Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:28 AM GMT

PDB ID	:	3M1R
Title	:	The crystal structure of formimidoylglutamase from Bacillus subtilis subsp. subtilis str. 168
Authors	:	Tan, K.; Bigelow, L.; Trevino, D.; Buck, K.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2010-03-05
Resolution	:	2.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

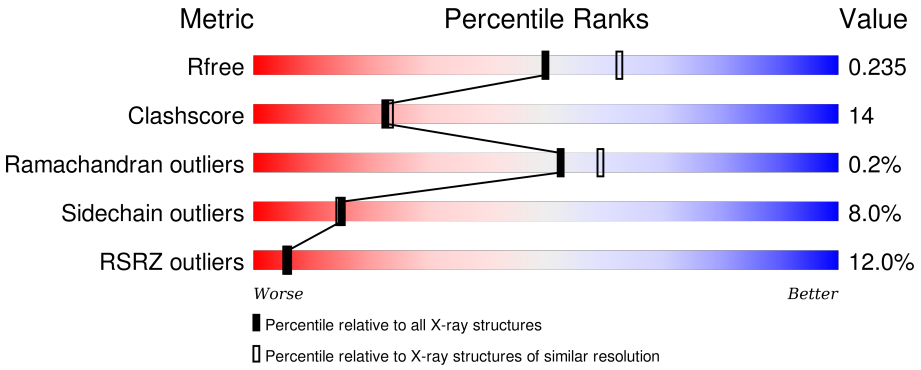
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	322	12% 69% 25% 5% •
1	B	322	14% 65% 29% 5% •
1	C	322	10% 75% 18% • •
1	D	322	11% 75% 21% •
1	E	322	11% 75% 20% • •

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Mol	Chain	Length	Quality of chain
1	F	322	11% 74% 22%

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	CL	A	320	-	-	-	X
2	CL	A	321	-	-	X	-
2	CL	B	320	-	-	-	X
2	CL	B	321	-	-	X	-
2	CL	C	321	-	-	-	X
2	CL	D	320	-	-	-	X
2	CL	E	321	-	-	-	X
3	CA	B	323	-	-	-	X
4	PEG	A	324	-	-	-	X
4	PEG	A	325	-	-	X	-
4	PEG	A	326	-	-	X	X
4	PEG	B	324	-	-	X	-
4	PEG	C	326	-	-	-	X
4	PEG	C	327	-	-	-	X
4	PEG	C	329	-	-	-	X
4	PEG	C	330	-	-	-	X
4	PEG	C	331	-	-	-	X
4	PEG	D	323	-	-	X	X
4	PEG	E	324	-	-	X	-
4	PEG	E	325	-	-	-	X
4	PEG	E	326	-	-	-	X
4	PEG	F	325	-	-	-	X
4	PEG	F	326	-	-	-	X
4	PEG	F	328	-	-	X	-
5	CAC	C	320[A]	-	-	-	X
5	CAC	C	320[B]	-	-	-	X
5	CAC	E	320[A]	-	-	-	X
5	CAC	E	320[B]	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15171 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 Formimidoylglutamase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	Se	0	0	0
			2462	1558	421	474	1	8			
1	B	317	Total	C	N	O	S	Se	0	0	0
			2449	1549	419	472	1	8			
1	C	316	Total	C	N	O	S	Se	0	0	0
			2441	1544	418	471	1	7			
1	D	321	Total	C	N	O	S	Se	0	0	0
			2479	1568	424	478	1	8			
1	E	316	Total	C	N	O	S	Se	0	0	0
			2441	1544	418	471	1	7			
1	F	316	Total	C	N	O	S	Se	0	0	0
			2444	1549	418	469	1	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP P42068
A	-1	ASN	-	EXPRESSION TAG	UNP P42068
A	0	ALA	-	EXPRESSION TAG	UNP P42068
B	-2	SER	-	EXPRESSION TAG	UNP P42068
B	-1	ASN	-	EXPRESSION TAG	UNP P42068
B	0	ALA	-	EXPRESSION TAG	UNP P42068
C	-2	SER	-	EXPRESSION TAG	UNP P42068
C	-1	ASN	-	EXPRESSION TAG	UNP P42068
C	0	ALA	-	EXPRESSION TAG	UNP P42068
D	-2	SER	-	EXPRESSION TAG	UNP P42068
D	-1	ASN	-	EXPRESSION TAG	UNP P42068
D	0	ALA	-	EXPRESSION TAG	UNP P42068
E	-2	SER	-	EXPRESSION TAG	UNP P42068
E	-1	ASN	-	EXPRESSION TAG	UNP P42068
E	0	ALA	-	EXPRESSION TAG	UNP P42068
F	-2	SER	-	EXPRESSION TAG	UNP P42068
F	-1	ASN	-	EXPRESSION TAG	UNP P42068

