Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 12:02 PM EDT

PDB ID	:	5SV0
Title	:	Structure of the ExbB/ExbD complex from E. coli at pH 7.0
Authors	:	Celia, H.; Botos, I.; Lloubes, R.; Buchanan, S.K.; Noinaj, N.
Deposited on	:	2016-08-04
Resolution	:	2.60 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:

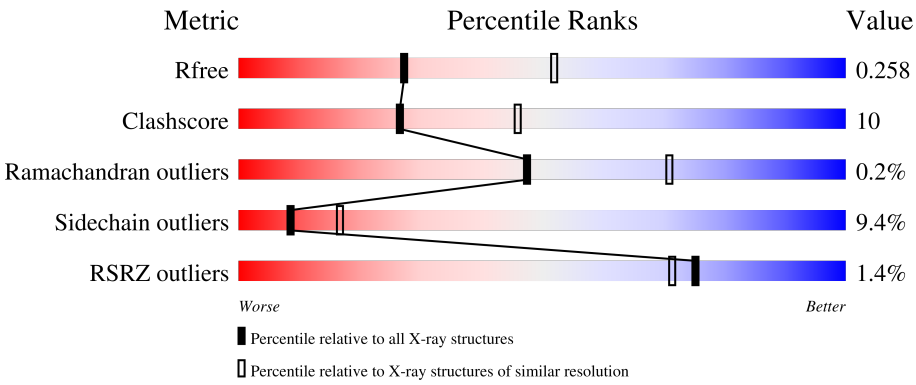
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	244	2%, 69%, 23%, • 5%
1	B	244	70%, 18%, • 8%
1	C	244	70%, 17%, • 9%
1	D	244	.%, 65%, 18%, 5%, 12%
1	E	244	2%, 65%, 20%, • • 11%

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Mol	Chain	Length	Quality of chain
1	F	244	3% 71% 18% 9%
1	G	244	% 70% 20% 6%
1	H	244	% 70% 20% 8%
1	I	244	64% 24% 9%
1	J	244	% 66% 19% 12%

2 Entry composition (i)

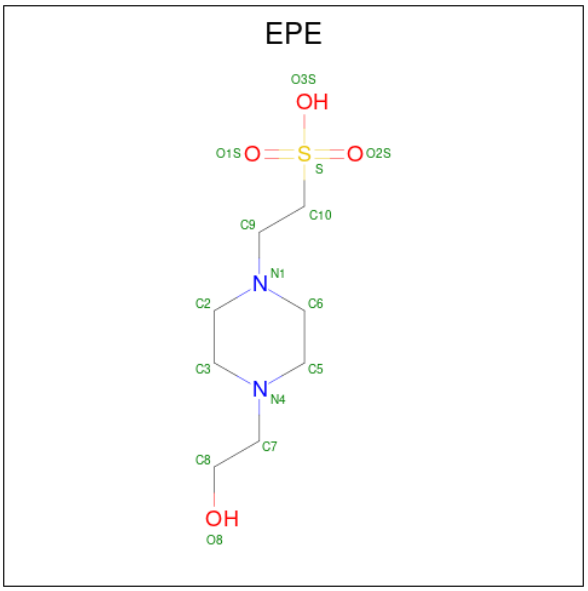
There are 4 unique types of molecules in this entry. The entry contains 16861 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Biopolymer transport protein ExbB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	225	1692	1080	295	311	6	0	0	0
			Total	C	N	O	S			
1	C	222	1651	1050	289	306	6	0	0	0
			Total	C	N	O	S			
1	D	215	1615	1028	282	300	5	0	0	0
			Total	C	N	O	S			
1	E	216	1609	1025	279	300	5	0	0	0
			Total	C	N	O	S			
1	F	223	1651	1050	290	306	5	0	0	0
			Total	C	N	O	S			
1	G	229	1731	1104	301	320	6	0	2	0
			Total	C	N	O	S			
1	H	225	1700	1085	296	313	6	0	0	0
			Total	C	N	O	S			
1	I	223	1678	1068	294	310	6	0	0	0
			Total	C	N	O	S			
1	J	214	1596	1017	279	295	5	0	0	0
			Total	C	N	O	S			
1	A	233	1749	1111	308	324	6	0	0	0

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	I	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	14	Total	O	0	0
			14	14		
4	C	11	Total	O	0	0
			11	11		
4	D	12	Total	O	0	0
			12	12		
4	E	16	Total	O	0	0
			16	16		

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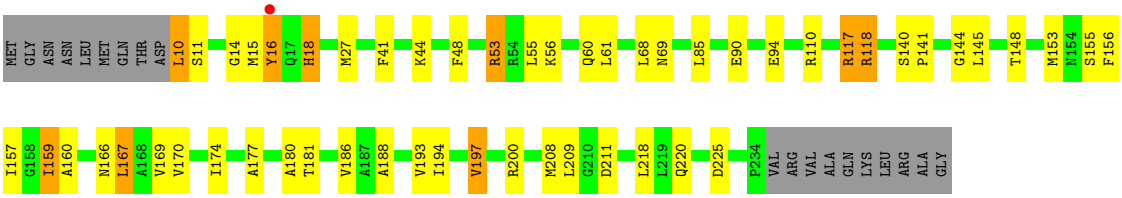
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	F	16	16	16	0	0
			Total	O		
4	G	15	15	15	0	0
			Total	O		
4	H	13	13	13	0	0
			Total	O		
4	I	15	15	15	0	0
			Total	O		
4	J	20	20	20	0	0
			Total	O		
4	A	10	10	10	0	0

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.

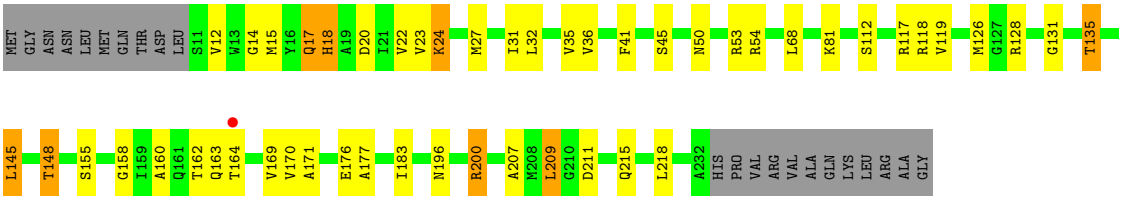
• Molecule 1: Biopolymer transport protein ExbB

Chain B: 70% 18% • 8%



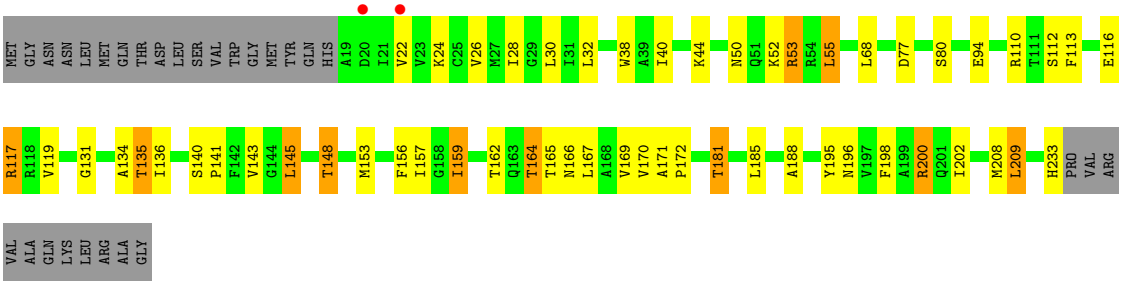
• Molecule 1: Biopolymer transport protein ExbB

