Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 02:17 AM EDT

PDB ID	:	4KI3
Title	:	1.70 Angstrom resolution crystal structure of outer-membrane lipoprotein carrier protein (lolA) from Yersinia pestis CO92
Authors	:	Halavaty, A.S.; Wawrzak, Z.; Kudritska, M.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2013-05-01
Resolution	:	1.70 Å(reported)

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

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

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

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

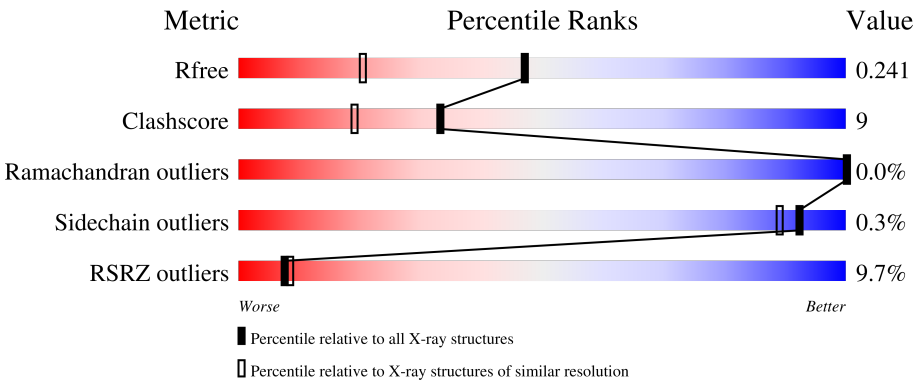
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.70 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 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	184	9%, 80%, 16%, •
1	B	184	5%, 76%, 16%, 8%
1	C	184	13%, 81%, 15%, •
1	D	184	9%, 87%, 10%, • •
1	E	184	7%, 78%, 14%, 8%

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Mol	Chain	Length	Quality of chain
1	F	184	9% 84% 11%
1	G	184	7% 83% 14%
1	H	184	4% 80% 13% 7%
1	I	184	9% 84% 14%
1	J	184	16% 81% 14%
1	K	184	8% 79% 14% 7%
1	L	184	16% 81% 15%

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	ACT	H	301	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19260 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 Outer-membrane lipoprotein carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	177	1490	933	251	304	2	0	12	0
1	B	169	1453	913	248	289	3	0	14	0
1	C	177	1491	936	253	299	3	0	12	0
1	D	179	1524	950	260	312	2	0	14	0
1	E	169	1409	887	237	283	2	0	9	0
1	F	177	1482	928	250	301	3	0	11	0
1	G	179	1520	950	253	315	2	0	15	0
1	H	172	1434	901	241	290	2	0	10	0
1	I	180	1494	937	252	302	3	0	10	0
1	J	177	1503	944	252	304	3	0	13	0
1	K	171	1389	874	232	280	3	0	5	0
1	L	176	1464	915	248	298	3	0	10	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	SER	-	expression tag	UNP E8P443
A	20	ASN	-	expression tag	UNP E8P443
B	19	SER	-	expression tag	UNP E8P443
B	20	ASN	-	expression tag	UNP E8P443
C	19	SER	-	expression tag	UNP E8P443

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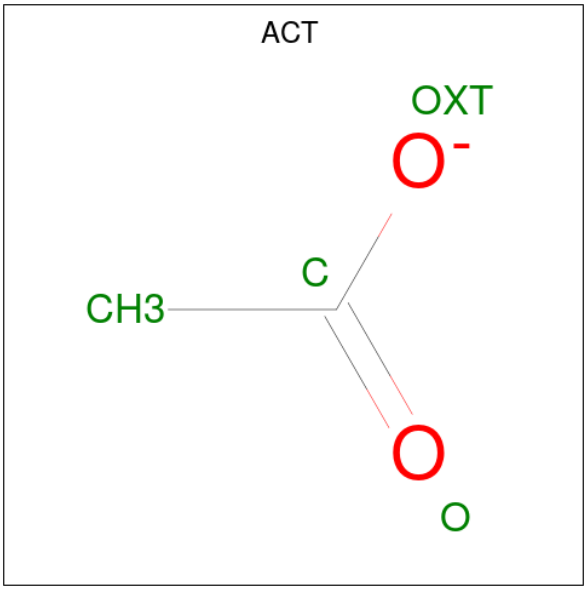
Chain	Residue	Modelled	Actual	Comment	Reference
C	20	ASN	-	expression tag	UNP E8P443
D	19	SER	-	expression tag	UNP E8P443
D	20	ASN	-	expression tag	UNP E8P443
E	19	SER	-	expression tag	UNP E8P443
E	20	ASN	-	expression tag	UNP E8P443
F	19	SER	-	expression tag	UNP E8P443
F	20	ASN	-	expression tag	UNP E8P443
G	19	SER	-	expression tag	UNP E8P443
G	20	ASN	-	expression tag	UNP E8P443
H	19	SER	-	expression tag	UNP E8P443
H	20	ASN	-	expression tag	UNP E8P443
I	19	SER	-	expression tag	UNP E8P443
I	20	ASN	-	expression tag	UNP E8P443
J	19	SER	-	expression tag	UNP E8P443
J	20	ASN	-	expression tag	UNP E8P443
K	19	SER	-	expression tag	UNP E8P443
K	20	ASN	-	expression tag	UNP E8P443
L	19	SER	-	expression tag	UNP E8P443
L	20	ASN	-	expression tag	UNP E8P443

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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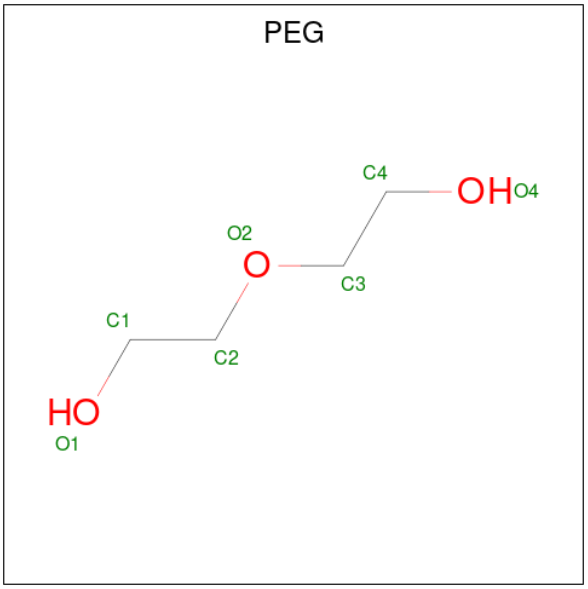
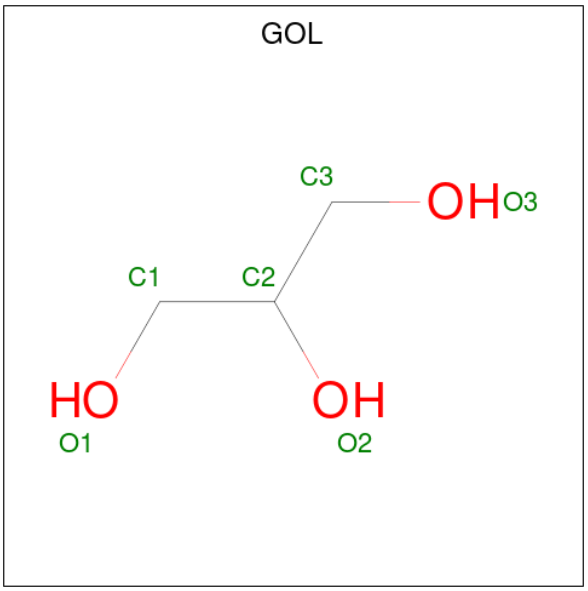
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	D	1	4	2	2	0	0
			Total	C	O		
2	F	1	4	2	2	0	0
			Total	C	O		
2	G	1	4	2	2	0	0
			Total	C	O		
2	H	1	4	2	2	0	0
			Total	C	O		
2	I	1	4	2	2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	7	4	3	0	0
			Total	C	O		
3	D	1	14	8	6	0	1
			Total	C	O		
3	J	1	7	4	3	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	H	1	6	3	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	143	144	144	0	3
			Total	O		
5	B	137	141	141	0	5
			Total	O		
5	C	122	128	128	0	7
			Total	O		
5	D	146	153	153	0	8
			Total	O		
5	E	100	102	102	0	2
			Total	O		
5	F	116	119	119	0	8
			Total	O		
5	G	133	139	139	0	8
			Total	O		
5	H	146	149	149	0	5
			Total	O		
5	I	137	138	138	0	3
			Total	O		
5	J	104	108	108	0	4

