD1	1:A:162:ASN:N	2.52	0.41
2:C:99:GLU:O	2:C:99:GLU:HG2	2.20	0.41
2:C:316:ARG:HE	2:C:330:THR:HG21	1.84	0.41
2:C:640:LYS:HE3	2:C:640:LYS:HB3	1.78	0.41
3:I:145:GLU:HB2	3:I:148:TRP:HD1	1.86	0.41
1:B:124:GLU:OE1	2:D:490:TYR:OH	2.33	0.41
2:C:381:GLU:HB2	2:C:438:TYR:CB	2.51	0.41
2:C:513:ARG:HB2	2:C:515:ASN:OD1	2.20	0.41
2:C:294:ASP:N	2:C:294:ASP:OD1	2.51	0.41
3:I:34:LEU:O	3:I:38:VAL:HB	2.19	0.41
2:C:608:ASN:HB3	2:C:611:VAL:HG22	2.03	0.41
2:D:320:LEU:HD11	2:D:328:THR:HG22	2.01	0.41
2:D:572:LEU:HA	2:D:575:HIS:CD2	2.55	0.41
3:K:72:VAL:HG21	3:K:120:VAL:HG22	2.03	0.41
2:C:206:ASN:OD1	2:C:206:ASN:N	2.52	0.41
2:C:229:LEU:HD11	2:C:505:GLN:NE2	2.36	0.41
2:C:249:GLY:HA3	2:C:338:ILE:HG21	2.01	0.41
2:C:333:LEU:HD12	2:C:334:THR:H	1.84	0.41
2:C:362:ILE:HD12	2:C:369:LEU:HD11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:587:ASN:HB2	2:D:626:ARG:CZ	2.51	0.41
2:C:115:LEU:HD12	2:C:115:LEU:HA	1.87	0.41
2:C:186:GLU:O	2:C:189:GLU:HG3	2.21	0.41
2:C:392:LEU:HB3	2:C:395:ASN:HD22	1.86	0.41
2:D:84:VAL:HG21	2:D:126:ARG:HB2	2.03	0.41
2:D:162:LEU:H	2:D:162:LEU:HD23	1.86	0.41
3:I:24:LEU:HD23	3:I:24:LEU:HA	1.92	0.41
3:J:43:ARG:HG2	3:J:79:GLN:OE1	2.20	0.41
2:C:159:GLU:O	2:C:163:ASN:HB2	2.21	0.41
2:C:287:GLN:OE1	2:C:287:GLN:N	2.54	0.41
2:C:640:LYS:HD2	2:C:641:LYS:HB2	2.01	0.41
1:A:250:LEU:O	1:A:254:THR:HG23	2.21	0.40
2:C:418:GLN:OE1	2:C:556:ALA:HB2	2.22	0.40
2:D:261:ILE:HG22	2:D:263:SER:HB3	2.03	0.40
2:D:310:PRO:HD2	2:D:313:SER:HB2	2.03	0.40
2:D:527:ASP:HB3	2:D:568:GLU:HG3	2.02	0.40
2:D:560:LYS:HE2	2:D:560:LYS:HB3	1.90	0.40
3:I:36:ARG:HH22	3:I:162:SER:HA	1.85	0.40
3:K:75:THR:HG21	3:K:122:ILE:HD11	2.03	0.40
1:B:103:GLY:O	1:B:107:THR:HG23	2.21	0.40
2:C:265:VAL:HG23	2:C:266:ALA:H	1.86	0.40
2:D:141:THR:HG21	2:D:609:TYR:HB2	2.04	0.40
2:D:656:LEU:O	2:D:660:VAL:HG23	2.20	0.40
3:I:48:TYR:CZ	3:I:140:ILE:HG13	2.56	0.40
3:I:67:ASP:CG	3:I:86:ARG:HH22	2.25	0.40
2:C:265:VAL:O	2:C:267:GLY:N	2.53	0.40
2:D:466:ARG:HE	2:D:466:ARG:HB3	1.72	0.40
3:I:88:THR:HG23	3:I:120:VAL:HB	2.02	0.40
1:A:242:LYS:HD2	1:A:242:LYS:HA	1.95	0.40
1:B:113:ASP:HA	1:B:116:TYR:CD2	2.56	0.40
2:C:81:SER:HB3	2:C:150:ARG:CG	2.51	0.40
2:D:190:THR:O	2:D:194:ARG:HG3	2.21	0.40
2:D:470:VAL:HG13	2:D:528:ILE:HB	2.04	0.40
2:C:81:SER:O	2:C:150:ARG:HG3	2.21	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	262/297 (88%)	255 (97%)	7 (3%)	0	100 100