Chain C: 70% 17% • 9%



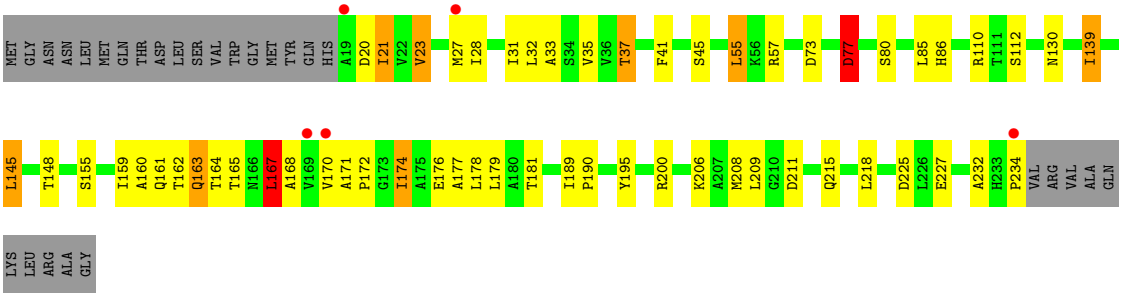
• Molecule 1: Biopolymer transport protein ExbB

Chain D: % 65% 18% 5% 12%



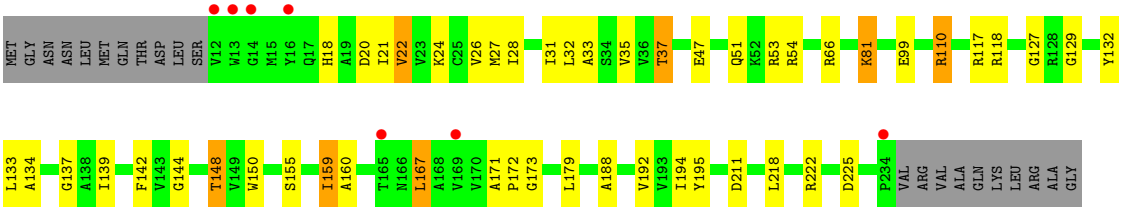
• Molecule 1: Biopolymer transport protein ExbB

Chain E: 2% 65% 20% • • 11%



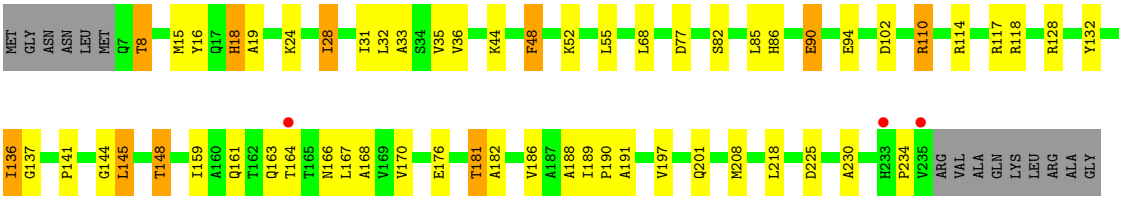
• Molecule 1: Biopolymer transport protein ExbB

Chain F:



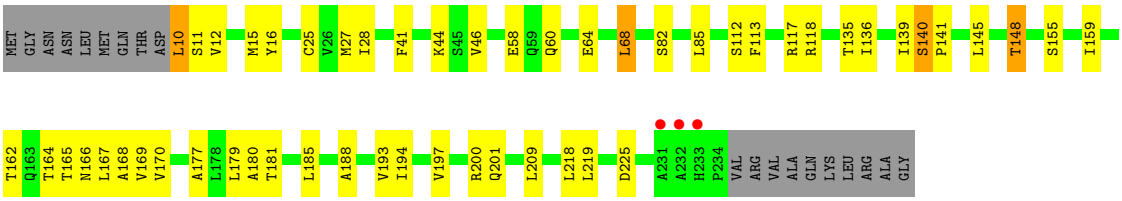
• Molecule 1: Biopolymer transport protein ExbB

Chain G:



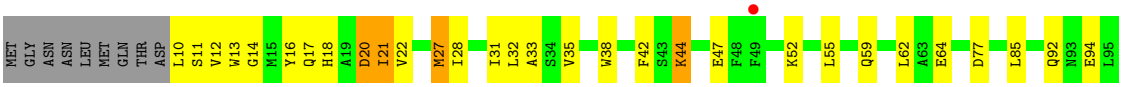
• Molecule 1: Biopolymer transport protein ExbB

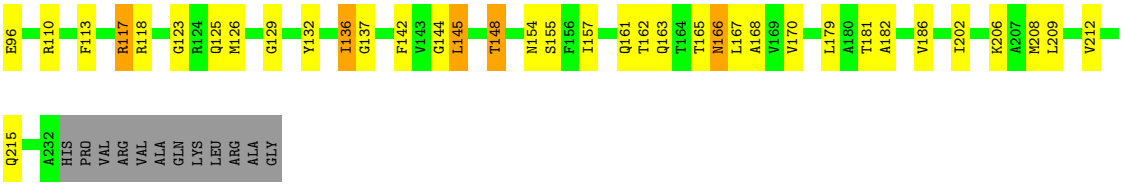
Chain H:



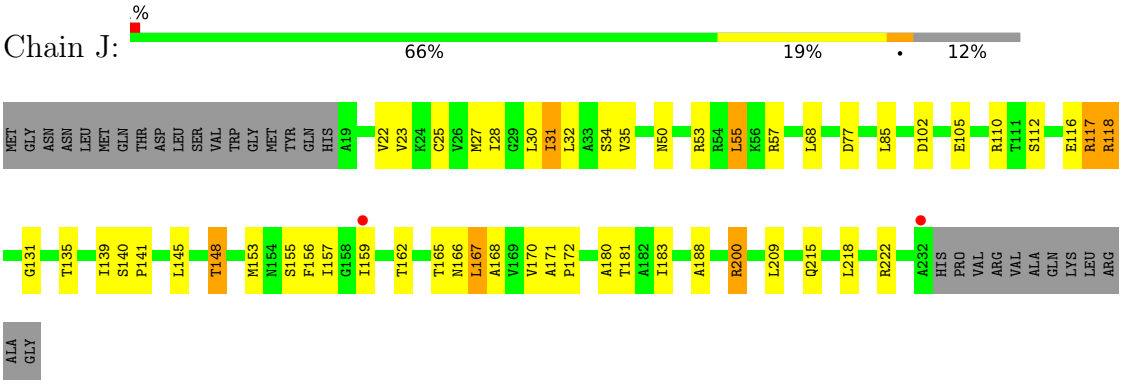
• Molecule 1: Biopolymer transport protein ExbB

Chain I:

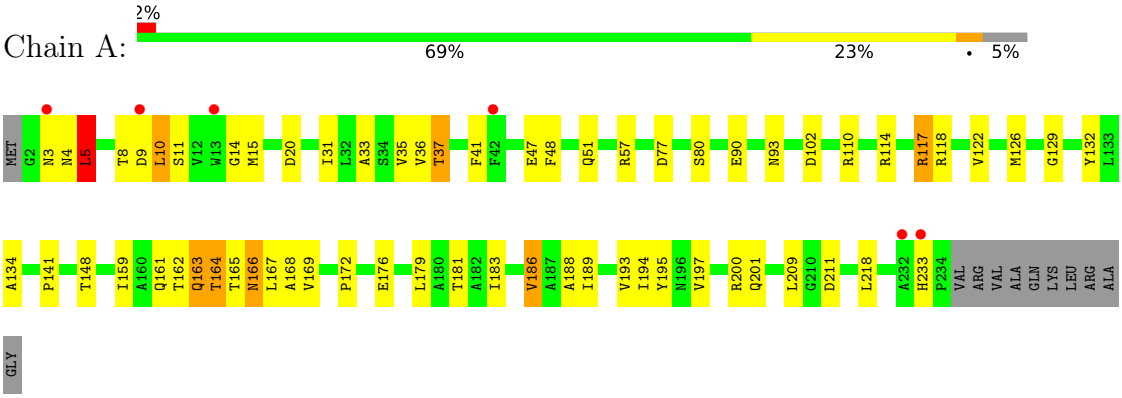




• Molecule 1: Biopolymer transport protein ExbB



• Molecule 1: Biopolymer transport protein ExbB



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	137.17Å 104.78Å 149.36Å 90.00° 91.77° 90.00°	Depositor
Resolution (Å)	46.00 – 2.60 49.76 – 2.58	Depositor EDS
% Data completeness (in resolution range)	94.4 (46.00-2.60) 89.3 (49.76-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.10_2142: ???)	Depositor
R, R_{free}	0.211 , 0.258 0.210 , 0.258	Depositor DCC
R_{free} test set	2008 reflections (1.59%)	wwPDB-VP
Wilson B-factor (Å^2)	55.7	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 59.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16861	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: CA, MLY, EPE