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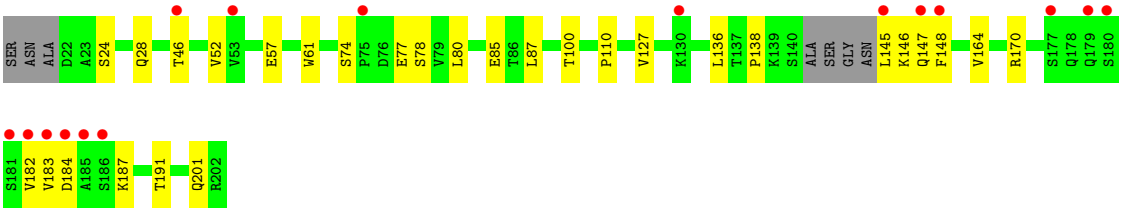
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	K	107	109	109	0	3
			Total	O		
5	L	106	109	109	0	3

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.

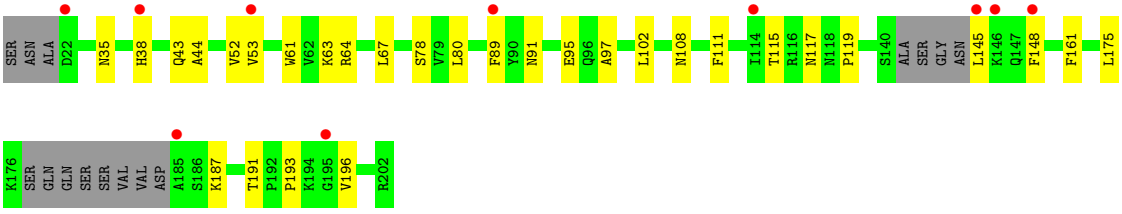
• Molecule 1: Outer-membrane lipoprotein carrier protein

Chain A:



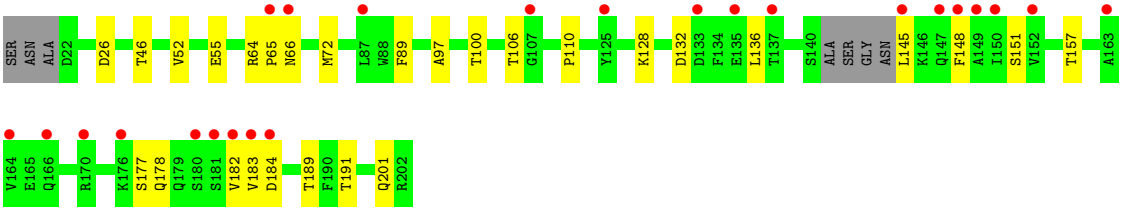
• Molecule 1: Outer-membrane lipoprotein carrier protein

Chain B:



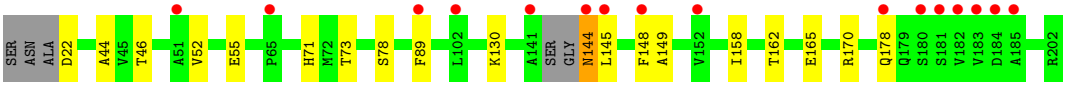
• Molecule 1: Outer-membrane lipoprotein carrier protein

Chain C:



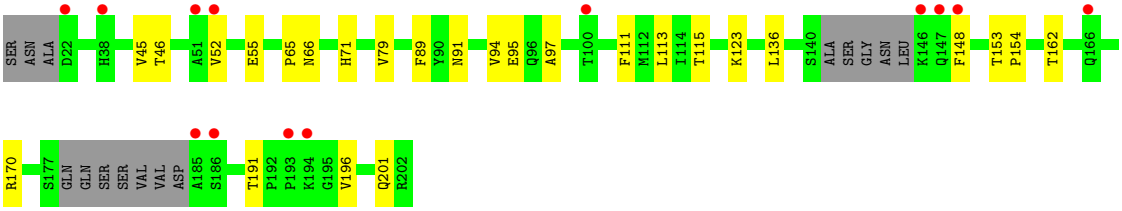
• Molecule 1: Outer-membrane lipoprotein carrier protein

Chain D:



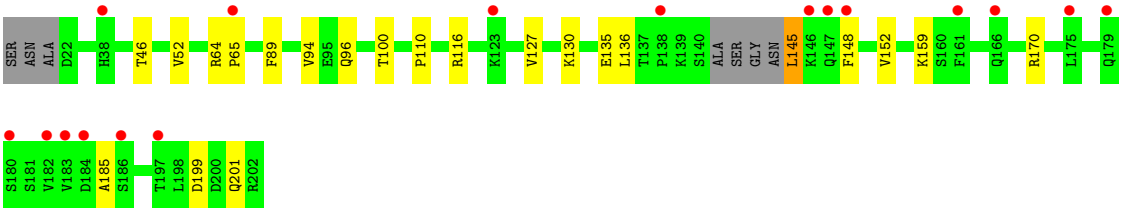
• Molecule 1: Outer-membrane lipoprotein carrier protein

Chain E:



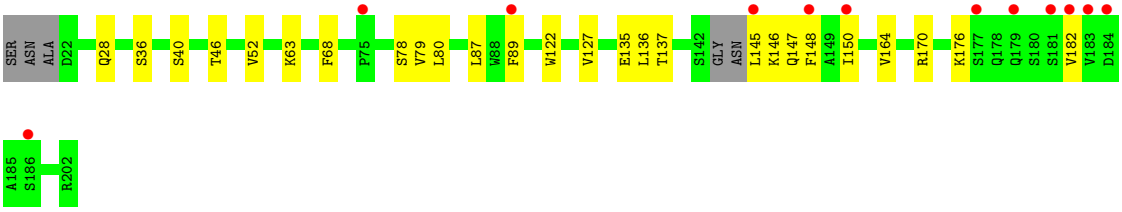
• Molecule 1: Outer-membrane lipoprotein carrier protein

Chain F:



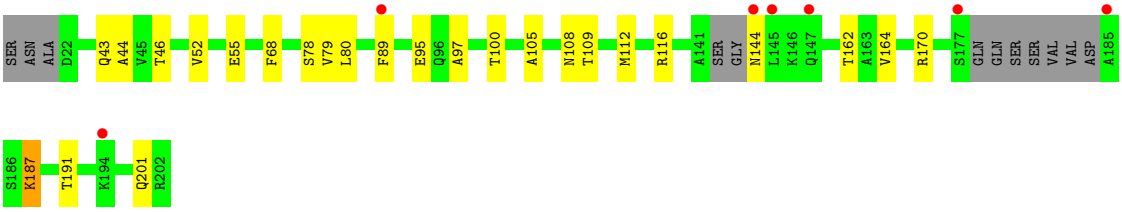
• Molecule 1: Outer-membrane lipoprotein carrier protein

Chain G:



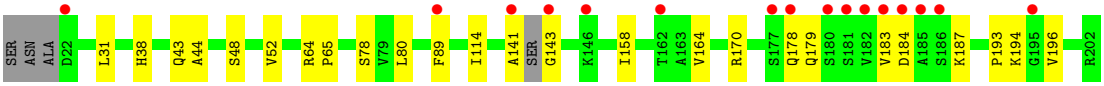
• Molecule 1: Outer-membrane lipoprotein carrier protein

Chain H:



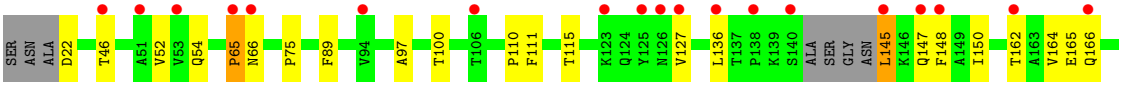
• Molecule 1: Outer-membrane lipoprotein carrier protein

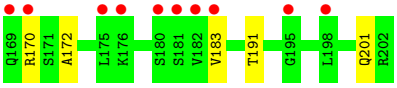
Chain I:



• Molecule 1: Outer-membrane lipoprotein carrier protein

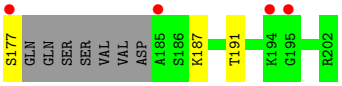
Chain J:





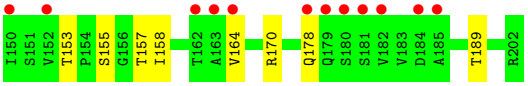
• Molecule 1: Outer-membrane lipoprotein carrier protein

Chain K:



• Molecule 1: Outer-membrane lipoprotein carrier protein

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.20Å 67.13Å 132.56Å 94.30° 94.01° 120.01°	Depositor
Resolution (Å)	29.09 – 1.70 29.08 – 1.70	Depositor EDS
% Data completeness (in resolution range)	93.8 (29.09-1.70) 93.8 (29.08-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.204 , 0.240 0.211 , 0.241	Depositor DCC
R_{free} test set	10416 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 35.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.277 for -k,-h,-l	Xtriage
Reported twinning fraction	0.749 for H, K, L 0.251 for -K, -H, -L	Depositor
Outliers	0 of 207034 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19260	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, GOL, PEG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.62	0/1524	0.80	0/2071
1	B	0.63	0/1487	0.84	0/2019
1	C	0.55	0/1525	0.82	0/2072
1	D	0.63	0/1558	0.79	0/2112
1	E	0.56	0/1443	0.78	0/1958
1	F	0.58	0/1515	0.81	0/2054
1	G	0.61	0/1554	0.83	0/2113
1	H	0.58	0/1467	0.80	0/1991
1	I	0.60	0/1529	0.79	0/2075
1	J	0.52	0/1538	0.78	0/2089
1	K	0.53	0/1420	0.77	0/1925
1	L	0.55	0/1498	0.78	0/2037
All	All	0.58	0/18058	0.80	0/24516

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 (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	1490	0	1411	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1453	0	1380	28	0
1	C	1491	0	1429	34	0
1	D	1524	0	1435	19	0
1	E	1409	0	1335	20	0
1	F	1482	0	1410	26	0
1	G	1520	0	1431	25	0
1	H	1434	0	1359	32	0
1	I	1494	0	1411	23	0
1	J	1503	0	1425	28	0
1	K	1389	0	1321	25	0
1	L	1464	0	1385	28	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	D	4	0	3	0	0
2	F	4	0	3	1	0
2	G	4	0	3	0	0
2	H	4	0	3	2	0
2	I	4	0	3	0	0
3	A	7	0	10	0	0
3	D	14	0	20	0	0
3	J	7	0	10	0	0
4	A	6	0	8	0	0
4	H	6	0	8	0	0
5	A	144	0	0	5	0
5	B	141	0	0	7	0
5	C	128	0	0	10	0
5	D	153	0	0	6	0
5	E	102	0	0	0	0
5	F	119	0	0	8	0
5	G	139	0	0	6	0
5	H	149	0	0	14	0
5	I	138	0	0	4	0
5	J	108	0	0	4	0
5	K	109	0	0	4	0
5	L	109	0	0	12	0
All	All	19260	0	16809	298	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 9.