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	EXPRESSION TAG	UNP P42068

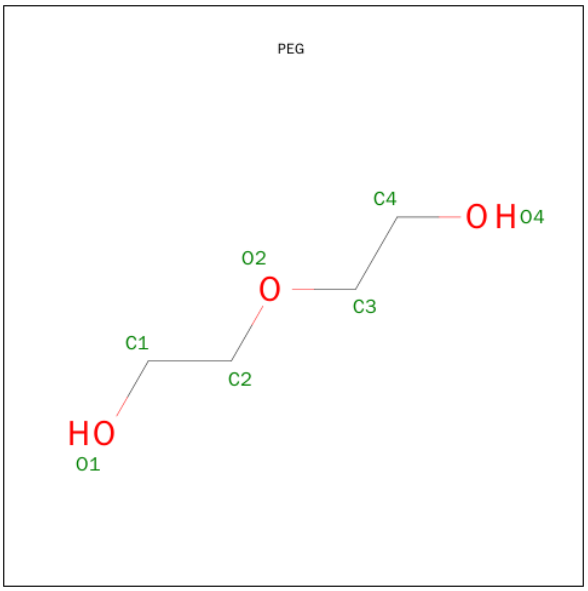
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	B	2	Total Cl 2 2	0	0
2	C	2	Total Cl 2 2	0	0
2	A	2	Total Cl 2 2	0	0
2	F	1	Total Cl 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	2	Total Ca 2 2	0	0
3	E	2	Total Ca 2 2	0	0
3	B	2	Total Ca 2 2	0	0
3	C	2	Total Ca 2 2	0	0
3	A	2	Total Ca 2 2	0	0
3	F	2	Total Ca 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0

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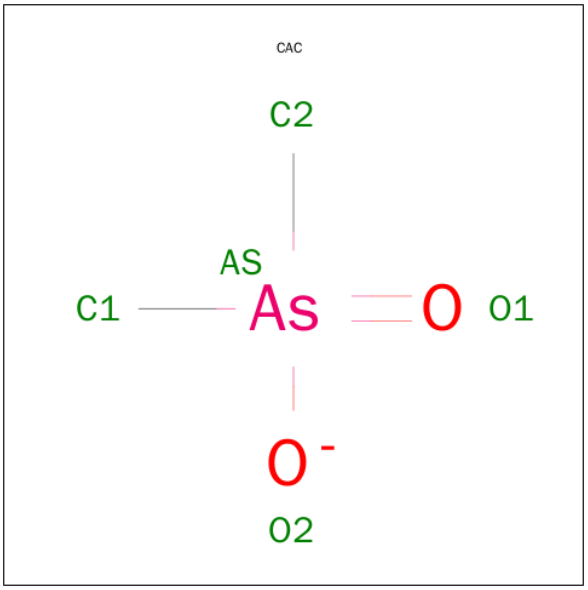
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0
4	F	1	Total C O 7 4 3	0	0
4	F	1	Total C O 7 4 3	0	0
4	F	1	Total C O 7 4 3	0	0
4	F	1	Total C O 7 4 3	0	0
4	F	1	Total C O 7 4 3	0	0
4	F	1	Total C O 7 4 3	0	0

- Molecule 5 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total As C O 10 2 4 4	0	1
5	E	1	Total As C O 10 2 4 4	0	1

- Molecule 6 is water.

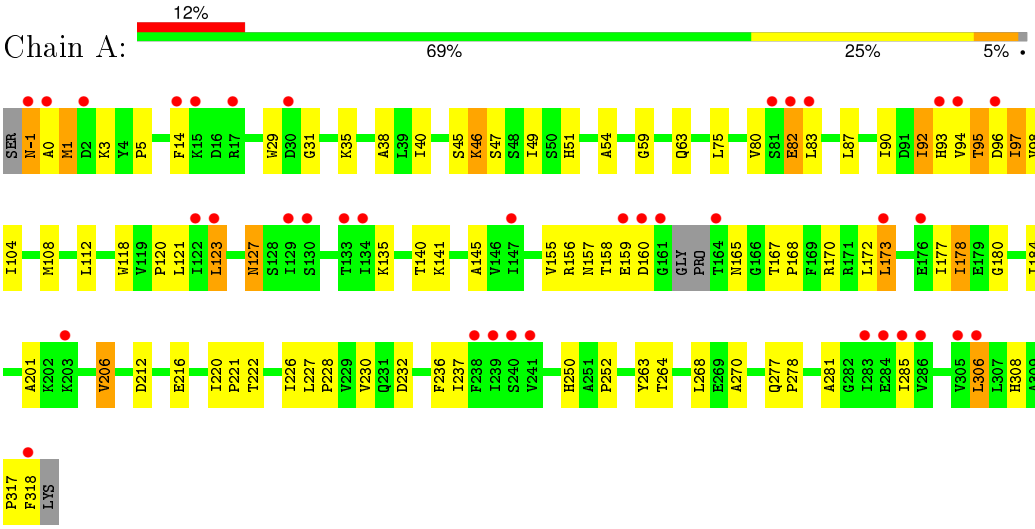
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	36	Total O 36 36	0	0
6	B	36	Total O 36 36	0	0
6	C	55	Total O 55 55	0	0
6	D	46	Total O 46 46	0	0
6	E	45	Total O 45 45	0	0
6	F	35	Total O 35 35	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

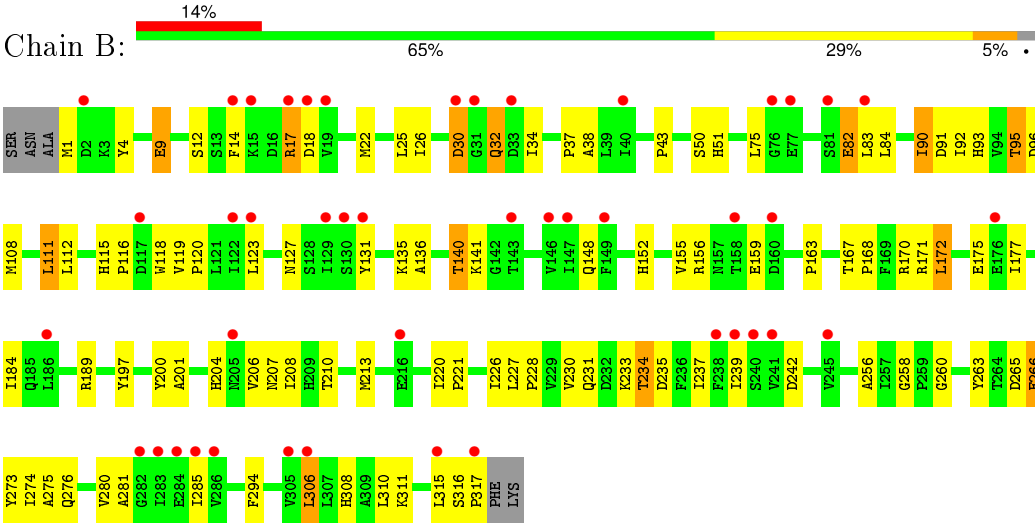
- Molecule 1: Formimidoylglutamase

Chain A:



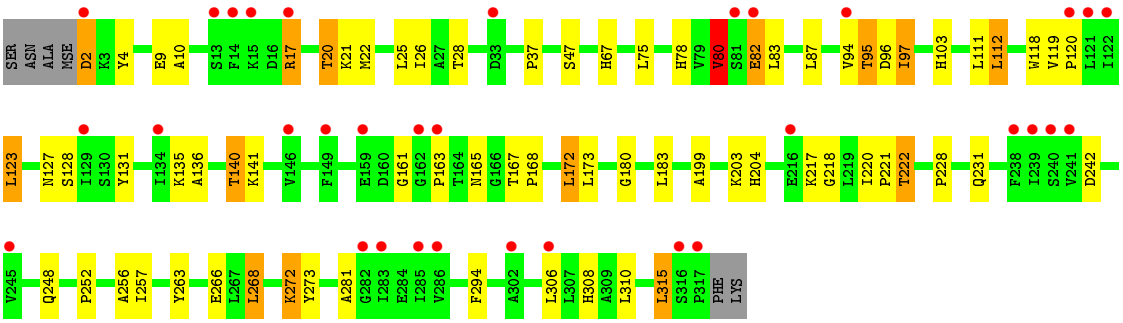
- Molecule 1: Formimidoylglutamase

Chain B:



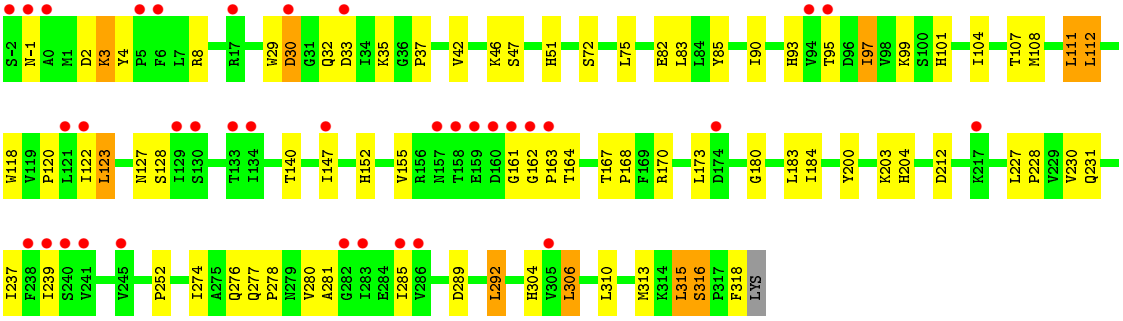
- Molecule 1: Formimidoylglutamase

Chain C:



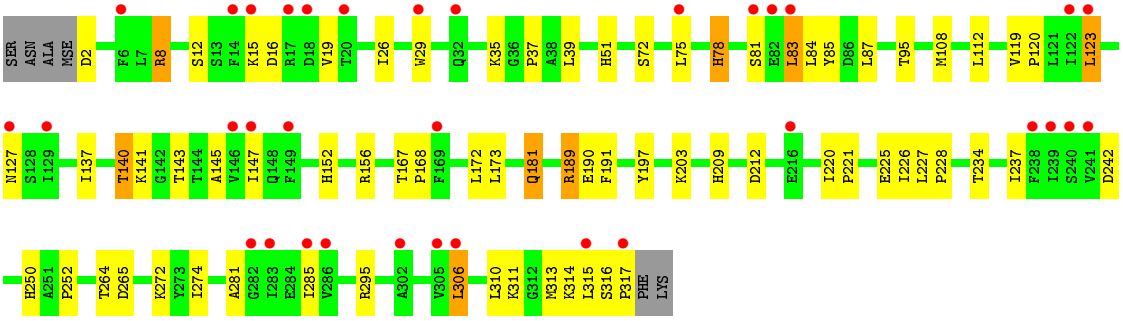
- Molecule 1: Formimidoylglutamase

Chain D:



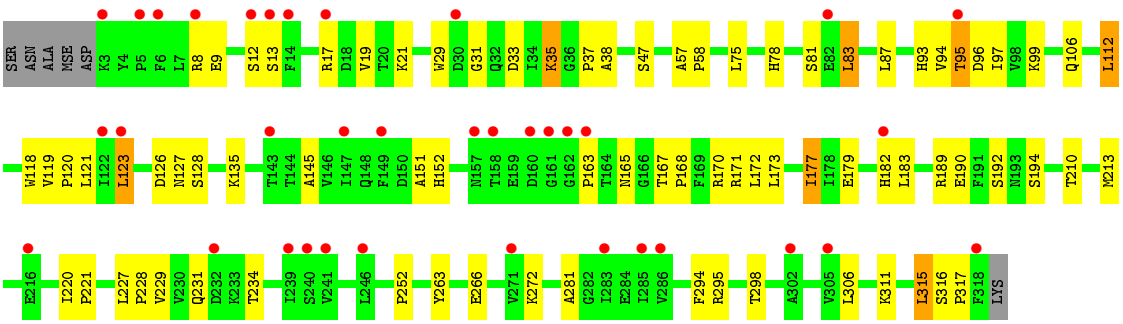
- Molecule 1: Formimidoylglutamase

Chain E:



- Molecule 1: Formimidoylglutamase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	142.04Å 118.98Å 123.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.47 – 2.20 32.47 – 2.20	Depositor EDS
% Data completeness (in resolution range)	88.0 (32.47-2.20) 96.5 (32.47-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.176 , 0.230 0.185 , 0.235	Depositor DCC
R_{free} test set	5124 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	40.6	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 62.8	EDS
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 102739 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15171	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CAC, CA, PEG, CL

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	0.39	0/2507	0.56	0/3388
1	B	0.37	0/2496	0.56	0/3377
1	C	0.42	0/2488	0.60	1/3367 (0.0%)
1	D	0.40	0/2526	0.57	0/3416
1	E	0.41	0/2488	0.60	0/3367
1	F	0.38	0/2492	0.56	0/3372
All	All	0.39	0/14997	0.58	1/20287 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	242	ASP	CB-CG-OD1	6.19	123.87	118.30

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	2462	0	2432	82	0
1	B	2449	0	2423	101	0
1	C	2441	0	2411	56	0
1	D	2479	0	2448	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2441	0	2411	59	0
1	F	2444	0	2416	59	0
2	A	2	0	0	4	0
2	B	2	0	0	3	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	21	0	30	11	0
4	B	14	0	20	4	0
4	C	49	0	70	5	0
4	D	14	0	20	5	0
4	E	21	0	30	7	0
4	F	42	0	60	7	0
5	C	10	0	0	3	0
5	E	10	0	0	1	0
6	A	36	0	0	1	0
6	B	36	0	0	2	0
6	C	55	0	0	1	0
6	D	46	0	0	1	0
6	E	45	0	0	0	0
6	F	35	0	0	0	0
All	All	15171	0	14771	408	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 14.