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	0.47	0/1764	0.63	0/2392
1	B	0.44	0/1707	0.68	0/2315
1	C	0.44	0/1661	0.61	0/2249
1	D	0.50	0/1625	0.62	0/2200
1	E	0.44	0/1619	0.64	2/2195 (0.1%)
1	F	0.48	0/1662	0.62	1/2253 (0.0%)
1	G	0.46	0/1747	0.66	1/2370 (0.0%)
1	H	0.46	0/1715	0.63	0/2324
1	I	0.48	0/1690	0.64	0/2289
1	J	0.52	0/1605	0.68	0/2174
All	All	0.47	0/16795	0.64	4/22761 (0.0%)

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	A	0	1
1	C	0	2
1	D	0	1
1	E	0	1
1	G	0	3
All	All	0	8

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	167	LEU	C-N-CA	6.74	138.55	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	77	ASP	C-N-CA	6.27	137.37	121.70
1	F	110	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	G	110	ARG	NE-CZ-NH2	-5.45	117.58	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	LEU	Peptide
1	C	17	GLN	Peptide
1	C	18	HIS	Peptide
1	D	162	THR	Peptide
1	E	167	LEU	Peptide
1	G	161	GLN	Peptide
1	G	166	ASN	Peptide
1	G	167	LEU	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	1749	0	1759	45	0
1	B	1692	0	1714	40	0
1	C	1651	0	1679	28	0
1	D	1615	0	1651	36	0
1	E	1609	0	1636	40	0
1	F	1651	0	1663	41	0
1	G	1731	0	1734	41	0
1	H	1700	0	1729	30	0
1	I	1678	0	1708	53	0
1	J	1596	0	1630	42	0
2	D	15	0	17	0	0
2	F	15	0	17	1	0
2	I	15	0	17	1	0
3	A	1	0	0	0	0
3	I	1	0	0	0	0
4	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	0	4	0
4	C	11	0	0	0	0
4	D	12	0	0	1	0
4	E	16	0	0	0	0
4	F	16	0	0	1	0
4	G	15	0	0	1	0
4	H	13	0	0	1	0
4	I	15	0	0	1	0
4	J	20	0	0	0	0
All	All	16861	0	16954	348	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 (348) 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:117:ARG:NH1	1:C:211:ASP:OD1	1.88	1.06
1:H:136:ILE:O	1:H:140:SER:HB3	1.68	0.93
1:B:90:GLU:HG3	1:B:118:ARG:HH22	1.33	0.92
1:C:196:ASN:HB3	1:C:200:ARG:HH11	1.39	0.87
1:A:141:PRO:HD3	1:A:188:ALA:HB2	1.54	0.87
1:E:211:ASP:OD1	1:J:117:ARG:NH1	2.08	0.86
1:A:167:LEU:O	1:A:169:VAL:N	2.08	0.85
1:J:159:ILE:HD11	1:J:170:VAL:HG21	1.60	0.84
1:I:165:THR:OG1	1:J:166:ASN:O	1.96	0.83
1:E:189:ILE:HG13	1:E:190:PRO:HD3	1.62	0.81
1:C:128:ARG:O	1:D:200:ARG:NH2	2.15	0.79
1:D:112:SER:O	1:D:116:GLU:HG2	1.83	0.78
1:C:160:ALA:O	1:C:163:GLN:NE2	2.18	0.75
1:B:11:SER:O	1:B:15:MET:HB2	1.86	0.75
1:B:110:ARG:HG2	1:C:218:LEU:HD23	1.69	0.74
1:C:162:THR:HG23	1:C:164:THR:H	1.53	0.72
1:I:162:THR:HG1	1:I:163:GLN:HA	1.53	0.71
1:E:159:ILE:HD13	1:E:165:THR:HG22	1.73	0.71
1:A:10:LEU:HB3	1:A:14:GLY:HA3	1.70	0.71
1:F:142:PHE:HB2	1:A:189:ILE:HD11	1.73	0.70
1:E:110:ARG:HG2	1:G:218:LEU:HD23	1.72	0.70
1:E:167:LEU:HD21	1:J:167:LEU:HD22	1.73	0.70
1:J:166:ASN:O	1:J:168:ALA:N	2.25	0.69
1:F:54:ARG:HH12	1:F:81:LYS:HG3	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:141:PRO:HD3	1:H:188:ALA:HB2	1.76	0.67
1:I:155:SER:HB3	1:I:170:VAL:HG23	1.75	0.67
1:I:94:GLU:OE1	1:I:110:ARG:NH1	2.27	0.67
1:I:21:ILE:HG23	1:I:22:VAL:H	1.58	0.67
1:F:142:PHE:CB	1:A:189:ILE:HD11	2.25	0.67
1:I:14:GLY:O	1:I:18:HIS:ND1	2.28	0.66
1:G:132[B]:TYR:O	1:G:136:ILE:HG23	1.95	0.66
1:B:200:ARG:HH12	1:A:132:TYR:HE1	1.43	0.66
1:G:128:ARG:O	1:H:200:ARG:NH2	2.29	0.66
1:B:148:THR:HG22	1:B:180:ALA:HB3	1.77	0.65
1:D:159:ILE:HD11	1:F:167:LEU:HB3	1.78	0.65
1:B:94:GLU:OE1	1:B:110:ARG:NH1	2.30	0.65
1:G:141:PRO:HD3	1:G:188:ALA:HB2	1.79	0.65
1:E:33:ALA:O	1:E:37:THR:HG23	1.97	0.64
1:G:19:ALA:HB2	1:G:176:GLU:HG2	1.80	0.64
1:I:110:ARG:HG2	1:J:218:LEU:HD23	1.80	0.64
1:I:162:THR:OG1	1:I:163:GLN:HA	1.98	0.64
1:B:148:THR:HG21	1:B:181:THR:OG1	1.98	0.63
1:G:15:MET:O	1:G:18:HIS:N	2.30	0.63
1:F:117:ARG:NH2	1:A:211:ASP:OD1	2.32	0.62
1:E:73:ASP:O	1:A:57:ARG:NH2	2.32	0.62
1:D:159:ILE:HG22	1:D:170:VAL:HG11	1.79	0.62
1:D:50:ASN:OD1	1:D:53:ARG:NH1	2.33	0.61
1:E:23:VAL:HG21	1:E:176:GLU:HG2	1.83	0.61
1:F:33:ALA:O	1:F:37:THR:HG23	2.00	0.61
1:B:90:GLU:HG3	1:B:118:ARG:NH2	2.10	0.60
1:F:47:GLU:O	1:F:51:GLN:HG3	2.01	0.60
1:I:62:LEU:O	1:I:215:GLN:NE2	2.32	0.60
1:J:27:MET:SD	1:J:183:ILE:HD12	2.42	0.60
1:G:118[B]:ARG:HE	1:G:118[B]:ARG:HA	1.66	0.60
1:B:117:ARG:HG2	1:B:117:ARG:HH11	1.67	0.60
1:J:166:ASN:C	1:J:168:ALA:H	2.05	0.59
1:G:141:PRO:HD3	1:G:188:ALA:CB	2.33	0.59
1:F:20:ASP:OD1	1:F:21:ILE:N	2.36	0.59
1:F:155:SER:HB3	1:F:173:GLY:HA3	1.84	0.59
1:D:148:THR:HG21	1:D:181:THR:OG1	2.03	0.59
1:J:141:PRO:HD3	1:J:188:ALA:HB2	1.86	0.58
1:H:68:LEU:HB2	1:H:219:LEU:HB3	1.85	0.58
1:B:141:PRO:HD3	1:B:188:ALA:HB2	1.86	0.57
1:E:148:THR:HG23	1:E:177:ALA:HB1	1.85	0.57
1:F:53:ARG:NH1	4:F:401:HOH:O	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:GLY:O	1:A:200:ARG:NH2	2.37	0.57
1:C:131:GLY:O	1:C:135:THR:HG22	2.04	0.57
1:F:18:HIS:O	1:F:18:HIS:ND1	2.38	0.57
1:D:145:LEU:HA	1:D:181:THR:HG23	1.86	0.57
1:B:159:ILE:HG13	1:B:160:ALA:N	2.18	0.57
1:H:193:VAL:O	1:H:197:VAL:HG23	2.05	0.57
1:J:50:ASN:OD1	1:J:53:ARG:NH2	2.38	0.57
1:I:44:LYS:HA	1:I:47:GLU:HG2	1.85	0.57
1:E:77:ASP:OD1	1:E:77:ASP:N	2.38	0.56
1:C:20:ASP:OD1	1:C:22:VAL:N	2.36	0.56
1:D:119:VAL:HG22	1:D:209:LEU:HD13	1.86	0.56
1:A:48:PHE:CZ	1:A:201:GLN:HB3	2.39	0.56
1:B:211:ASP:OD1	1:A:117:ARG:NH1	2.38	0.56
1:I:52:LYS:HE3	1:I:208:MET:HE1	1.88	0.56
1:D:156:PHE:HA	1:D:159:ILE:HG23	1.87	0.56
1:H:148:THR:HG22	1:H:177:ALA:O	2.06	0.56
1:D:164:THR:HG21	1:D:169:VAL:HG21	1.88	0.56
1:F:54:ARG:HH12	1:F:81:LYS:CG	2.19	0.55
1:H:159:ILE:HD11	1:H:170:VAL:HG21	1.87	0.55
1:C:32:LEU:O	1:C:36:VAL:HG12	2.06	0.55
1:I:129:GLY:H	1:J:200:ARG:NH1	2.05	0.55
1:E:170:VAL:O	1:E:174:ILE:HG23	2.06	0.55
1:J:77:ASP:OD1	1:J:77:ASP:N	2.33	0.55
1:A:15:MET:HB3	1:A:176:GLU:OE1	2.06	0.55
1:J:112:SER:O	1:J:116:GLU:HG2	2.06	0.55
1:D:117:ARG:NH1	1:F:211:ASP:OD1	2.40	0.55
1:B:218:LEU:HD23	1:A:110:ARG:HG2	1.88	0.54
1:I:117:ARG:HG2	1:I:117:ARG:HH11	1.71	0.54
1:G:31:ILE:O	1:G:35:VAL:HG23	2.07	0.54
1:A:3:ASN:OD1	1:A:4:ASN:N	2.40	0.54