1	B	262/297 (88%)	255 (97%)	7 (3%)	0	100 100
2	C	645/688 (94%)	592 (92%)	52 (8%)	1 (0%)	47 81
2	D	649/688 (94%)	591 (91%)	56 (9%)	2 (0%)	41 75
3	I	140/168 (83%)	132 (94%)	8 (6%)	0	100 100
3	J	145/168 (86%)	135 (93%)	10 (7%)	0	100 100
3	K	138/168 (82%)	129 (94%)	9 (6%)	0	100 100
3	L	146/168 (87%)	136 (93%)	10 (7%)	0	100 100
All	All	2387/2642 (90%)	2225 (93%)	159 (7%)	3 (0%)	51 84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	267	GLY
2	D	266	ALA
2	C	265	VAL

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	225/254 (89%)	222 (99%)	3 (1%)	69 86
1	B	225/254 (89%)	223 (99%)	2 (1%)	78 90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	557/588 (95%)	547 (98%)	10 (2%)	59 81
2	D	559/588 (95%)	551 (99%)	8 (1%)	67 85
3	I	124/146 (85%)	122 (98%)	2 (2%)	62 83
3	J	129/146 (88%)	126 (98%)	3 (2%)	50 77
3	K	122/146 (84%)	121 (99%)	1 (1%)	81 91
3	L	130/146 (89%)	130 (100%)	0	100 100
All	All	2071/2268 (91%)	2042 (99%)	29 (1%)	67 85

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	159	ASP
1	A	162	ASN
1	B	159	ASP
1	B	179	GLU
2	C	126	ARG
2	C	138	MET
2	C	150	ARG
2	C	197	PHE
2	C	354	LYS
2	C	374	LYS
2	C	457	PHE
2	C	578	ARG
2	C	601	LYS
2	C	640	LYS
2	D	123	ARG
2	D	162	LEU
2	D	197	PHE
2	D	336	GLU
2	D	366	TYR
2	D	425	LYS
2	D	457	PHE
2	D	648	ASP
3	I	131	HIS
3	I	153	ASN
3	J	43	ARG
3	J	118	ARG
3	J	131	HIS
3	K	131	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	418	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

14 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	$\#\|Z\| > 2$
6	PO4	K	205	-	4,4,4	0.92	0	6,6,6	0.43	0
6	PO4	L	202	-	4,4,4	0.92	0	6,6,6	0.44	0
6	PO4	I	202	-	4,4,4	0.91	0	6,6,6	0.46	0
6	PO4	K	203	-	4,4,4	0.92	0	6,6,6	0.43	0
6	PO4	K	204	-	4,4,4	0.91	0	6,6,6	0.43	0
6	PO4	J	203	-	4,4,4	0.92	0	6,6,6	0.43	0
6	PO4	L	201	-	4,4,4	0.93	0	6,6,6	0.46	0
6	PO4	K	202	-	4,4,4	0.92	0	6,6,6	0.43	0
6	PO4	I	201	-	4,4,4	0.94	0	6,6,6	0.41	0
6	PO4	K	201	-	4,4,4	0.92	0	6,6,6	0.42	0
6	PO4	J	202	-	4,4,4	0.92	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PO4	I	203	-	4,4,4	0.91	0	6,6,6	0.47	0
6	PO4	J	201	-	4,4,4	0.92	0	6,6,6	0.39	0
6	PO4	I	204	-	4,4,4	0.92	0	6,6,6	0.43	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	201	PO4	1	0
6	J	201	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	264/297 (88%)	0.03	1 (0%) 92 90	75, 100, 148, 257	0