All (408) 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:D:152:HIS:HE2	4:D:323:PEG:H11	1.27	0.98
1:F:93:HIS:HD2	1:F:95:THR:H	1.12	0.96
1:D:93:HIS:HD2	1:D:95:THR:H	1.14	0.94
1:E:295:ARG:H	4:E:325:PEG:H21	1.33	0.93
1:F:135:LYS:HA	1:F:177:ILE:CD1	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:HIS:CD2	1:F:95:THR:H	1.90	0.89
1:E:37:PRO:HG3	1:E:313:MSE:HE1	1.56	0.88
1:D:152:HIS:CE1	4:D:323:PEG:H42	2.09	0.88
4:A:325:PEG:H21	4:A:326:PEG:H42	1.56	0.87
1:B:152:HIS:HE2	4:B:324:PEG:H11	1.40	0.86
1:A:93:HIS:HD2	1:A:95:THR:H	1.23	0.86
2:B:321:CL:CL	1:E:51:HIS:NE2	2.44	0.86
1:B:182:HIS:HE1	1:B:233:LYS:O	1.61	0.83
1:B:183:LEU:HB3	1:B:206:VAL:HG23	1.59	0.83
1:E:152:HIS:CE1	4:E:324:PEG:H11	2.14	0.82
1:B:91:ASP:HB2	1:D:8:ARG:HD2	1.60	0.82
1:F:93:HIS:CD2	1:F:96:ASP:H	1.99	0.81
1:C:112:LEU:HB3	1:C:140:THR:HG21	1.62	0.81
1:B:9:GLU:CD	1:B:9:GLU:H	1.84	0.80
1:D:93:HIS:CD2	1:D:95:THR:H	2.00	0.79
1:A:157:ASN:HA	1:A:170:ARG:HH11	1.47	0.78
1:A:40:ILE:HD13	1:A:108:MSE:HE1	1.66	0.78
1:D:237:ILE:HD11	1:D:280:VAL:HG22	1.65	0.78
1:D:93:HIS:ND1	1:D:99:LYS:HD2	2.00	0.77
1:B:30:ASP:HB2	1:B:32:GLN:NE2	1.99	0.76
1:B:201:ALA:HB1	1:B:206:VAL:HG11	1.68	0.76
1:E:295:ARG:N	4:E:325:PEG:H21	2.00	0.76
1:A:135:LYS:HE2	1:A:177:ILE:HD11	1.69	0.74
1:C:25:LEU:HD13	1:C:80:VAL:O	1.87	0.74
1:B:75:LEU:HD11	1:B:315:LEU:HD13	1.69	0.74
1:D:42:VAL:HG22	1:D:90:ILE:HD12	1.68	0.74
1:C:128:SER:HB3	1:C:165:ASN:HA	1.70	0.73
1:B:163:PRO:HD2	1:E:95:THR:HG21	1.69	0.73
1:A:145:ALA:HB3	1:A:237:ILE:HG22	1.70	0.73
1:C:141:LYS:HZ2	4:C:329:PEG:H31	1.54	0.73
1:A:93:HIS:CD2	1:A:95:THR:H	2.07	0.72
1:A:92:ILE:HD13	1:A:92:ILE:H	1.55	0.72
1:B:93:HIS:HD2	1:B:95:THR:H	1.36	0.72
1:E:250:HIS:HD2	1:E:264:THR:H	1.38	0.71
1:D:123:LEU:HD11	1:D:306:LEU:HD21	1.71	0.71
1:D:152:HIS:NE2	4:D:323:PEG:H11	2.03	0.71
1:E:123:LEU:HD11	1:E:306:LEU:HD21	1.71	0.71
1:A:40:ILE:HD13	1:A:108:MSE:CE	2.20	0.71
1:E:315:LEU:O	1:E:315:LEU:HD12	1.90	0.70
1:C:228:PRO:HA	1:C:231:GLN:HE21	1.54	0.70
1:B:91:ASP:HB2	1:D:8:ARG:CD	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:HIS:CD2	1:B:95:THR:H	2.11	0.69
1:C:82:GLU:CD	1:C:82:GLU:H	1.93	0.69
1:B:159:GLU:HB2	1:C:17:ARG:HH12	1.56	0.69
1:B:135:LYS:HG3	1:B:177:ILE:HD12	1.74	0.68
1:B:51:HIS:NE2	2:B:321:CL:CL	2.62	0.68
1:F:135:LYS:HA	1:F:177:ILE:HD13	1.75	0.68
1:A:93:HIS:CD2	1:A:96:ASP:H	2.12	0.67
1:E:145:ALA:HB3	1:E:237:ILE:HG22	1.76	0.67
1:E:272:LYS:HD3	1:E:311:LYS:HE2	1.75	0.67
1:A:59:GLY:HA3	4:A:324:PEG:H11	1.76	0.66
1:A:0:ALA:C	1:A:1:MSE:HE3	2.15	0.66
1:D:32:GLN:HG3	1:D:85:TYR:OH	1.96	0.66
1:D:304:HIS:HD2	4:D:324:PEG:O1	1.79	0.66
1:B:34:ILE:H	1:B:115:HIS:HD2	1.44	0.66
1:B:260:GLY:HA3	4:C:328:PEG:H31	1.78	0.66
1:A:59:GLY:HA3	4:A:324:PEG:H31	1.79	0.65
1:F:272:LYS:HD2	1:F:311:LYS:HE2	1.79	0.65
1:C:75:LEU:HD11	1:C:315:LEU:CD2	2.27	0.64
1:E:181:GLN:HE21	1:E:181:GLN:H	1.45	0.64
1:B:93:HIS:CD2	1:B:96:ASP:H	2.16	0.64
1:D:97:ILE:HD13	1:D:101:HIS:HD2	1.62	0.64
1:B:140:THR:HG23	1:B:141:LYS:HG2	1.80	0.63
1:B:9:GLU:HG2	1:B:12:SER:OG	1.97	0.63
1:E:147:ILE:HD13	1:E:274:ILE:HD13	1.79	0.63
1:B:123:LEU:HD21	1:B:306:LEU:HD21	1.81	0.63
1:D:292:LEU:HD12	4:F:323:PEG:H41	1.81	0.63
1:F:93:HIS:HD2	1:F:95:THR:N	1.91	0.63
1:E:137:ILE:O	1:E:141:LYS:HB2	1.99	0.63