1:D:165:THR:HG22	1:D:166:ASN:H	1.72	0.54
1:I:145:LEU:HA	1:I:148:THR:HG23	1.88	0.54
1:D:110:ARG:NH2	1:F:225:ASP:OD2	2.40	0.54
1:E:218:LEU:HD23	1:J:110:ARG:HG2	1.89	0.54
1:C:23:VAL:HG21	1:C:176:GLU:HG2	1.90	0.54
1:C:145:LEU:HA	1:C:148:THR:HG23	1.90	0.54
1:I:142:PHE:HA	1:I:145:LEU:HD23	1.89	0.53
1:G:182:ALA:O	1:G:186:VAL:HG23	2.08	0.53
1:H:16:TYR:HD1	1:H:27:MET:HE3	1.72	0.53
1:I:59:GLN:HG3	1:I:212:VAL:HG22	1.91	0.53
1:A:11:SER:O	1:A:15:MET:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:ALA:HB2	1:F:195:TYR:CE1	2.44	0.53
1:D:136:ILE:O	1:D:140:SER:HB2	2.09	0.53
1:I:77:ASP:OD1	1:I:77:ASP:N	2.42	0.53
1:A:4:ASN:O	1:A:5:LEU:HD22	2.09	0.52
1:A:41:PHE:HB2	1:A:194:ILE:HD13	1.91	0.52
1:H:166:ASN:O	1:H:169:VAL:HG22	2.09	0.52
1:J:148:THR:HG22	1:J:180:ALA:HB3	1.92	0.52
1:B:166:ASN:O	1:B:169:VAL:HG22	2.09	0.52
1:F:118:ARG:HH22	2:F:301:EPE:H81	1.74	0.52
1:B:41:PHE:HB2	1:B:194:ILE:HD13	1.92	0.52
1:I:118:ARG:NH2	4:I:402:HOH:O	2.41	0.52
1:I:132:TYR:O	1:I:136:ILE:HG23	2.10	0.52
1:A:33:ALA:O	1:A:37:THR:HG23	2.09	0.52
1:I:136:ILE:HG13	1:I:137:GLY:N	2.23	0.52
1:B:148:THR:HG22	1:B:177:ALA:O	2.10	0.52
1:G:77:ASP:OD1	1:G:77:ASP:N	2.41	0.52
1:I:166:ASN:ND2	1:I:166:ASN:O	2.43	0.52
1:A:193:VAL:O	1:A:197:VAL:HG23	2.10	0.51
1:G:90:GLU:HG3	1:G:114:ARG:HH11	1.75	0.51
1:I:123:GLY:HA3	1:I:206:LYS:HE2	1.91	0.51
1:B:11:SER:O	1:B:15:MET:CB	2.58	0.51
1:E:41:PHE:O	1:E:45:SER:HB2	2.09	0.51
1:B:140:SER:HB2	1:B:188:ALA:HB2	1.91	0.51
1:B:170:VAL:O	1:B:174:ILE:HD13	2.10	0.51
1:C:31:ILE:O	1:C:35:VAL:HG23	2.11	0.51
1:I:11:SER:O	1:I:13:TRP:N	2.43	0.51
1:J:131:GLY:O	1:J:135:THR:HG23	2.11	0.51
1:I:161:GLN:O	1:I:163:GLN:HA	2.11	0.51
1:J:159:ILE:HG13	1:J:170:VAL:HG11	1.93	0.51
1:F:129:GLY:HA2	1:F:132:TYR:CD1	2.46	0.50
1:F:28:ILE:O	1:F:32:LEU:HG	2.11	0.50
1:E:161:GLN:HA	1:G:8:THR:HG23	1.93	0.50
1:G:33:ALA:O	1:G:36:VAL:HG22	2.12	0.50
1:H:113:PHE:O	1:H:117:ARG:HB2	2.12	0.50
1:G:145:LEU:O	1:G:148:THR:HG23	2.12	0.50
1:A:8:THR:HG22	1:A:9:ASP:H	1.75	0.50
1:G:90:GLU:HG2	1:G:114:ARG:HD2	1.94	0.50
1:G:52:LYS:HE3	1:G:208:MET:HE1	1.94	0.49
1:J:148:THR:HG21	1:J:181:THR:OG1	2.12	0.49
1:D:24:LYS:O	1:D:28:ILE:HG23	2.12	0.49
1:I:117:ARG:HG2	1:I:117:ARG:NH1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:58:GLU:OE2	1:H:82:SER:OG	2.25	0.49
1:C:148:THR:HA	1:C:177:ALA:HA	1.94	0.49
1:F:22:VAL:HG11	1:F:150:TRP:NE1	2.27	0.49
1:G:82:SER:O	1:G:86:HIS:HD2	1.95	0.49
1:F:110:ARG:HG2	1:A:218:LEU:HD23	1.93	0.49
1:G:136:ILE:HG13	1:G:137:GLY:N	2.27	0.49
1:D:159:ILE:CD1	1:F:167:LEU:HB3	2.42	0.49
1:D:233:HIS:O	1:D:233:HIS:ND1	2.42	0.49
1:I:110:ARG:HG2	1:J:218:LEU:CD2	2.43	0.49
1:I:126:MET:HE2	1:I:202:ILE:HG12	1.94	0.49
1:G:136:ILE:HD11	1:G:191:ALA:HB2	1.95	0.49
1:J:25:CYS:O	1:J:28:ILE:HG12	2.13	0.49
1:J:153:MET:O	1:J:157:ILE:HG13	2.13	0.49
1:E:162:THR:O	1:E:162:THR:OG1	2.31	0.48
1:G:230:ALA:O	1:G:234:PRO:HD2	2.12	0.48
1:A:129:GLY:HA2	1:A:132:TYR:CE2	2.47	0.48
1:E:110:ARG:NH2	1:G:225:ASP:OD2	2.46	0.48
1:B:193:VAL:O	1:B:197:VAL:HG13	2.13	0.48
1:C:169:VAL:HG23	1:C:170:VAL:HG23	1.94	0.48
1:D:110:ARG:HG2	1:F:218:LEU:HD23	1.94	0.48
1:E:232:ALA:O	1:E:234:PRO:HD3	2.12	0.48
1:I:33:ALA:HB1	1:I:136:ILE:HD13	1.95	0.48
1:A:48:PHE:CE2	1:A:201:GLN:HB3	2.48	0.48
1:C:27:MET:HG2	1:C:183:ILE:HD12	1.96	0.48
1:A:169:VAL:O	1:A:172:PRO:HD2	2.13	0.48
1:J:27:MET:O	1:J:31:ILE:HG23	2.12	0.48
1:B:160:ALA:HB2	1:C:171:ALA:HB3	1.96	0.48
1:H:10:LEU:HD23	1:H:11:SER:N	2.29	0.48
1:I:13:TRP:O	1:I:16:TYR:N	2.46	0.48
1:B:10:LEU:HD23	1:B:14:GLY:HA3	1.96	0.47
1:F:27:MET:O	1:F:31:ILE:HG23	2.14	0.47
1:A:163:GLN:CD	1:A:164:THR:H	2.18	0.47
1:H:41:PHE:HB2	1:H:194:ILE:HD13	1.96	0.47
1:A:31:ILE:O	1:A:35:VAL:HG23	2.14	0.47
1:H:148:THR:HG22	1:H:180:ALA:HB3	1.95	0.47
1:I:32:LEU:O	1:I:35:VAL:HG22	2.14	0.47
1:I:167:LEU:HA	1:I:170:VAL:HG12	1.96	0.47
1:D:131:GLY:O	1:D:135:THR:HG23	2.14	0.47
1:H:10:LEU:HD23	1:H:11:SER:H	1.80	0.47
1:D:38:TRP:HA	1:D:38:TRP:CE3	2.49	0.47
1:F:54:ARG:HH22	1:F:81:LYS:HG3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:197:VAL:O	1:H:201:GLN:HG2	2.14	0.47
1:B:225:ASP:OD2	1:A:110:ARG:NH2	2.48	0.47
1:I:154:ASN:O	1:I:157:ILE:HG13	2.15	0.47
1:I:165:THR:HG21	1:J:167:LEU:HB2	1.96	0.47
1:J:28:ILE:O	1:J:32:LEU:HG	2.13	0.47
1:G:148:THR:HG21	1:G:181:THR:OG1	2.14	0.47
1:G:164:THR:H	1:H:168:ALA:HB2	1.79	0.47
1:C:119:VAL:HG22	1:C:209:LEU:HD13	1.97	0.47
1:E:145:LEU:HA	1:E:145:LEU:HD22	1.61	0.47
1:B:16:TYR:HD1	1:B:27:MET:HE3	1.80	0.46
1:J:31:ILE:O	1:J:35:VAL:HG23	2.15	0.46
1:A:93:ASN:HB3	1:A:114:ARG:HH22	1.80	0.46
1:A:167:LEU:C	1:A:169:VAL:H	2.05	0.46
1:D:94:GLU:OE2	1:F:222:ARG:NH1	2.49	0.46
1:E:80:SER:O	1:E:86:HIS:NE2	2.48	0.46
1:I:44:LYS:HE2	1:I:47:GLU:OE1	2.15	0.46
1:I:62:LEU:C	1:I:215:GLN:HE22	2.18	0.46
1:A:33:ALA:O	1:A:36:VAL:HG22	2.15	0.46
1:D:134:ALA:HB2	1:D:195:TYR:CE1	2.50	0.46
1:E:139:ILE:HD13	1:E:139:ILE:HA	1.68	0.46
1:F:144:GLY:O	1:F:148:THR:HG23	2.16	0.46
1:G:159:ILE:HD11	1:G:170:VAL:HG11	1.97	0.46
1:B:140:SER:N	1:B:141:PRO:HD2	2.31	0.46
1:H:225:ASP:OD2	4:H:301:HOH:O	2.20	0.46
1:A:4:ASN:HB3	1:A:5:LEU:H	1.46	0.46
1:A:148:THR:OG1	1:A:181:THR:OG1	2.20	0.46
1:D:26:VAL:HG13	1:D:143:VAL:HG23	1.97	0.46
1:C:50:ASN:O	1:C:53:ARG:NH1	2.49	0.46
1:F:54:ARG:NH1	1:F:81:LYS:HG3	2.30	0.45
1:A:122:VAL:O	1:A:126:MET:HG2	2.16	0.45
1:I:20:ASP:O	1:I:22:VAL:N	2.50	0.45
1:H:140:SER:N	1:H:141:PRO:HD2	2.31	0.45
1:J:31:ILE:HG13	1:J:32:LEU:N	2.30	0.45
1:F:137:GLY:HA3	1:F:192:VAL:HG12	1.99	0.45
1:H:68:LEU:O	1:H:68:LEU:HG	2.17	0.45
1:A:134:ALA:HB2	1:A:195:TYR:CE1	2.51	0.45
1:C:14:GLY:O	1:C:18:HIS:HB2	2.16	0.45
1:E:174:ILE:HD11	1:J:156:PHE:CD1	2.52	0.45
1:H:141:PRO:HD3	1:H:188:ALA:CB	2.44	0.45
1:J:135:THR:O	1:J:139:ILE:HG13	2.16	0.45