1	B	264/297 (88%)	-0.00	4 (1%) 73 68	75, 102, 153, 250	0
2	C	647/688 (94%)	1.17	167 (25%) 0 0	116, 237, 331, 402	0
2	D	651/688 (94%)	1.07	136 (20%) 1 1	117, 235, 329, 487	0
3	I	142/168 (84%)	0.38	5 (3%) 44 39	90, 124, 178, 230	0
3	J	147/168 (87%)	0.04	3 (2%) 65 60	102, 136, 188, 303	0
3	K	140/168 (83%)	0.25	4 (2%) 51 45	90, 117, 170, 229	0
3	L	148/168 (88%)	0.14	6 (4%) 37 33	89, 145, 188, 271	0
4	M	0/8	-	-	-	-
5	N	0/9	-	-	-	-
All	All	2403/2659 (90%)	0.66	326 (13%) 3 4	75, 165, 311, 487	0

All (326) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	358	GLY	14.8
2	D	131	LEU	10.5
2	D	323	GLY	10.4
2	D	432	THR	9.3
2	C	607	LEU	9.1
2	D	186	GLU	8.8
2	D	247	GLY	8.6
2	D	132	SER	8.5
2	D	321	PRO	8.4
2	D	322	ALA	8.1
2	D	282	ILE	8.0
2	C	331	VAL	8.0
2	C	190	THR	8.0
2	D	344	ALA	7.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	276	ILE	7.6
2	D	181	GLY	7.5
2	C	606	SER	7.4
2	C	385	VAL	7.2
2	D	355	GLU	7.1
2	D	190	THR	6.9
2	C	326	THR	6.9
2	C	557	THR	6.7
2	C	247	GLY	6.5
2	D	354	LYS	6.4
2	D	385	VAL	6.4
2	C	143	ASN	6.4
2	C	642	LEU	6.3
2	C	595	PHE	6.2
2	D	133	VAL	6.1
2	C	332	THR	6.0
2	D	332	THR	5.8
2	D	378	GLN	5.8
2	D	191	LEU	5.7
2	C	253	GLN	5.5
2	D	434	GLY	5.5
2	D	595	PHE	5.5
2	C	649	TYR	5.4
2	C	643	ASP	5.3
2	D	281	LYS	5.2
2	C	363	PRO	5.2
2	C	575	HIS	5.2
2	C	559	VAL	5.2
2	D	671	LYS	5.1
2	C	665	ASP	5.1
2	C	281	LYS	5.1
2	D	348	SER	5.0
2	D	435	GLN	5.0
2	C	664	LEU	5.0
2	C	639	LEU	5.0
2	D	318	GLU	5.0
2	D	606	SER	4.9
2	D	428	GLU	4.9
2	C	191	LEU	4.9
2	C	353	GLY	4.8
2	C	637	PRO	4.8
2	C	375	VAL	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	325	GLY	4.8
2	C	569	PRO	4.8
2	C	553	ILE	4.7
2	C	666	LEU	4.7
2	D	374	LYS	4.7
2	C	310	PRO	4.7
2	D	327	LYS	4.7
2	C	147	ASN	4.7
2	D	567	PHE	4.7
2	C	420	ARG	4.6
2	C	330	THR	4.5
2	C	155	TRP	4.5
3	L	165	HIS	4.4
2	D	672	ALA	4.4
2	C	311	LYS	4.4
2	D	644	ASP	4.4
2	C	327	LYS	4.4
2	C	526	PRO	4.3
2	D	260	VAL	4.3
2	C	180	THR	4.3
2	C	573	LYS	4.2
2	C	627	LEU	4.2
2	C	25	ASP	4.2
2	D	645	LEU	4.2
2	C	259	THR	4.2
2	C	144	ASP	4.1
2	D	192	THR	4.1
2	C	350	LYS	4.1
2	C	361	ASP	4.1
2	C	625	ALA	4.0
2	D	183	THR	4.0
2	D	326	THR	4.0
2	C	563	ASP	4.0
3	K	131	HIS	3.9
2	C	349	VAL	3.9
2	D	353	GLY	3.9
2	C	260	VAL	3.9
2	D	561	SER	3.9
2	C	142	GLY	3.9
2	D	331	VAL	3.9
2	C	261	ILE	3.9
2	C	408	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	346	LYS	3.8
2	D	464	TYR	3.8
2	C	289	GLY	3.8
2	D	670	GLU	3.8