1:C:123:LEU:HD11	1:C:306:LEU:HD11	1.81	0.63
1:A:93:HIS:HD2	1:A:95:THR:N	1.96	0.63
1:E:250:HIS:CD2	1:E:264:THR:H	2.17	0.62
1:B:285:ILE:CD1	1:B:306:LEU:HD13	2.29	0.62
1:B:285:ILE:HD11	1:B:306:LEU:HD13	1.81	0.62
1:D:167:THR:N	1:D:168:PRO:HD3	2.14	0.62
1:B:201:ALA:O	1:B:206:VAL:HG12	1.99	0.62
1:E:285:ILE:HD11	1:E:306:LEU:HD13	1.81	0.62
1:E:272:LYS:HE2	1:E:311:LYS:HD3	1.82	0.62
1:A:112:LEU:HB3	1:A:140:THR:HG21	1.82	0.62
1:A:108:MSE:HE2	1:A:108:MSE:HA	1.80	0.62
1:D:278:PRO:HG3	1:D:318:PHE:CZ	2.35	0.62
2:A:321:CL:CL	1:D:51:HIS:NE2	2.68	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ALA:O	1:C:140:THR:HB	2.00	0.61
1:A:83:LEU:C	1:A:83:LEU:HD12	2.21	0.61
1:A:317:PRO:HG2	1:A:318:PHE:CE2	2.36	0.61
4:A:325:PEG:H12	4:A:326:PEG:H21	1.83	0.61
1:A:51:HIS:CD2	2:A:321:CL:CL	2.91	0.61
1:B:22:MSE:O	1:B:26:ILE:HG13	2.01	0.60
1:D:239:ILE:HD11	1:D:274:ILE:HG22	1.83	0.60
1:F:123:LEU:HD11	1:F:306:LEU:HD11	1.82	0.60
1:A:99:LYS:HE2	1:A:103:HIS:CE1	2.36	0.60
1:E:152:HIS:CE1	4:E:324:PEG:C1	2.84	0.59
1:B:227:LEU:O	1:B:231:GLN:HG3	2.02	0.59
1:C:218:GLY:O	1:C:222:THR:CG2	2.49	0.59
1:F:172:LEU:HD22	1:F:177:ILE:HG12	1.84	0.59
1:D:83:LEU:HD12	1:D:83:LEU:C	2.23	0.59
1:E:120:PRO:HD2	1:E:281:ALA:O	2.03	0.59
1:B:105:PHE:CE2	1:B:135:LYS:HD2	2.37	0.58
1:B:140:THR:CG2	1:B:141:LYS:HG2	2.33	0.58
1:C:218:GLY:O	1:C:222:THR:HG23	2.02	0.58
1:B:82:GLU:HG3	1:B:83:LEU:H	1.68	0.58
1:F:227:LEU:HB3	1:F:228:PRO:HD3	1.84	0.58
1:D:276:GLN:O	1:D:316:SER:HB2	2.03	0.58
1:D:289:ASP:OD2	1:D:292:LEU:HD22	2.03	0.58
1:B:237:ILE:HD11	1:B:280:VAL:HG22	1.84	0.58
1:B:131:TYR:CD1	1:B:172:LEU:HD13	2.39	0.58
1:F:135:LYS:HA	1:F:177:ILE:HD11	1.85	0.58
1:E:37:PRO:HG3	1:E:313:MSE:CE	2.30	0.58
1:C:294:PHE:CD2	5:C:320[A]:CAC:C1	2.86	0.58
1:F:93:HIS:HD2	1:F:96:ASP:H	1.47	0.58
1:B:210:THR:OG1	1:B:213:MSE:HG3	2.04	0.57
1:F:151:ALA:HB3	4:F:328:PEG:H42	1.85	0.57
1:D:152:HIS:CE1	4:D:323:PEG:C4	2.86	0.57
1:C:131:TYR:HD1	1:C:172:LEU:HD13	1.69	0.57
1:F:295:ARG:HG2	4:F:323:PEG:H31	1.85	0.57
1:B:272:LYS:HG3	1:B:273:TYR:N	2.19	0.57
1:C:75:LEU:HD11	1:C:315:LEU:HD22	1.87	0.57
1:C:112:LEU:HD13	1:C:118:TRP:CE3	2.40	0.57
1:A:1:MSE:HE1	1:F:31:GLY:HA3	1.87	0.57
1:F:189:ARG:NH1	4:F:328:PEG:H31	2.20	0.56
1:D:97:ILE:HD13	1:D:101:HIS:CD2	2.41	0.56
1:B:38:ALA:HB3	1:B:118:TRP:NE1	2.20	0.56
1:E:72:SER:OG	1:E:75:LEU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:325:PEG:H21	4:A:326:PEG:C4	2.33	0.56
1:C:131:TYR:CD1	1:C:172:LEU:HD13	2.41	0.56
1:B:105:PHE:CD2	1:B:135:LYS:HD2	2.41	0.56
1:C:256:ALA:HB1	4:C:327:PEG:H22	1.87	0.56
1:C:167:THR:N	1:C:168:PRO:HD2	2.21	0.56
1:A:100:SER:O	1:A:104:ILE:HG13	2.06	0.56
1:B:152:HIS:NE2	4:B:324:PEG:H11	2.18	0.56
1:B:231:GLN:HA	1:B:234:THR:HG22	1.87	0.56
1:C:128:SER:HB3	1:C:165:ASN:CA	2.36	0.55
1:C:180:GLY:HA3	1:C:204:HIS:O	2.07	0.55
1:C:163:PRO:HD2	1:F:95:THR:HG21	1.88	0.55
1:A:167:THR:N	1:A:168:PRO:CD	2.70	0.55
1:B:131:TYR:HD1	1:B:172:LEU:HD13	1.71	0.55
1:A:167:THR:N	1:A:168:PRO:HD2	2.21	0.55
4:A:325:PEG:C2	4:A:326:PEG:H42	2.31	0.55
1:E:78:HIS:N	1:E:78:HIS:HD1	2.05	0.55
1:E:152:HIS:HE1	4:E:324:PEG:H11	1.68	0.54
1:F:227:LEU:O	1:F:231:GLN:HB2	2.06	0.54
6:D:341:HOH:O	1:F:78:HIS:HE1	1.90	0.54
1:D:112:LEU:HD13	1:D:118:TRP:CE3	2.43	0.54