All (298) 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:J:46[A]:THR:HG22	1:J:52:VAL:HG22	1.62	0.81
1:C:65[B]:PRO:HB3	5:C:409:HOH:O	1.79	0.81
1:L:153[B]:THR:HG22	1:L:157:THR:H	1.47	0.78
1:G:80[B]:LEU:HD21	1:G:87:LEU:HD11	1.67	0.77
1:F:145:LEU:HD21	1:F:148:PHE:CZ	2.20	0.77
1:H:79:VAL:HG13	5:H:514:HOH:O	1.85	0.75
1:K:46:THR:HG22	1:K:52:VAL:HG22	1.68	0.74
1:G:89[A]:PHE:HZ	5:H:406:HOH:O	1.71	0.73
1:H:89[A]:PHE:HZ	5:H:491:HOH:O	1.72	0.73
1:G:164:VAL:HG22	1:G:170:ARG:HG2	1.69	0.72
1:C:46[A]:THR:HG22	1:C:52:VAL:HG22	1.70	0.72
1:B:89[A]:PHE:HZ	5:B:440:HOH:O	1.72	0.71
1:L:72[B]:MET:SD	5:L:338:HOH:O	2.47	0.71
1:L:153[B]:THR:HG21	5:L:374:HOH:O	1.90	0.71
1:B:108:ASN:ND2	5:B:519:HOH:O	2.24	0.70
1:L:71[B]:HIS:CD2	1:L:79:VAL:HG22	2.27	0.69
1:C:189:THR:HG22	5:C:357[B]:HOH:O	1.92	0.69
1:E:136:LEU:HD22	1:E:148[B]:PHE:CZ	2.28	0.69
1:I:183:VAL:HG11	1:I:187:LYS:HG3	1.74	0.68
1:L:189:THR:HG22	5:L:352[B]:HOH:O	1.94	0.68
1:E:136:LEU:HD13	1:E:148[B]:PHE:CE2	2.29	0.68
1:L:35[B]:ASN:OD1	1:L:35[B]:ASN:O	2.12	0.68
1:I:183:VAL:CG2	5:I:523:HOH:O	2.42	0.67
1:I:183:VAL:CG1	1:I:184:ASP:N	2.57	0.67
1:K:113:LEU:HD13	1:K:148:PHE:CZ	2.30	0.67
1:E:113:LEU:HD13	1:E:148[B]:PHE:CZ	2.30	0.67
1:E:201[A]:GLN:NE2	1:F:135:GLU:OE2	2.29	0.66
1:H:108:ASN:HD21	2:H:301:ACT:H2	1.60	0.65
1:C:128[B]:LYS:HB2	1:C:128[B]:LYS:NZ	2.13	0.64
1:H:89[A]:PHE:CZ	5:H:491:HOH:O	2.48	0.64
1:H:46[B]:THR:HG22	5:H:475:HOH:O	1.98	0.64
1:L:52:VAL:HG11	1:L:55:GLU:HG3	1.78	0.64
1:K:176:LYS:O	1:K:177[B]:SER:HB3	1.97	0.63
1:D:162:THR:HG21	1:D:170[B]:ARG:HD2	1.80	0.63
1:E:191[A]:THR:HG23	1:E:191[A]:THR:O	1.96	0.63
1:I:183:VAL:HG12	1:I:184:ASP:N	2.11	0.63
1:C:65[B]:PRO:O	1:C:66[B]:ASN:HB2	1.98	0.62
1:G:137[B]:THR:HG23	5:G:445:HOH:O	2.00	0.62
1:C:52:VAL:HG11	1:C:55:GLU:HG3	1.82	0.62
1:C:177:SER:C	5:C:329:HOH:O	2.38	0.62
1:B:145:LEU:HD13	1:B:148:PHE:CZ	2.35	0.61
1:B:191[A]:THR:HG23	5:B:486:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:110:PRO:HB3	1:J:148[B]:PHE:CE1	2.35	0.60
1:C:157:THR:HA	1:C:178:GLN:HE22	1.65	0.60
1:K:136:LEU:HD22	1:K:148:PHE:CZ	2.36	0.60
1:A:77:GLU:HG2	5:A:497:HOH:O	2.01	0.60
1:E:52:VAL:HG11	1:E:55:GLU:HG3	1.83	0.60
1:J:165[A]:GLU:HG2	1:J:166:GLN:N	2.17	0.60
1:A:61:TRP:CE2	1:A:187:LYS:HE2	2.36	0.59
1:C:136:LEU:HD12	1:C:136:LEU:N	2.17	0.59
1:F:65:PRO:HA	5:F:444:HOH:O	2.02	0.59
1:D:158:ILE:O	1:D:178:GLN:NE2	2.35	0.59
1:G:68:PHE:HE1	1:G:80[B]:LEU:HD22	1.67	0.59
1:K:148:PHE:HB2	1:K:162:THR:O	2.03	0.59
1:I:184:ASP:HB3	5:I:515:HOH:O	2.02	0.58
1:A:191[A]:THR:HG23	1:A:191[A]:THR:O	2.03	0.58
1:A:80:LEU:HD11	1:A:87:LEU:HD11	1.84	0.58
1:K:65:PRO:HA	5:K:310:HOH:O	2.04	0.58
1:F:46[B]:THR:CG2	1:F:170:ARG:HB2	2.34	0.58
1:E:123[B]:LYS:HE2	5:I:514:HOH:O	2.04	0.57
1:J:22:ASP:N	5:J:490:HOH:O	2.36	0.57
1:F:136:LEU:N	1:F:136:LEU:HD12	2.19	0.57
1:L:94:VAL:HG21	5:L:360:HOH:O	2.04	0.57
1:F:46[B]:THR:HG22	5:F:426:HOH:O	2.04	0.56
1:F:199:ASP:OD1	1:F:201[A]:GLN:NE2	2.32	0.56
1:G:147:GLN:NE2	5:G:435:HOH:O	2.38	0.56
1:B:80:LEU:HD13	1:B:89[B]:PHE:CE2	2.41	0.56
1:F:89:PHE:HZ	5:F:451:HOH:O	1.87	0.56
1:J:54:GLN:NE2	1:J:75:PRO:CG	2.69	0.56
1:I:158:ILE:H	1:I:178:GLN:HE22	1.54	0.56
1:L:164:VAL:HG22	1:L:170:ARG:HG2	1.87	0.56
1:L:71[A]:HIS:NE2	1:L:73:THR:HG22	2.21	0.56
1:A:61:TRP:CD2	1:A:187:LYS:HE2	2.41	0.55
1:D:144:ASN:O	1:D:144:ASN:ND2	2.29	0.55
1:D:149:ALA:HB2	5:D:444:HOH:O	2.06	0.55
1:K:176:LYS:O	1:K:177[B]:SER:CB	2.55	0.55
1:L:136:LEU:N	1:L:136:LEU:HD12	2.22	0.55
1:D:89:PHE:HZ	5:D:417:HOH:O	1.90	0.55
1:E:46:THR:HG22	1:E:52:VAL:HG22	1.88	0.54
1:H:105:ALA:HB3	5:H:498:HOH:O	2.08	0.54
1:J:164:VAL:HG22	1:J:170:ARG:HG2	1.89	0.54
1:J:172:ALA:HB1	5:L:360:HOH:O	2.07	0.54
1:G:89[A]:PHE:CZ	5:H:406:HOH:O	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:ALA:HB1	5:F:446:HOH:O	2.07	0.54
1:J:65[A]:PRO:C	1:J:66[A]:ASN:OD1	2.46	0.54
1:J:162:THR:HG21	1:J:170:ARG:NH2	2.22	0.54
1:C:89:PHE:HZ	5:C:316:HOH:O	1.90	0.54
1:E:71:HIS:CD2	1:E:79:VAL:HG22	2.42	0.54
1:L:43:GLN:HG2	1:L:44:ALA:N	2.22	0.54
1:G:78[A]:SER:HB3	1:H:52:VAL:HG23	1.90	0.54
1:H:68:PHE:CZ	5:H:543:HOH:O	2.60	0.54
1:K:71:HIS:CD2	1:K:79:VAL:HG22	2.43	0.54
1:C:178:GLN:N	5:C:329:HOH:O	2.41	0.53
1:B:193:PRO:HD2	1:B:196:VAL:HG21	1.91	0.53
1:K:145:LEU:C	1:K:145:LEU:HD12	2.29	0.53
1:C:182:VAL:HG23	1:C:182:VAL:O	2.09	0.53
1:J:46[B]:THR:HG22	5:J:461:HOH:O	2.07	0.53
1:K:124:GLN:HG2	5:K:385:HOH:O	2.09	0.53
1:J:52:VAL:HG23	1:L:78[B]:SER:OG	2.08	0.53
1:I:164:VAL:HG22	1:I:170:ARG:HG2	1.91	0.53
1:C:128[B]:LYS:HB2	1:C:128[B]:LYS:HZ3	1.73	0.52
1:J:172:ALA:CB	5:L:360:HOH:O	2.56	0.52
1:J:54:GLN:NE2	1:J:75:PRO:HG3	2.24	0.52
1:L:158:ILE:H	1:L:178:GLN:HE22	1.56	0.52
1:B:91[B]:ASN:ND2	1:D:44:ALA:HB1	2.24	0.52
1:E:95:GLU:OE1	1:E:196:VAL:HG22	2.09	0.52
1:H:144:ASN:ND2	5:H:474[A]:HOH:O	2.42	0.52
1:H:187:LYS:NZ	1:H:187:LYS:HA	2.25	0.52
1:L:46[B]:THR:HG21	1:L:170:ARG:NH1	2.24	0.52
1:C:145:LEU:HD11	1:C:148:PHE:CZ	2.44	0.52