2	C	433	ASP	3.7
2	C	187	ILE	3.7
2	D	193	ARG	3.7
2	D	148	LEU	3.7
2	D	149	ASP	3.7
2	D	565	THR	3.7
3	L	103	LEU	3.7
2	C	644	ASP	3.7
2	D	156	PRO	3.7
2	D	646	PRO	3.7
2	D	674	PRO	3.7
2	C	359	VAL	3.7
2	D	521	ARG	3.7
2	D	592	ILE	3.7
2	D	542	LYS	3.6
3	K	69	SER	3.6
2	C	431	ASP	3.6
2	D	352	VAL	3.6
2	C	322	ALA	3.6
2	C	669	LEU	3.6
3	K	121	GLY	3.6
2	D	187	ILE	3.6
2	C	539	THR	3.6
3	J	103	LEU	3.6
2	C	357	VAL	3.6
3	I	121	GLY	3.6
2	D	433	ASP	3.5
3	L	21	THR	3.5
2	D	188	ARG	3.5
2	D	599	LYS	3.5
2	D	343	ARG	3.4
2	D	603	ASN	3.4
2	C	280	ASP	3.4
2	C	554	ASP	3.4
2	D	431	ASP	3.4
2	D	262	ASN	3.4
2	D	27	THR	3.4
2	D	568	GLU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	321	PRO	3.4
2	D	137	PRO	3.4
2	D	320	LEU	3.4
2	C	27	THR	3.4
2	C	668	LYS	3.4
3	I	141	SER	3.3
2	D	333	LEU	3.3
2	C	449	PHE	3.3
2	D	194	ARG	3.3
2	C	258	TYR	3.3
3	J	155	ALA	3.3
2	D	25	ASP	3.3
2	C	540	GLY	3.3
2	D	643	ASP	3.3
2	D	607	LEU	3.3
2	C	249	GLY	3.3
2	D	280	ASP	3.3
2	C	566	ALA	3.3
2	C	134	LEU	3.2
2	C	354	LYS	3.2
2	D	294	ASP	3.2
2	C	636	LYS	3.2
2	D	26	ILE	3.2
2	C	648	ASP	3.2
2	C	177	LEU	3.2
3	L	64	LYS	3.2
2	C	176	SER	3.2
2	C	124	PHE	3.2
2	C	605	VAL	3.2
2	D	184	ASP	3.1
2	C	501	LEU	3.1
2	D	596	ASN	3.1
2	C	282	ILE	3.1
2	C	364	GLY	3.1
2	C	623	ARG	3.0
2	C	478	GLY	3.0
2	D	649	TYR	3.0
2	D	122	ARG	3.0
2	C	336	GLU	3.0
2	C	352	VAL	3.0
2	C	667	ALA	3.0
2	D	639	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	278	VAL	3.0
2	C	156	PRO	3.0
2	D	185	LYS	2.9
2	C	186	GLU	2.9
3	I	160	SER	2.9
2	C	319	ILE	2.9
2	C	351	THR	2.9
2	C	432	THR	2.9
2	D	189	GLU	2.9
2	C	576	ASN	2.9
2	D	175	LEU	2.9
2	C	435	GLN	2.8
2	D	330	THR	2.8
2	C	325	GLY	2.8
2	D	261	ILE	2.8
2	C	146	TYR	2.8
2	D	316	ARG	2.8
2	D	279	GLY	2.8
2	D	520	GLN	2.8
2	C	570	GLU	2.8
2	D	347	MET	2.8
2	C	645	LEU	2.8
2	D	379	LYS	2.8
2	D	569	PRO	2.8
2	C	574	GLU	2.8
2	C	558	TYR	2.8
2	C	205	THR	2.8
2	D	397	GLY	2.8
2	D	648	ASP	2.8
2	D	604	ILE	2.7
2	C	318	GLU	2.7
2	C	604	ILE	2.7
2	D	541	GLU	2.7
2	D	399	ALA	2.7
2	C	634	GLU	2.7
2	D	627	LEU	2.7
2	C	457	PHE	2.7
2	C	561	SER	2.7
2	D	336	GLU	2.7
2	C	251	VAL	2.7
2	C	88	SER	2.7
2	C	584	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	174	GLU	2.6
3	L	168	HIS	2.6
2	D	558	TYR	2.6
2	C	641	LYS	2.6
2	D	637	PRO	2.6
3	I	151	ARG	2.6
2	C	204	GLN	2.6
2	D	134	LEU	2.6
2	D	628	ASN	2.6
2	D	641	LYS	2.6
2	D	668	LYS	2.6
2	C	188	ARG	2.6
2	D	346	LYS	2.6
2	C	626	ARG	2.6
2	C	521	ARG	2.5