1:C:161:GLY:O	1:F:95:THR:HB	2.07	0.54
1:B:82:GLU:CG	1:B:83:LEU:H	2.19	0.54
1:C:167:THR:N	1:C:168:PRO:CD	2.70	0.54
1:E:143:THR:HG22	1:E:234:THR:HG22	1.90	0.54
1:D:37:PRO:HG3	1:D:313:MSE:CE	2.38	0.54
1:E:8:ARG:HD3	1:E:12:SER:HB2	1.88	0.54
1:B:83:LEU:C	1:B:83:LEU:HD12	2.28	0.54
1:F:210:THR:OG1	1:F:213:MSE:HG3	2.08	0.54
1:F:120:PRO:HD2	1:F:281:ALA:O	2.08	0.54
1:F:172:LEU:CD2	1:F:177:ILE:HG12	2.37	0.54
1:A:264:THR:O	1:A:268:LEU:HG	2.08	0.53
1:A:45:SER:HB3	1:A:54:ALA:HB3	1.89	0.53
1:A:285:ILE:HD11	1:A:306:LEU:HD13	1.91	0.53
1:B:180:GLY:HA3	1:B:204:HIS:O	2.08	0.53
1:C:75:LEU:HD11	1:C:315:LEU:HD21	1.91	0.52
1:B:184:ILE:HD11	1:B:230:VAL:HG21	1.91	0.52
1:F:8:ARG:NH2	1:F:13:SER:O	2.43	0.52
1:F:316:SER:OG	1:F:317:PRO:HD3	2.09	0.52
1:F:145:ALA:HB2	1:F:234:THR:HG21	1.89	0.52
1:A:220:ILE:HB	1:A:221:PRO:HD3	1.92	0.52
1:F:210:THR:HG23	1:F:213:MSE:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:PRO:HD2	1:C:281:ALA:O	2.10	0.52
1:C:9:GLU:HG2	6:C:385:HOH:O	2.09	0.52
1:F:75:LEU:HD11	1:F:315:LEU:CD2	2.40	0.52
1:D:252:PRO:HB2	1:F:294:PHE:CE1	2.44	0.52
1:B:210:THR:HG23	1:B:213:MSE:HE3	1.92	0.52
1:C:82:GLU:HG2	1:C:83:LEU:H	1.75	0.52
1:D:75:LEU:HD11	1:D:315:LEU:HD22	1.92	0.52
1:B:152:HIS:HE2	4:B:324:PEG:C1	2.18	0.52
1:D:101:HIS:HE1	1:D:128:SER:O	1.92	0.52
1:B:17:ARG:NE	1:B:18:ASP:OD2	2.43	0.52
1:D:47:SER:HB3	1:D:97:ILE:HD11	1.92	0.51
1:B:227:LEU:HB3	1:B:228:PRO:HD3	1.91	0.51
1:C:22:MSE:O	1:C:26:ILE:HG13	2.10	0.51
1:A:45:SER:CB	1:A:54:ALA:HB3	2.40	0.51
1:C:82:GLU:CD	1:C:82:GLU:N	2.64	0.51
1:A:180:GLY:O	1:A:206:VAL:HA	2.10	0.51
1:B:9:GLU:HG2	1:B:12:SER:HG	1.75	0.51
1:A:135:LYS:HE2	1:A:177:ILE:CD1	2.40	0.51
1:E:19:VAL:HG23	1:F:194:SER:OG	2.10	0.51
1:A:3:LYS:O	1:A:5:PRO:HD3	2.11	0.51
1:E:272:LYS:HZ2	1:E:311:LYS:HZ3	1.59	0.51
1:B:104:ILE:O	1:B:108:MSE:HB2	2.11	0.50
1:C:20:THR:HG21	1:C:78:HIS:NE2	2.27	0.50
1:C:272:LYS:HG3	1:C:273:TYR:N	2.26	0.50
1:A:127:ASN:OD1	2:A:320:CL:CL	2.66	0.50
1:C:308:HIS:CE1	4:C:328:PEG:H21	2.46	0.50
1:D:167:THR:N	1:D:168:PRO:CD	2.75	0.50
1:F:152:HIS:CE1	4:F:328:PEG:H41	2.46	0.50
1:F:112:LEU:HD13	1:F:118:TRP:CE3	2.47	0.50
1:C:128:SER:CB	1:C:165:ASN:HA	2.39	0.50
1:E:75:LEU:HD11	1:E:315:LEU:HD23	1.94	0.50
1:D:237:ILE:HG12	1:D:280:VAL:HA	1.93	0.49
1:E:252:PRO:HG3	5:E:320[A]:CAC:C1	2.42	0.49
1:C:95:THR:HG22	1:C:96:ASP:N	2.27	0.49
1:A:38:ALA:HB3	1:A:118:TRP:NE1	2.26	0.49
1:F:29:TRP:CD2	1:F:87:LEU:HD22	2.47	0.49
1:C:268:LEU:HD23	4:C:328:PEG:H32	1.94	0.49
1:B:239:ILE:HD11	1:B:274:ILE:HG22	1.93	0.49
4:A:325:PEG:O4	1:B:308:HIS:HE1	1.96	0.49
1:A:38:ALA:HB1	1:A:87:LEU:HD13	1.93	0.49
4:A:325:PEG:C1	4:A:326:PEG:H21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:MSE:HE1	1:A:118:TRP:HH2	1.76	0.49
1:A:250:HIS:CD2	1:A:264:THR:H	2.29	0.49
1:A:82:GLU:CD	1:A:82:GLU:H	2.16	0.49
1:E:83:LEU:HD12	1:E:83:LEU:C	2.33	0.49
1:F:167:THR:N	1:F:168:PRO:CD	2.76	0.49
1:A:-1:ASN:OD1	1:A:-1:ASN:N	2.45	0.49
1:C:217:LYS:O	1:C:217:LYS:HG3	2.13	0.49
1:A:184:ILE:HD11	1:A:230:VAL:HG21	1.95	0.49
1:B:93:HIS:HD2	1:B:96:ASP:H	1.58	0.49
1:B:156:ARG:HA	1:B:197:TYR:CZ	2.48	0.49
1:A:155:VAL:HG23	1:A:197:TYR:HB3	1.94	0.49
1:B:207:ASN:OD1	1:B:226:ILE:HD11	2.13	0.49
1:A:201:ALA:O	1:A:206:VAL:HG13	2.13	0.48
1:D:108:MSE:HE2	1:D:122:ILE:HD11	1.95	0.48