1:H:80:LEU:HD13	1:H:89[B]:PHE:CE2	2.45	0.52
1:A:138:PRO:HG3	1:A:145[A]:LEU:HD12	1.91	0.51
1:F:46[A]:THR:HG22	1:F:52:VAL:HG22	1.93	0.51
1:F:130[B]:LYS:O	1:F:130[B]:LYS:HD3	2.10	0.51
1:F:100:THR:HG22	1:F:201[A]:GLN:HB2	1.92	0.51
1:F:145:LEU:HD21	1:F:148:PHE:CE1	2.44	0.51
1:H:191[A]:THR:HG23	1:H:191[A]:THR:O	2.10	0.51
1:K:52:VAL:HG11	1:K:55:GLU:HG3	1.91	0.51
1:K:127:VAL:HG22	1:K:136:LEU:HG	1.91	0.51
1:G:40:SER:OG	1:G:176:LYS:HD2	2.10	0.51
1:F:127:VAL:HG22	1:F:136:LEU:HG	1.92	0.51
1:H:78[A]:SER:OG	1:H:89[A]:PHE:CE1	2.64	0.51
1:A:182:VAL:HG23	1:A:182:VAL:O	2.10	0.51
1:H:109:THR:N	5:H:518:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:149:ALA:HB1	5:K:341:HOH:O	2.11	0.50
1:H:187:LYS:HA	1:H:187:LYS:HZ3	1.76	0.50
1:I:141:ALA:O	1:I:143:GLY:N	2.44	0.50
1:E:65[B]:PRO:O	1:E:66[B]:ASN:HB2	2.11	0.50
1:E:191[A]:THR:O	1:E:191[A]:THR:CG2	2.60	0.50
1:A:127:VAL:HG22	1:A:136:LEU:HG	1.92	0.50
1:K:187:LYS:NZ	5:K:396:HOH:O	2.42	0.50
1:B:61:TRP:CZ3	1:B:187:LYS:HE2	2.47	0.50
1:C:106:THR:HG23	5:C:404:HOH:O	2.11	0.50
1:J:191[A]:THR:HG23	1:J:191[A]:THR:O	2.10	0.50
1:B:61:TRP:CH2	1:B:187:LYS:HE2	2.46	0.50
1:L:35[B]:ASN:OD1	1:L:35[B]:ASN:C	2.49	0.50
1:J:148[B]:PHE:CZ	1:J:150:ILE:HB	2.47	0.49
1:F:159:LYS:CD	5:F:501:HOH:O	2.60	0.49
1:C:145:LEU:HD11	1:C:148:PHE:CE1	2.48	0.49
1:G:46[A]:THR:HG21	1:I:89[A]:PHE:CZ	2.48	0.49
1:D:22:ASP:N	5:D:543:HOH:O	2.46	0.49
1:D:145:LEU:HD13	1:D:148:PHE:CZ	2.48	0.49
1:H:170:ARG:NH1	5:H:523:HOH:O	2.46	0.49
1:L:71[A]:HIS:CD2	1:L:73:THR:CG2	2.95	0.49
1:B:53:VAL:HG21	5:B:416:HOH:O	2.12	0.49
1:I:183:VAL:HG22	5:I:523:HOH:O	2.09	0.48
1:J:183:VAL:O	5:J:472:HOH:O	2.20	0.48
1:H:78[A]:SER:OG	1:H:89[A]:PHE:CZ	2.66	0.48
1:H:89[B]:PHE:O	1:H:97:ALA:HA	2.14	0.48
1:J:165[A]:GLU:CG	1:J:166:GLN:N	2.76	0.48
1:C:66[B]:ASN:N	5:C:359:HOH:O	2.46	0.48
1:G:46[B]:THR:HG21	5:G:461:HOH:O	2.13	0.48
1:A:85[B]:GLU:OE2	5:A:508:HOH:O	2.20	0.48
1:L:46[B]:THR:HG22	5:L:372:HOH:O	2.13	0.47
1:C:132:ASP:O	1:C:151:SER:HA	2.13	0.47
2:H:301:ACT:H3	1:I:48:SER:O	2.13	0.47
1:H:112:MET:SD	5:H:543:HOH:O	2.60	0.47
1:L:71[A]:HIS:CD2	1:L:73:THR:HG22	2.50	0.47
1:F:46[B]:THR:HG22	1:F:170:ARG:HB2	1.96	0.47
1:J:100:THR:HG22	1:J:201[B]:GLN:HB2	1.97	0.47
1:A:61:TRP:CZ2	1:A:187:LYS:HE2	2.50	0.47
1:A:183:VAL:HG22	1:A:184:ASP:N	2.30	0.47
1:C:46[A]:THR:CG2	1:C:52:VAL:HG22	2.42	0.47
1:D:170[B]:ARG:CZ	5:D:416:HOH:O	2.63	0.47
1:G:79:VAL:HG13	5:G:520:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:136:LEU:N	1:K:136:LEU:HD12	2.29	0.47
1:L:65:PRO:HA	5:L:308:HOH:O	2.15	0.47
1:B:64[B]:ARG:NH2	1:B:117:ASN:HB2	2.29	0.46
1:D:130[B]:LYS:NZ	1:D:130[B]:LYS:CB	2.78	0.46
1:G:89[A]:PHE:CZ	1:H:46[A]:THR:HG21	2.50	0.46
1:C:145:LEU:CD1	1:C:148:PHE:CE1	2.98	0.46
1:A:46[A]:THR:HG21	1:D:89:PHE:CZ	2.50	0.46
1:B:67:LEU:HD13	5:B:511:HOH:O	2.14	0.46
1:B:78[B]:SER:HB2	1:D:52:VAL:HG23	1.98	0.46
1:G:78[B]:SER:HB2	1:H:52:VAL:HG23	1.95	0.46
1:E:136:LEU:HD22	1:E:148[B]:PHE:HZ	1.79	0.46
1:K:191[A]:THR:HG23	1:K:191[A]:THR:O	2.14	0.46
1:B:191[A]:THR:HG23	1:B:191[A]:THR:O	2.15	0.46
1:D:46[B]:THR:HG22	5:D:418:HOH:O	2.14	0.46
1:C:52:VAL:HG11	1:C:55:GLU:CG	2.46	0.46
1:I:80:LEU:HD13	1:I:89[B]:PHE:CE2	2.51	0.46
1:I:193:PRO:HD2	1:I:196:VAL:HG21	1.97	0.46
1:A:77:GLU:CG	5:A:497:HOH:O	2.60	0.46
1:B:161:PHE:CE2	1:B:175:LEU:HD11	2.51	0.45
1:C:191[A]:THR:HG23	1:C:191[A]:THR:O	2.15	0.45
1:D:158:ILE:N	1:D:178:GLN:HE22	2.15	0.45
1:L:153[B]:THR:HG23	1:L:155:SER:H	1.81	0.45
1:I:38[B]:HIS:CE1	1:I:179:GLN:HB2	2.51	0.45
1:J:65[A]:PRO:O	1:J:66[A]:ASN:OD1	2.35	0.45
1:A:145[A]:LEU:HD13	1:A:146:LYS:N	2.32	0.45
1:F:116:ARG:HA	2:F:301:ACT:H2	1.98	0.45
1:C:157:THR:HA	1:C:178:GLN:NE2	2.32	0.45
1:F:145:LEU:CD2	1:F:148:PHE:CE1	3.00	0.45
1:C:89:PHE:O	1:C:97:ALA:HA	2.17	0.45
1:J:136:LEU:HD12	1:J:136:LEU:N	2.32	0.45
1:B:63:LYS:HD2	1:B:67:LEU:HD12	1.97	0.45
1:B:38[B]:HIS:HB3	1:B:61:TRP:CD1	2.52	0.44
1:E:91:ASN:OD1	1:E:94:VAL:HG22	2.17	0.44
1:K:187:LYS:HE3	1:K:187:LYS:HA	1.99	0.44
1:L:60:LEU:HD12	1:L:60:LEU:O	2.18	0.44
1:B:95:GLU:OE1	1:B:196:VAL:HG22	2.18	0.44
1:J:100:THR:HG22	1:J:201[A]:GLN:HB2	2.00	0.44
1:J:127:VAL:HG22	1:J:136:LEU:HG	1.99	0.44
1:K:61:TRP:CD2	1:K:187:LYS:HD3	2.53	0.44
1:F:145:LEU:CD2	1:F:148:PHE:CZ	2.97	0.44
1:B:89[A]:PHE:CZ	5:B:440:HOH:O	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:PHE:O	1:B:115:THR:HG23	2.18	0.44
1:G:135[A]:GLU:HG3	1:G:147:GLN:OE1	2.18	0.44
1:A:57:GLU:HG2	1:A:74[B]:SER:HB3	2.00	0.43
1:A:164:VAL:HG22	1:A:170:ARG:HG2	2.00	0.43
1:B:35:ASN:HB3	1:B:64[B]:ARG:HB2	2.00	0.43
1:F:94:VAL:HG23	1:F:96[B]:GLN:HG2	2.00	0.43
1:H:100:THR:HG22	1:H:201[A]:GLN:HB2	2.00	0.43
1:C:106:THR:CG2	5:C:404:HOH:O	2.64	0.43
1:E:89:PHE:O	1:E:97:ALA:HA	2.19	0.43
1:H:116:ARG:NH1	5:H:498:HOH:O	2.50	0.43
1:B:102:LEU:HD23	5:B:509:HOH:O	2.19	0.43
1:G:52:VAL:HG23	1:I:78:SER:HB2	2.00	0.43
1:K:113:LEU:CD1	1:K:148:PHE:CZ	2.99	0.43