1:A:47:GLU:O	1:A:51:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:38:TRP:O	1:I:42:PHE:HD1	1.99	0.45
1:B:14:GLY:O	1:B:18:HIS:HB2	2.16	0.45
1:C:158:GLY:O	1:C:162:THR:HG22	2.17	0.45
1:F:24:LYS:O	1:F:28:ILE:HG23	2.16	0.45
1:G:110:ARG:HG2	1:H:218:LEU:HD23	1.97	0.45
1:E:171:ALA:N	1:E:172:PRO:HD2	2.32	0.45
1:F:133:LEU:HD13	1:F:194:ILE:HG22	1.98	0.45
4:B:301:HOH:O	1:C:207:ALA:HA	2.17	0.45
1:F:171:ALA:N	1:F:172:PRO:HD2	2.32	0.45
1:A:189:ILE:HD13	1:A:189:ILE:HA	1.73	0.45
1:D:80:SER:N	4:D:405:HOH:O	2.50	0.44
1:E:167:LEU:HD12	1:J:159:ILE:HG21	2.00	0.44
1:F:139:ILE:HB	1:A:189:ILE:HD12	1.99	0.44
1:I:94:GLU:OE2	1:J:222:ARG:NH1	2.50	0.44
1:D:141:PRO:HD3	1:D:188:ALA:HB2	1.98	0.44
1:B:44:LYS:HE3	1:B:48:PHE:CE1	2.53	0.44
1:J:118:ARG:HA	1:J:118:ARG:HD3	1.61	0.44
1:E:130:ASN:HB3	1:E:195:TYR:CE1	2.53	0.44
1:H:148:THR:HG21	1:H:181:THR:OG1	2.17	0.44
1:I:148:THR:HG21	1:I:181:THR:OG1	2.16	0.44
1:A:183:ILE:O	1:A:186:VAL:HG12	2.17	0.44
1:B:153:MET:O	1:B:157:ILE:HG13	2.18	0.44
1:I:110:ARG:NH1	1:J:222:ARG:HD3	2.32	0.44
1:J:165:THR:OG1	1:J:166:ASN:N	2.51	0.44
1:C:17:GLN:CB	1:C:24:LYS:HD2	2.48	0.44
1:G:94:GLU:OE1	1:G:110:ARG:HD2	2.18	0.44
1:I:166:ASN:HD21	1:I:168:ALA:HB3	1.83	0.44
1:B:117:ARG:NH2	4:B:301:HOH:O	2.32	0.44
1:F:99:GLU:OE2	1:G:230:ALA:HA	2.18	0.44
1:G:28:ILE:O	1:G:32:LEU:HG	2.17	0.44
1:I:167:LEU:O	1:I:170:VAL:HG12	2.18	0.44
1:C:41:PHE:O	1:C:45:SER:CB	2.66	0.43
1:A:77:ASP:OD1	1:A:77:ASP:N	2.50	0.43
1:H:167:LEU:HD23	1:H:167:LEU:HA	1.82	0.43
1:G:90:GLU:HG3	1:G:114:ARG:NH1	2.33	0.43
1:E:174:ILE:HD11	1:J:156:PHE:CG	2.53	0.43
1:D:117:ARG:HA	1:D:117:ARG:HD2	1.79	0.43
1:E:232:ALA:C	1:E:234:PRO:HD3	2.39	0.43
1:J:57:ARG:HG3	1:J:57:ARG:HH11	1.83	0.43
1:C:145:LEU:HA	1:C:145:LEU:HD12	1.77	0.43
1:G:197:VAL:O	1:G:201:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:182:ALA:O	1:I:186:VAL:HG23	2.18	0.43
1:C:27:MET:O	1:C:31:ILE:HG12	2.19	0.42
1:E:163:GLN:O	1:E:164:THR:HG23	2.19	0.42
1:G:86:HIS:HB3	1:G:118[A]:ARG:HE	1.83	0.42
1:H:25:CYS:O	1:H:28:ILE:HG13	2.19	0.42
1:I:92:GLN:HG3	1:I:96:GLU:OE2	2.19	0.42
1:B:144:GLY:O	1:B:148:THR:HG23	2.20	0.42
1:F:159:ILE:HG12	1:F:160:ALA:N	2.35	0.42
1:F:28:ILE:O	1:F:31:ILE:HG13	2.19	0.42
1:B:167:LEU:HD13	1:A:159:ILE:HG21	2.01	0.42
1:D:153:MET:O	1:D:157:ILE:HG13	2.19	0.42
1:E:20:ASP:OD1	1:E:21:ILE:N	2.53	0.42
1:F:31:ILE:O	1:F:35:VAL:HG23	2.18	0.42
1:E:148:THR:HG1	1:E:181:THR:HG1	1.61	0.42
1:E:225:ASP:OD2	1:J:110:ARG:NH2	2.52	0.42
1:H:117:ARG:HD2	1:H:117:ARG:HA	1.75	0.42
1:J:140:SER:N	1:J:141:PRO:HD2	2.35	0.42
1:D:30:LEU:HD21	1:D:143:VAL:HG22	2.01	0.42
1:G:144:GLY:O	1:G:148:THR:HG22	2.19	0.42
1:E:170:VAL:HG12	1:E:174:ILE:CG2	2.49	0.42
1:H:12:VAL:HA	1:H:15:MET:HE3	2.02	0.42
1:I:144:GLY:O	1:I:148:THR:HG23	2.18	0.42
2:I:302:EPE:H51	2:I:302:EPE:H81	1.71	0.42
1:A:93:ASN:OD1	1:A:114:ARG:NH2	2.48	0.42
1:C:41:PHE:O	1:C:45:SER:OG	2.32	0.42
1:D:198:PHE:O	1:D:202:ILE:HG13	2.19	0.42
1:B:68:LEU:HD12	1:B:220:GLN:HA	2.02	0.42
1:J:171:ALA:N	1:J:172:PRO:HD2	2.35	0.42
1:A:10:LEU:CB	1:A:14:GLY:HA3	2.44	0.42
1:D:171:ALA:N	1:D:172:PRO:HD2	2.35	0.41
1:E:55:LEU:HD13	1:E:208:MET:HG2	2.02	0.41
1:B:56:LYS:HZ2	1:B:60:GLN:HG3	1.85	0.41
1:D:55:LEU:HD13	1:D:208:MET:HB3	2.03	0.41
1:G:15:MET:C	1:G:18:HIS:H	2.22	0.41
1:B:208:MET:O	1:B:211:ASP:HB2	2.19	0.41
1:C:164:THR:HG23	1:C:169:VAL:HG11	2.02	0.41
1:D:40:ILE:O	1:D:44:LYS:HB2	2.20	0.41
1:E:27:MET:O	1:E:31:ILE:HG12	2.20	0.41
1:G:16:TYR:CE1	1:G:24:LYS:HG2	2.54	0.41
1:H:185:LEU:HA	1:H:185:LEU:HD23	1.83	0.41
1:C:135:THR:HB	1:D:196:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:LEU:N	1:E:168:ALA:HB3	2.36	0.41
1:F:132:TYR:H	1:F:132:TYR:HD1	1.67	0.41
1:A:165:THR:OG1	1:A:166:ASN:N	2.53	0.41
1:D:141:PRO:HB3	1:D:185:LEU:HD23	2.02	0.41
1:I:113:PHE:O	1:I:117:ARG:HB2	2.21	0.41
1:I:162:THR:CB	1:I:163:GLN:HA	2.50	0.41
1:J:55:LEU:HD23	1:J:55:LEU:HA	1.81	0.41
1:A:161:GLN:HG3	1:A:162:THR:HG23	2.03	0.41
1:B:53:ARG:HA	1:B:53:ARG:HD2	1.86	0.41
1:B:110:ARG:NH2	4:B:303:HOH:O	2.52	0.41
1:E:31:ILE:O	1:E:35:VAL:HG13	2.20	0.41
1:E:139:ILE:HD12	1:G:189:ILE:HG23	2.03	0.41
1:F:188:ALA:O	1:F:192:VAL:HG13	2.21	0.41
1:D:32:LEU:HA	1:D:32:LEU:HD13	1.77	0.41
1:E:160:ALA:C	1:E:162:THR:H	2.24	0.41
1:I:20:ASP:O	1:I:21:ILE:C	2.59	0.41
1:I:64:GLU:OE2	1:I:64:GLU:N	2.44	0.41
1:A:117:ARG:CG	1:A:117:ARG:HH11	2.34	0.41
1:B:156:PHE:HA	1:B:159:ILE:HG23	2.03	0.41
1:G:44:LYS:O	1:G:48:PHE:HB2	2.21	0.41
1:G:163:GLN:HB2	1:H:168:ALA:HB1	2.03	0.41
1:G:190:PRO:HG2	4:G:309:HOH:O	2.20	0.41
1:I:27:MET:HE1	1:I:179:LEU:HG	2.03	0.41
1:I:28:ILE:O	1:I:32:LEU:HG	2.21	0.41
1:I:31:ILE:O	1:I:35:VAL:HG13	2.21	0.41
1:I:129:GLY:H	1:J:200:ARG:HH11	1.66	0.41
1:G:19:ALA:HB2	1:G:176:GLU:CG	2.49	0.41
1:B:61:LEU:HD23	1:B:61:LEU:HA	1.85	0.40
1:E:41:PHE:O	1:E:45:SER:CB	2.68	0.40
1:H:135:THR:O	1:H:139:ILE:HG12	2.21	0.40
1:J:31:ILE:O	1:J:34:SER:HB3	2.21	0.40
1:B:69:ASN:ND2	4:B:304:HOH:O	2.54	0.40
1:E:159:ILE:HG22	1:G:168:ALA:HA	2.04	0.40
1:E:206:LYS:HB2	1:E:206:LYS:HE3	1.91	0.40
1:D:165:THR:HA	1:F:167:LEU:HD13	2.04	0.40
1:F:27:MET:HE1	1:F:179:LEU:HG	2.03	0.40
1:J:30:LEU:HA	1:J:30:LEU:HD23	1.88	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	230/244 (94%)	216 (94%)	12 (5%)	2 (1%)	17	35
1	B	222/244 (91%)	215 (97%)	7 (3%)	0	100	100
1	C	219/244 (90%)	217 (99%)	2 (1%)	0	100	100
1	D	212/244 (87%)	206 (97%)	6 (3%)	0	100	100
1	E	213/244 (87%)	206 (97%)	7 (3%)	0	100	100
1	F	220/244 (90%)	214 (97%)	6 (3%)	0	100	100
1	G	228/244 (93%)	222 (97%)	6 (3%)	0	100	100
1	H	222/244 (91%)	214 (96%)	7 (3%)	1 (0%)	29	52
1	I	220/244 (90%)	215 (98%)	3 (1%)	2 (1%)	17	35
1	J	211/244 (86%)	207 (98%)	4 (2%)	0	100	100
All	All	2197/2440 (90%)	2132 (97%)	60 (3%)	5 (0%)	47	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	12	VAL
1	A	168	ALA
1	H	68	LEU
1	I	21	ILE
1	A	166	ASN