2	C	185	LYS	2.5
2	C	444	VAL	2.5
2	C	632	LYS	2.5
2	C	418	GLN	2.5
2	C	635	GLY	2.5
2	C	624	LEU	2.5
2	D	439	LYS	2.5
2	D	566	ALA	2.5
2	D	390	ILE	2.5
2	D	144	ASP	2.5
2	C	192	THR	2.5
2	D	580	ALA	2.5
2	D	319	ILE	2.5
3	J	104	ARG	2.5
2	C	562	GLY	2.5
2	C	342	ASP	2.5
2	C	316	ARG	2.4
2	C	290	LYS	2.4
2	C	599	LYS	2.4
2	C	374	LYS	2.4
2	C	183	THR	2.4
1	B	286	ASP	2.4
2	C	450	SER	2.4
2	C	275	ALA	2.4
2	C	671	LYS	2.4
2	C	598	MET	2.4
2	C	525	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	251	VAL	2.4
2	D	287	GLN	2.4
2	D	636	LYS	2.4
2	C	31	GLN	2.3
2	D	328	THR	2.3
2	D	252	LEU	2.3
2	C	398	GLY	2.3
2	D	145	THR	2.3
2	C	26	ILE	2.3
3	K	68	CYS	2.3
2	C	312	GLY	2.3
2	C	535	GLU	2.3
2	D	598	MET	2.3
2	C	384	ASN	2.3
2	D	315	VAL	2.3
2	D	171	LYS	2.3
3	I	21	THR	2.3
2	C	531	PRO	2.3
2	D	182	LYS	2.3
2	C	85	LEU	2.2
2	D	573	LYS	2.2
2	C	424	GLY	2.2
2	D	136	LYS	2.2
2	D	31	GLN	2.2
2	D	384	ASN	2.2
2	C	89	ASP	2.2
2	D	478	GLY	2.2
2	C	663	ALA	2.2
2	D	363	PRO	2.2
2	D	371	ASP	2.2
2	D	310	PRO	2.2
2	D	334	THR	2.2
2	C	628	ASN	2.2
2	C	323	GLY	2.2
2	C	458	ALA	2.2
1	B	288	LEU	2.2
2	C	597	ALA	2.1
2	C	189	GLU	2.1
2	C	175	LEU	2.1
2	C	333	LEU	2.1
2	C	262	ASN	2.1
1	B	287	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	572	LEU	2.1
2	D	590	LYS	2.1
1	A	285	GLN	2.1
2	C	434	GLY	2.1
2	D	180	THR	2.1
2	D	535	GLU	2.1
2	C	248	ILE	2.1
2	D	424	GLY	2.1
2	C	362	ILE	2.1
2	C	138	MET	2.1
2	C	541	GLU	2.1
2	D	602	ARG	2.1
2	C	367	VAL	2.0
1	B	285	GLN	2.0
3	L	81	GLY	2.0
2	D	675	ALA	2.0
2	C	328	THR	2.0
2	C	317	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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
6	PO4	K	201	5/5	0.69	0.25	175,185,221,227	0
6	PO4	K	204	5/5	0.75	0.25	182,187,222,240	0
6	PO4	I	202	5/5	0.79	0.22	164,164,192,200	0
6	PO4	K	203	5/5	0.84	0.20	165,177,211,226	0
6	PO4	I	201	5/5	0.85	0.23	195,204,212,215	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PO4	J	203	5/5	0.86	0.21	162,199,226,242	0
6	PO4	I	203	5/5	0.86	0.25	120,169,174,175	0
6	PO4	I	204	5/5	0.88	0.50	176,180,209,227	0
6	PO4	L	202	5/5	0.88	0.28	136,166,191,204	0
6	PO4	K	202	5/5	0.90	0.17	131,149,177,193	0
6	PO4	J	202	5/5	0.91	0.19	143,144,153,162	0
6	PO4	L	201	5/5	0.92	0.19	122,157,181,208	0
6	PO4	K	205	5/5	0.93	0.17	121,138,170,188	0
6	PO4	J	201	5/5	0.97	0.25	123,127,178,192	0

6.5 Other polymers (i)

There are no such residues in this entry.