1:A:78:SER:HB2	1:B:52:VAL:HG23	2.01	0.43
1:H:43:GLN:HG2	1:H:44:ALA:N	2.34	0.43
1:H:52:VAL:HG11	1:H:55:GLU:HG3	2.01	0.43
1:A:52:VAL:HG23	1:D:78:SER:HB2	2.00	0.43
1:A:183:VAL:HG22	1:A:184:ASP:H	1.83	0.43
1:C:26:ASP:OD1	5:C:398[B]:HOH:O	2.21	0.43
1:C:183:VAL:HG22	1:C:184:ASP:N	2.33	0.43
1:D:52:VAL:HG11	1:D:55:GLU:HG3	2.00	0.43
1:G:145:LEU:N	1:G:145:LEU:HD23	2.34	0.43
1:K:71:HIS:CE1	1:K:73:THR:HG22	2.54	0.43
1:E:153:THR:HB	1:E:154:PRO:HD2	2.00	0.43
1:B:64[B]:ARG:NH2	1:B:117:ASN:CB	2.82	0.42
1:C:145:LEU:CD1	1:C:148:PHE:CZ	3.02	0.42
1:G:150:ILE:O	1:G:150:ILE:HG23	2.19	0.42
1:A:46[B]:THR:HG22	5:A:425:HOH:O	2.19	0.42
1:J:54:GLN:NE2	1:J:75:PRO:HG2	2.33	0.42
1:J:191[A]:THR:HG22	5:J:455:HOH:O	2.19	0.42
1:K:43:GLN:HG2	1:K:44:ALA:N	2.34	0.42
1:L:46[B]:THR:HG23	5:L:346:HOH:O	2.19	0.42
1:C:100:THR:HG22	1:C:201[A]:GLN:HB2	2.01	0.42
1:E:162:THR:HG21	1:E:170:ARG:NH2	2.33	0.42
1:H:95:GLU:HA	1:H:95:GLU:OE1	2.19	0.42
1:A:147:GLN:HB2	5:A:503:HOH:O	2.18	0.42
1:F:110:PRO:HD3	1:F:148:PHE:CE1	2.54	0.42
1:B:80:LEU:HD13	1:B:89[B]:PHE:CD2	2.54	0.42
1:F:46[A]:THR:HG22	1:F:52:VAL:HA	2.01	0.42
1:H:89[A]:PHE:O	1:H:97:ALA:HA	2.19	0.42
1:H:164:VAL:HG22	1:H:170:ARG:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:PRO:HD3	1:A:148:PHE:CE1	2.55	0.42
1:J:89:PHE:O	1:J:97:ALA:HA	2.19	0.42
1:F:64:ARG:HA	1:F:65:PRO:HA	1.80	0.42
1:F:100:THR:HG22	1:F:201[B]:GLN:HB2	2.00	0.42
1:G:182:VAL:HG23	1:G:182:VAL:O	2.20	0.42
1:B:43:GLN:HG2	1:B:44:ALA:N	2.34	0.41
1:H:162:THR:HG21	1:H:170:ARG:NH1	2.35	0.41
1:C:100:THR:HG22	1:C:201[B]:GLN:HB2	2.01	0.41
1:C:110:PRO:HG3	1:C:148:PHE:CD1	2.54	0.41
1:C:110:PRO:HD3	1:C:148:PHE:CE1	2.55	0.41
1:G:147:GLN:CG	1:G:148:PHE:N	2.83	0.41
1:I:43:GLN:HG2	1:I:44:ALA:N	2.35	0.41
1:K:52:VAL:HG11	1:K:55:GLU:CG	2.49	0.41
1:L:46[A]:THR:HG22	1:L:52:VAL:HG22	2.03	0.41
1:J:111:PHE:O	1:J:115:THR:HG23	2.21	0.41
1:A:24:SER:O	1:A:28:GLN:HG3	2.21	0.41
1:A:191[A]:THR:O	1:A:191[A]:THR:CG2	2.68	0.41
1:B:89[B]:PHE:O	1:B:97:ALA:HA	2.20	0.41
1:F:152:VAL:CG2	5:F:474:HOH:O	2.67	0.41
1:G:146:LYS:HD2	5:G:524:HOH:O	2.19	0.41
1:J:145:LEU:HD12	1:J:147:GLN:CA	2.49	0.41
1:G:127:VAL:HG22	1:G:136:LEU:HG	2.03	0.41
1:A:100:THR:HG22	1:A:201[A]:GLN:HB2	2.03	0.41
1:K:89:PHE:O	1:K:97:ALA:HA	2.20	0.41
1:H:78[B]:SER:HB3	1:I:52:VAL:HG23	2.02	0.41
1:I:64:ARG:HA	1:I:65:PRO:HA	1.82	0.41
1:I:194:LYS:CD	1:K:59[B]:GLU:HG3	2.51	0.41
1:A:61:TRP:CE3	1:A:187:LYS:HE2	2.55	0.41
1:C:72[A]:MET:SD	5:C:351:HOH:O	2.63	0.41
1:D:71:HIS:CE1	1:D:73:THR:HG22	2.56	0.41
1:I:31:LEU:HD22	1:I:114[B]:ILE:HD12	2.02	0.41
1:I:194:LYS:HD3	1:K:59[B]:GLU:HG3	2.02	0.41
1:L:25[A]:THR:HG23	5:L:393:HOH:O	2.20	0.41
1:A:136:LEU:HD12	1:A:136:LEU:N	2.35	0.41
1:C:64[A]:ARG:HA	1:C:65[A]:PRO:HA	1.50	0.41
1:E:136:LEU:HD12	1:E:136:LEU:N	2.35	0.41
1:G:28:GLN:HG2	1:G:122:TRP:CD1	2.56	0.41
1:B:89[A]:PHE:CZ	1:D:46[A]:THR:HG21	2.56	0.40
1:E:111:PHE:O	1:E:115:THR:HG23	2.21	0.40
1:G:36[B]:SER:OG	1:G:63:LYS:HG3	2.22	0.40
1:J:162:THR:HG21	1:J:170:ARG:CZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:22:ASP:N	5:L:355:HOH:O	2.54	0.40
1:E:45:VAL:HG21	5:F:511:HOH:O	2.22	0.40
1:F:159:LYS:HD2	5:F:501:HOH:O	2.21	0.40
1:L:72[A]:MET:O	1:L:77:GLU:HA	2.21	0.40
1:D:165[A]:GLU:OE1	5:D:516:HOH:O	2.22	0.40
1:H:68:PHE:CE2	5:H:543:HOH:O	2.57	0.40
1:I:183:VAL:CG1	1:I:184:ASP:H	2.34	0.40
1:G:146:LYS:HE3	5:G:435:HOH:O	2.20	0.40
1:H:78[A]:SER:HB2	1:I:52:VAL:HG23	2.03	0.40
1:L:85:GLU:HB2	5:L:322:HOH:O	2.22	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	184/184 (100%)	180 (98%)	4 (2%)	0	100	100
1	B	177/184 (96%)	174 (98%)	3 (2%)	0	100	100
1	C	185/184 (100%)	179 (97%)	6 (3%)	0	100	100
1	D	189/184 (103%)	185 (98%)	4 (2%)	0	100	100
1	E	172/184 (94%)	166 (96%)	6 (4%)	0	100	100
1	F	184/184 (100%)	176 (96%)	8 (4%)	0	100	100
1	G	190/184 (103%)	185 (97%)	5 (3%)	0	100	100
1	H	176/184 (96%)	173 (98%)	3 (2%)	0	100	100
1	I	186/184 (101%)	181 (97%)	5 (3%)	0	100	100
1	J	186/184 (101%)	182 (98%)	2 (1%)	2 (1%)	14	3
1	K	169/184 (92%)	165 (98%)	4 (2%)	0	100	100
1	L	182/184 (99%)	180 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2180/2208 (99%)	2126 (98%)	52 (2%)	2 (0%)	100 33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	65[A]	PRO
1	J	65[B]	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	169/161 (105%)	169 (100%)	0	100 100
1	B	163/161 (101%)	162 (99%)	1 (1%)	86 80
1	C	169/161 (105%)	169 (100%)	0	100 100
1	D	172/161 (107%)	171 (99%)	1 (1%)	86 80
1	E	158/161 (98%)	158 (100%)	0	100 100
1	F	168/161 (104%)	167 (99%)	1 (1%)	86 80
1	G	173/161 (108%)	173 (100%)	0	100 100
1	H	161/161 (100%)	160 (99%)	1 (1%)	86 80
1	I	168/161 (104%)	168 (100%)	0	100 100
1	J	170/161 (106%)	169 (99%)	1 (1%)	86 80
1	K	155/161 (96%)	155 (100%)	0	100 100
1	L	166/161 (103%)	166 (100%)	0	100 100
All	All	1992/1932 (103%)	1987 (100%)	5 (0%)	92 89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	119	PRO
1	D	144	ASN