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	176/189 (93%)	161 (92%)	15 (8%)	10	21
1	B	171/189 (90%)	156 (91%)	15 (9%)	10	19
1	C	166/189 (88%)	149 (90%)	17 (10%)	7	14
1	D	164/189 (87%)	147 (90%)	17 (10%)	7	13
1	E	162/189 (86%)	140 (86%)	22 (14%)	3	6
1	F	163/189 (86%)	155 (95%)	8 (5%)	25	48
1	G	173/189 (92%)	159 (92%)	14 (8%)	11	23
1	H	173/189 (92%)	156 (90%)	17 (10%)	8	15
1	I	170/189 (90%)	156 (92%)	14 (8%)	11	22
1	J	160/189 (85%)	142 (89%)	18 (11%)	6	10
All	All	1678/1890 (89%)	1521 (91%)	157 (9%)	8	17

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	10	LEU
1	B	16	TYR
1	B	18	HIS
1	B	53	ARG
1	B	55	LEU
1	B	85	LEU
1	B	117	ARG
1	B	118	ARG
1	B	145	LEU
1	B	155	SER
1	B	159	ILE
1	B	167	LEU
1	B	186	VAL
1	B	197	VAL
1	B	209	LEU
1	C	12	VAL
1	C	15	MET
1	C	24	LYS
1	C	54	ARG
1	C	68	LEU
1	C	81	LYS
1	C	112	SER
1	C	117	ARG
1	C	118	ARG

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Mol	Chain	Res	Type
1	C	126	MET
1	C	135	THR
1	C	145	LEU
1	C	148	THR
1	C	155	SER
1	C	200	ARG
1	C	209	LEU
1	C	215	GLN
1	D	22	VAL
1	D	52	LYS
1	D	53	ARG
1	D	55	LEU
1	D	68	LEU
1	D	77	ASP
1	D	113	PHE
1	D	117	ARG
1	D	135	THR
1	D	145	LEU
1	D	148	THR
1	D	159	ILE
1	D	164	THR
1	D	167	LEU
1	D	181	THR
1	D	200	ARG
1	D	209	LEU
1	E	21	ILE
1	E	23	VAL
1	E	28	ILE
1	E	32	LEU
1	E	37	THR
1	E	55	LEU
1	E	57	ARG
1	E	77	ASP
1	E	85	LEU
1	E	112	SER
1	E	139	ILE
1	E	145	LEU
1	E	155	SER
1	E	163	GLN
1	E	167	LEU
1	E	174	ILE
1	E	178	LEU

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Mol	Chain	Res	Type
1	E	179	LEU
1	E	200	ARG
1	E	209	LEU
1	E	215	GLN
1	E	227	GLU
1	F	22	VAL
1	F	26	VAL
1	F	37	THR
1	F	66	ARG
1	F	81	LYS
1	F	148	THR
1	F	159	ILE
1	F	167	LEU
1	G	8	THR
1	G	18	HIS
1	G	28	ILE
1	G	48	PHE
1	G	55	LEU
1	G	68	LEU
1	G	85	LEU
1	G	90	GLU
1	G	102	ASP
1	G	117	ARG
1	G	136	ILE
1	G	145	LEU
1	G	148	THR
1	G	181	THR
1	H	10	LEU
1	H	44	LYS
1	H	46	VAL
1	H	60	GLN
1	H	64	GLU
1	H	85	LEU
1	H	112	SER
1	H	118	ARG
1	H	140	SER
1	H	145	LEU
1	H	148	THR
1	H	155	SER
1	H	162	THR
1	H	164	THR
1	H	165	THR

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Mol	Chain	Res	Type
1	H	179	LEU
1	H	209	LEU
1	I	10	LEU
1	I	17	GLN
1	I	20	ASP
1	I	27	MET
1	I	44	LYS
1	I	55	LEU
1	I	85	LEU
1	I	117	ARG
1	I	125	GLN
1	I	136	ILE
1	I	145	LEU
1	I	148	THR
1	I	166	ASN
1	I	209	LEU
1	J	22	VAL
1	J	23	VAL
1	J	31	ILE
1	J	55	LEU
1	J	68	LEU
1	J	85	LEU
1	J	102	ASP
1	J	105	GLU
1	J	117	ARG
1	J	118	ARG
1	J	145	LEU
1	J	148	THR
1	J	155	SER
1	J	162	THR
1	J	167	LEU
1	J	200	ARG
1	J	209	LEU
1	J	215	GLN
1	A	5	LEU
1	A	10	LEU
1	A	20	ASP
1	A	37	THR
1	A	80	SER
1	A	90	GLU
1	A	102	ASP
1	A	117	ARG