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Mol	Chain	Res	Type
1	F	145	LEU
1	H	187	LYS
1	J	145	LEU

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

Mol	Chain	Res	Type
1	E	38	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

13 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	ACT	G	301	-	3,3,3	0.78	0	3,3,3	1.12	0
2	ACT	A	301	-	3,3,3	0.81	0	3,3,3	1.17	0
2	ACT	I	301	-	3,3,3	0.83	0	3,3,3	1.40	0
3	PEG	D	302[B]	-	6,6,6	0.41	0	5,5,5	0.35	0
4	GOL	A	303	-	5,5,5	0.42	0	5,5,5	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACT	H	301	-	3,3,3	0.75	0	3,3,3	1.25	0
3	PEG	D	302[A]	-	6,6,6	0.45	0	5,5,5	0.25	0
2	ACT	F	301	-	3,3,3	0.68	0	3,3,3	1.32	0
2	ACT	B	301	-	3,3,3	0.67	0	3,3,3	1.38	0
3	PEG	A	302	-	6,6,6	0.44	0	5,5,5	0.24	0
4	GOL	H	302	-	5,5,5	0.33	0	5,5,5	0.32	0
3	PEG	J	301	-	6,6,6	0.41	0	5,5,5	0.33	0
2	ACT	D	301	-	3,3,3	0.78	0	3,3,3	1.42	0

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
4	GOL	A	303	-	-	0/4/4/4	-
3	PEG	D	302[B]	-	-	2/4/4/4	-
3	PEG	D	302[A]	-	-	4/4/4/4	-
3	PEG	A	302	-	-	3/4/4/4	-
4	GOL	H	302	-	-	2/4/4/4	-
3	PEG	J	301	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	302	GOL	C1-C2-C3-O3
4	H	302	GOL	O2-C2-C3-O3
3	A	302	PEG	O1-C1-C2-O2
3	D	302[A]	PEG	O2-C3-C4-O4
3	A	302	PEG	O2-C3-C4-O4
3	D	302[A]	PEG	O1-C1-C2-O2
3	J	301	PEG	C1-C2-O2-C3
3	D	302[A]	PEG	C4-C3-O2-C2
3	D	302[B]	PEG	O2-C3-C4-O4
3	J	301	PEG	O2-C3-C4-O4
3	D	302[B]	PEG	C4-C3-O2-C2
3	A	302	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	J	301	PEG	C4-C3-O2-C2
3	D	302[A]	PEG	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	301	ACT	2	0
2	F	301	ACT	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 (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	177/184 (96%)	0.66	16 (9%)	9	10	18, 24, 38, 51	0
1	B	169/184 (91%)	0.62	10 (5%)	22	24	18, 24, 33, 40	0
1	C	177/184 (96%)	0.96	24 (13%)	3	3	19, 28, 44, 48	0
1	D	179/184 (97%)	0.62	16 (8%)	9	11	18, 24, 39, 47	0
1	E	169/184 (91%)	0.78	13 (7%)	13	15	19, 28, 40, 48	0
1	F	177/184 (96%)	0.84	17 (9%)	8	9	20, 27, 42, 46	0
1	G	179/184 (97%)	0.74	12 (6%)	17	20	18, 25, 41, 52	0
1	H	172/184 (93%)	0.61	7 (4%)	37	41	19, 25, 36, 42	0
1	I	180/184 (97%)	0.67	16 (8%)	9	11	18, 25, 41, 48	0
1	J	177/184 (96%)	1.07	29 (16%)	1	1	20, 29, 45, 50	0
1	K	171/184 (92%)	0.87	15 (8%)	10	11	21, 30, 43, 52	0
1	L	176/184 (95%)	0.97	29 (16%)	1	1	22, 29, 44, 49	0
All	All	2103/2208 (95%)	0.78	204 (9%)	7	8	18, 27, 42, 52	0