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Mol	Chain	Res	Type
1	A	118	ARG
1	A	163	GLN
1	A	164	THR
1	A	179	LEU
1	A	186	VAL
1	A	209	LEU
1	A	233	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	MLY	D	108	1	9,10,11	0.81	0	6,11,13	0.77	0
1	MLY	E	108	1	9,10,11	0.82	0	6,11,13	0.81	0
1	MLY	C	108	1	9,10,11	0.88	0	6,11,13	0.80	0
1	MLY	G	108	1	9,10,11	0.81	0	6,11,13	0.79	0
1	MLY	H	108	1	9,10,11	0.94	0	6,11,13	0.97	0
1	MLY	I	108	1	9,10,11	0.77	0	6,11,13	0.66	0
1	MLY	F	108	1	9,10,11	0.66	0	6,11,13	0.82	0
1	MLY	A	108	1	9,10,11	0.60	0	6,11,13	0.82	0
1	MLY	B	108	1	9,10,11	0.79	0	6,11,13	0.83	0
1	MLY	J	108	1	9,10,11	0.68	0	6,11,13	0.74	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
1	MLY	D	108	1	-	2/8/9/11	-
1	MLY	E	108	1	-	1/8/9/11	-
1	MLY	C	108	1	-	1/8/9/11	-
1	MLY	G	108	1	-	0/8/9/11	-
1	MLY	H	108	1	-	1/8/9/11	-
1	MLY	I	108	1	-	0/8/9/11	-
1	MLY	F	108	1	-	1/8/9/11	-
1	MLY	A	108	1	-	0/8/9/11	-
1	MLY	B	108	1	-	1/8/9/11	-
1	MLY	J	108	1	-	0/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	108	MLY	CD-CE-NZ-CH2
1	E	108	MLY	CD-CE-NZ-CH2
1	F	108	MLY	CD-CE-NZ-CH2
1	C	108	MLY	CD-CE-NZ-CH2
1	D	108	MLY	CD-CE-NZ-CH1
1	H	108	MLY	CD-CE-NZ-CH2
1	B	108	MLY	CD-CE-NZ-CH2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	EPE	F	301	-	15,15,15	0.93	1 (6%)	18,20,20	2.17	5 (27%)
2	EPE	I	302	-	15,15,15	0.91	1 (6%)	18,20,20	2.03	7 (38%)
2	EPE	D	301	-	15,15,15	0.95	1 (6%)	18,20,20	1.86	7 (38%)

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	EPE	F	301	-	-	4/9/19/19	0/1/1/1
2	EPE	I	302	-	-	4/9/19/19	0/1/1/1
2	EPE	D	301	-	-	3/9/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	EPE	C10-S	3.27	1.82	1.77
2	I	302	EPE	C10-S	3.11	1.81	1.77
2	D	301	EPE	C10-S	2.89	1.81	1.77

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	EPE	C5-N4-C3	5.67	121.58	108.83
2	I	302	EPE	C7-N4-C5	4.09	121.69	111.23
2	I	302	EPE	C5-N4-C3	4.08	118.01	108.83
2	F	301	EPE	O1S-S-C10	3.93	111.64	106.92
2	D	301	EPE	C5-N4-C3	3.69	117.13	108.83
2	F	301	EPE	C7-N4-C5	3.59	120.41	111.23
2	I	302	EPE	C7-N4-C3	3.46	120.09	111.23
2	D	301	EPE	C7-N4-C3	2.90	118.66	111.23
2	D	301	EPE	O3S-S-C10	2.88	110.43	105.77
2	I	302	EPE	O1S-S-C10	2.74	110.21	106.92
2	I	302	EPE	C6-N1-C2	2.59	114.65	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	EPE	O3S-S-C10	2.57	109.93	105.77
2	F	301	EPE	C7-N4-C3	2.41	117.41	111.23
2	D	301	EPE	C7-N4-C5	2.33	117.20	111.23
2	D	301	EPE	C9-N1-C2	-2.31	105.32	111.23
2	I	302	EPE	O3S-S-C10	2.23	109.38	105.77
2	D	301	EPE	C6-N1-C2	2.12	113.60	108.83
2	I	302	EPE	O2S-S-C10	2.11	109.46	106.92
2	D	301	EPE	C9-N1-C6	-2.11	105.84	111.23

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	EPE	C9-C10-S-O2S
2	D	301	EPE	C9-C10-S-O3S
2	F	301	EPE	C8-C7-N4-C5
2	F	301	EPE	C9-C10-S-O2S
2	F	301	EPE	C9-C10-S-O3S
2	I	302	EPE	C8-C7-N4-C5
2	I	302	EPE	S-C10-C9-N1
2	D	301	EPE	C9-C10-S-O1S
2	F	301	EPE	C9-C10-S-O1S
2	I	302	EPE	C10-C9-N1-C6
2	I	302	EPE	C9-C10-S-O2S

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	EPE	1	0
2	I	302	EPE	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	232/244 (95%)	-0.11	6 (2%)	56	50	42, 74, 134, 191	0
1	B	224/244 (91%)	-0.31	1 (0%)	92	91	46, 76, 121, 164	0
1	C	221/244 (90%)	-0.26	1 (0%)	91	89	42, 77, 115, 160	0
1	D	214/244 (87%)	-0.21	2 (0%)	84	82	41, 68, 128, 200	0
1	E	215/244 (88%)	-0.12	5 (2%)	60	54	42, 76, 134, 164	0
1	F	222/244 (90%)	-0.13	7 (3%)	47	40	43, 73, 147, 218	0
1	G	228/244 (93%)	-0.27	3 (1%)	77	73	44, 76, 132, 214	0
1	H	224/244 (91%)	-0.36	3 (1%)	77	73	46, 75, 116, 197	0
1	I	222/244 (90%)	-0.32	1 (0%)	91	89	45, 77, 123, 155	0
1	J	213/244 (87%)	-0.32	2 (0%)	84	82	40, 70, 142, 181	0
All	All	2215/2440 (90%)	-0.24	31 (1%)	75	71	40, 75, 132, 218	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	13	TRP	5.8
1	J	232	ALA	5.8
1	A	3	ASN	4.8
1	F	12	VAL	4.2
1	E	234	PRO	4.1
1	F	16	TYR	4.0
1	F	165	THR	3.8
1	A	9	ASP	3.2
1	G	164	THR	3.1
1	G	235	VAL	3.1
1	E	169	VAL	2.9
1	B	16	TYR	2.7
1	E	170	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	19	ALA	2.6
1	J	159	ILE	2.6
1	F	14	GLY	2.6
1	H	233	HIS	2.5
1	D	22	VAL	2.3
1	H	232	ALA	2.3
1	F	169	VAL	2.3
1	A	233	HIS	2.2
1	I	49	PHE	2.2
1	A	13	TRP	2.2
1	H	231	ALA	2.2
1	F	234	PRO	2.2
1	A	42	PHE	2.1
1	D	20	ASP	2.1
1	E	27	MET	2.1
1	C	164	THR	2.0
1	G	233	HIS	2.0
1	A	232	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	MLY	B	108	11/12	0.97	0.17	38,43,50,53	0
1	MLY	C	108	11/12	0.97	0.14	38,44,60,61	0
1	MLY	D	108	11/12	0.98	0.14	36,40,49,56	0
1	MLY	E	108	11/12	0.98	0.19	52,56,68,73	0
1	MLY	F	108	11/12	0.98	0.16	44,49,62,66	0
1	MLY	G	108	11/12	0.98	0.12	32,43,52,53	0
1	MLY	I	108	11/12	0.98	0.11	33,39,65,67	0
1	MLY	J	108	11/12	0.98	0.13	31,40,59,65	0
1	MLY	H	108	11/12	0.99	0.11	35,45,57,60	0
1	MLY	A	108	11/12	0.99	0.13	33,37,55,65	0

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	EPE	D	301	15/15	0.76	0.15	95,119,159,163	0
3	CA	I	301	1/1	0.81	0.16	104,104,104,104	0
2	EPE	I	302	15/15	0.82	0.14	85,127,167,169	0
2	EPE	F	301	15/15	0.86	0.29	88,114,157,161	0
3	CA	A	301	1/1	0.97	0.16	97,97,97,97	0

6.5 Other polymers (i)

There are no such residues in this entry.