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	182	VAL	8.3
1	J	182	VAL	7.7
1	C	182	VAL	6.7
1	D	183	VAL	6.0
1	A	182	VAL	5.9
1	I	182	VAL	5.9
1	E	148[A]	PHE	5.8
1	J	166	GLN	5.7
1	I	143	GLY	5.7
1	G	183	VAL	5.6
1	D	182	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	180	SER	5.1
1	H	177	SER	5.0
1	J	148[A]	PHE	5.0
1	H	185	ALA	5.0
1	J	145	LEU	4.9
1	F	183	VAL	4.8
1	F	166	GLN	4.8
1	I	141	ALA	4.7
1	A	183	VAL	4.5
1	F	182	VAL	4.2
1	B	185	ALA	4.0
1	J	176	LYS	4.0
1	H	144	ASN	3.8
1	K	166	GLN	3.8
1	B	195	GLY	3.7
1	D	89	PHE	3.7
1	A	181	SER	3.7
1	C	176	LYS	3.7
1	L	182	VAL	3.6
1	L	146	LYS	3.6
1	C	181	SER	3.6
1	L	148	PHE	3.5
1	G	177	SER	3.5
1	C	148	PHE	3.5
1	C	164	VAL	3.5
1	G	145	LEU	3.4
1	L	164	VAL	3.4
1	J	180	SER	3.4
1	K	148	PHE	3.4
1	B	145	LEU	3.4
1	L	185	ALA	3.3
1	J	181	SER	3.3
1	E	166	GLN	3.3
1	C	180	SER	3.2
1	C	145	LEU	3.2
1	K	185	ALA	3.2
1	F	148	PHE	3.2
1	K	194	LYS	3.2
1	K	141	ALA	3.2
1	L	131	GLY	3.2
1	G	184	ASP	3.1
1	K	195	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	181	SER	3.1
1	D	148	PHE	3.0
1	G	148	PHE	3.0
1	I	146	LYS	3.0
1	I	185	ALA	3.0
1	K	147	GLN	3.0
1	A	145[A]	LEU	3.0
1	D	180	SER	2.9
1	A	184	ASP	2.9
1	I	184	ASP	2.9
1	J	106	THR	2.9
1	H	89[A]	PHE	2.9
1	J	183	VAL	2.9
1	I	178	GLN	2.9
1	C	166	GLN	2.9
1	J	66[A]	ASN	2.8
1	L	65	PRO	2.8
1	E	185	ALA	2.8
1	D	145	LEU	2.8
1	L	61	TRP	2.8
1	C	66[A]	ASN	2.8
1	J	126	ASN	2.8
1	D	181	SER	2.8
1	F	147	GLN	2.8
1	G	89[A]	PHE	2.8
1	I	89[A]	PHE	2.8
1	L	180	SER	2.8
1	K	135[A]	GLU	2.7
1	E	186	SER	2.7
1	B	89[A]	PHE	2.7
1	K	170	ARG	2.7
1	K	177[A]	SER	2.7
1	A	185	ALA	2.7
1	C	183	VAL	2.7
1	A	46[A]	THR	2.7
1	F	138	PRO	2.7
1	J	46[A]	THR	2.7
1	C	152	VAL	2.6
1	F	175	LEU	2.6
1	G	75	PRO	2.6
1	L	137	THR	2.6
1	J	175[A]	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	146	LYS	2.6
1	J	195	GLY	2.6
1	J	94	VAL	2.6
1	K	145	LEU	2.6
1	J	125	TYR	2.6
1	A	147	GLN	2.6
1	C	137	THR	2.5
1	A	186	SER	2.5
1	G	179	GLN	2.5
1	C	184	ASP	2.5
1	D	185	ALA	2.5
1	A	148	PHE	2.5
1	A	179	GLN	2.5
1	C	87[A]	LEU	2.5
1	A	177	SER	2.5
1	B	22	ASP	2.5
1	D	65	PRO	2.4
1	C	163	ALA	2.4
1	E	38	HIS	2.4
1	E	194	LYS	2.4
1	C	150[A]	ILE	2.4
1	J	53	VAL	2.4
1	L	136	LEU	2.4
1	F	180	SER	2.4
1	L	147	GLN	2.4
1	L	178	GLN	2.4
1	F	197	THR	2.4
1	J	136	LEU	2.4
1	L	38	HIS	2.4
1	D	144	ASN	2.3
1	C	149	ALA	2.3
1	E	51	ALA	2.3
1	E	100	THR	2.3
1	J	162	THR	2.3
1	F	184	ASP	2.3
1	D	184[A]	ASP	2.3
1	I	22	ASP	2.3
1	L	184	ASP	2.3
1	F	179	GLN	2.3
1	A	130	LYS	2.3
1	L	25[A]	THR	2.3
1	F	123	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	102	LEU	2.3
1	G	150	ILE	2.3
1	I	181	SER	2.3
1	J	170	ARG	2.3
1	C	125	TYR	2.3
1	B	53	VAL	2.2
1	F	65	PRO	2.2
1	I	180	SER	2.2
1	I	183	VAL	2.2
1	K	22	ASP	2.2
1	D	178	GLN	2.2
1	J	169	GLN	2.2
1	L	179	GLN	2.2
1	B	38[A]	HIS	2.2
1	L	123	LYS	2.2
1	L	150	ILE	2.2
1	I	186	SER	2.2
1	E	22	ASP	2.2
1	B	146	LYS	2.2
1	E	52	VAL	2.2
1	B	114	ILE	2.2
1	C	135	GLU	2.2
1	L	51	ALA	2.2
1	C	133	ASP	2.2
1	L	181	SER	2.2
1	D	152	VAL	2.2
1	A	75	PRO	2.2
1	C	107	GLY	2.2
1	I	162	THR	2.2
1	L	162	THR	2.2
1	L	163	ALA	2.2
1	C	170	ARG	2.1
1	K	161	PHE	2.1
1	K	66	ASN	2.1
1	C	147	GLN	2.1
1	J	138	PRO	2.1
1	L	122	TRP	2.1
1	J	147	GLN	2.1
1	L	152	VAL	2.1
1	L	140	SER	2.1
1	J	123	LYS	2.1
1	F	38	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	168	GLY	2.1
1	B	148	PHE	2.1
1	G	186[A]	SER	2.1
1	J	127	VAL	2.1
1	D	141	ALA	2.1
1	J	51	ALA	2.1
1	F	161	PHE	2.1
1	H	147	GLN	2.1
1	E	146	LYS	2.1
1	J	198	LEU	2.1
1	H	194	LYS	2.0
1	E	193	PRO	2.0
1	J	65[A]	PRO	2.0
1	D	51	ALA	2.0
1	A	53	VAL	2.0
1	F	186	SER	2.0
1	I	177	SER	2.0
1	E	147	GLN	2.0
1	I	195	GLY	2.0
1	J	140	SER	2.0
1	H	145	LEU	2.0
1	L	41	PHE	2.0
1	L	22	ASP	2.0
1	L	106	THR	2.0
1	C	65[A]	PRO	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACT	A	301	4/4	0.55	0.23	36,37,37,38	0
2	ACT	I	301	4/4	0.68	0.21	38,38,38,38	0
2	ACT	H	301	4/4	0.70	0.18	37,37,38,39	0
3	PEG	D	302[A]	7/7	0.71	0.19	31,38,39,40	7
3	PEG	D	302[B]	7/7	0.71	0.19	40,43,44,44	7
4	GOL	H	302	6/6	0.78	0.15	47,48,48,48	0
2	ACT	B	301	4/4	0.84	0.15	38,38,38,39	0
3	PEG	J	301	7/7	0.85	0.17	42,43,43,44	0
2	ACT	D	301	4/4	0.86	0.20	44,45,45,45	0
3	PEG	A	302	7/7	0.87	0.20	32,40,44,44	0
4	GOL	A	303	6/6	0.88	0.14	31,36,37,39	0
2	ACT	G	301	4/4	0.88	0.16	42,42,43,43	0
2	ACT	F	301	4/4	0.89	0.13	39,39,40,41	0

6.5 Other polymers (i)

There are no such residues in this entry.