1:D:161:GLY:HA3	1:D:164:THR:HG21	1.94	0.48
1:B:30:ASP:HB2	1:B:32:GLN:CD	2.33	0.48
1:A:250:HIS:CE1	1:A:263:TYR:HD2	2.31	0.48
1:A:120:PRO:HD2	1:A:281:ALA:O	2.14	0.48
1:F:128:SER:HB3	1:F:165:ASN:HA	1.96	0.48
1:F:179:GLU:HB2	1:F:182:HIS:ND1	2.29	0.48
1:A:157:ASN:HA	1:A:170:ARG:NH1	2.23	0.48
1:B:167:THR:N	1:B:168:PRO:CD	2.77	0.48
1:B:17:ARG:HG3	1:B:18:ASP:N	2.29	0.48
1:D:29:TRP:CD1	1:D:30:ASP:O	2.67	0.48
1:D:120:PRO:HD2	1:D:281:ALA:O	2.14	0.47
1:C:2:ASP:HB2	1:C:4:TYR:H	1.78	0.47
1:E:19:VAL:HG13	1:E:19:VAL:O	2.13	0.47
1:A:220:ILE:HD11	1:A:270:ALA:HA	1.96	0.47
1:D:276:GLN:HE21	1:D:315:LEU:HB3	1.80	0.47
1:E:156:ARG:HA	1:E:197:TYR:CZ	2.49	0.47
1:B:38:ALA:HB3	1:B:118:TRP:HE1	1.79	0.47
1:A:90:ILE:HD11	1:A:108:MSE:HE3	1.97	0.47
1:B:32:GLN:OE1	1:B:32:GLN:N	2.42	0.47
1:D:47:SER:HB3	1:D:97:ILE:CD1	2.44	0.47
1:F:38:ALA:HB3	1:F:118:TRP:NE1	2.29	0.47
1:A:190:GLU:O	4:A:325:PEG:H41	2.14	0.47
1:A:1:MSE:N	1:A:1:MSE:HE3	2.30	0.47
1:B:230:VAL:O	1:B:234:THR:HB	2.15	0.47
1:C:97:ILE:HD11	1:C:163:PRO:HG2	1.97	0.47
1:A:112:LEU:CB	1:A:140:THR:HG21	2.44	0.47
1:C:252:PRO:HG3	5:C:320[B]:CAC:C2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:324:PEG:H11	4:A:324:PEG:H31	1.73	0.46
1:B:34:ILE:H	1:B:115:HIS:CD2	2.28	0.46
1:B:268:LEU:HG	1:B:308:HIS:ND1	2.31	0.46
1:B:93:HIS:HD2	1:B:95:THR:N	2.09	0.46
1:E:83:LEU:O	1:E:83:LEU:HD12	2.15	0.46
1:A:156:ARG:HA	1:A:197:TYR:CZ	2.50	0.46
1:F:152:HIS:HD2	1:F:192:SER:O	1.98	0.46
1:F:8:ARG:HG2	1:F:12:SER:OG	2.16	0.46
1:E:81:SER:HB3	1:E:314:LYS:NZ	2.31	0.46
1:B:220:ILE:HB	1:B:221:PRO:HD3	1.98	0.46
1:A:83:LEU:O	1:A:83:LEU:HD12	2.16	0.46
1:D:83:LEU:HD12	1:D:83:LEU:O	2.15	0.46
1:B:207:ASN:HB3	1:B:226:ILE:CD1	2.46	0.46
1:D:3:LYS:HE3	1:D:4:TYR:CZ	2.51	0.46
1:F:263:TYR:O	1:F:266:GLU:HB3	2.16	0.46
1:E:16:ASP:HB3	1:E:19:VAL:CG1	2.46	0.46
1:E:190:GLU:O	1:E:191:PHE:HB2	2.16	0.46
1:B:308:HIS:HD2	6:B:360:HOH:O	1.99	0.46
1:C:131:TYR:OH	1:C:135:LYS:HE3	2.16	0.45
1:C:199:ALA:O	1:C:203:LYS:HD3	2.16	0.45
1:A:157:ASN:OD1	1:A:170:ARG:NH1	2.49	0.45
1:E:78:HIS:ND1	1:E:78:HIS:N	2.64	0.45
1:C:228:PRO:HA	1:C:231:GLN:NE2	2.28	0.45
1:F:220:ILE:HB	1:F:221:PRO:HD3	1.97	0.45
1:D:35:LYS:NZ	1:D:35:LYS:HB2	2.31	0.45
1:B:108:MSE:HB3	1:B:136:ALA:CB	2.47	0.45
1:B:43:PRO:HD2	1:B:92:ILE:HG12	1.97	0.45
1:C:220:ILE:HB	1:C:221:PRO:HD3	1.98	0.45
1:B:256:ALA:O	4:B:324:PEG:C4	2.65	0.45
1:B:82:GLU:CG	1:B:83:LEU:N	2.79	0.45
1:A:250:HIS:CE1	1:A:263:TYR:CD2	3.04	0.45
1:F:37:PRO:HA	1:F:119:VAL:O	2.16	0.45
1:A:1:MSE:HE1	1:F:31:GLY:CA	2.46	0.45
1:E:37:PRO:HA	1:E:119:VAL:O	2.17	0.45
1:F:252:PRO:HD2	1:F:298:THR:OG1	2.17	0.45
1:C:263:TYR:O	1:C:266:GLU:HB2	2.16	0.45
1:B:201:ALA:HB1	1:B:206:VAL:CG1	2.41	0.45
1:E:272:LYS:NZ	1:E:311:LYS:NZ	2.65	0.45
1:E:265:ASP:N	1:E:265:ASP:OD1	2.49	0.45
1:A:277:GLN:HB3	1:A:278:PRO:CD	2.47	0.45
1:D:184:ILE:HD11	1:D:230:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:75:LEU:HD11	1:F:315:LEU:HD21	1.99	0.44
1:A:29:TRP:CZ2	1:A:31:GLY:HA2	2.52	0.44
1:E:272:LYS:NZ	1:E:311:LYS:HZ3	2.15	0.44
1:F:151:ALA:CB	4:F:328:PEG:H42	2.48	0.44
1:E:81:SER:HB3	1:E:314:LYS:HZ1	1.82	0.44
1:B:112:LEU:HD13	1:B:140:THR:HG21	1.98	0.44
1:B:4:TYR:CE2	1:D:111:LEU:HD13	2.52	0.44
1:D:155:VAL:O	1:D:170:ARG:HD2	2.18	0.44
2:B:321:CL:CL	1:E:51:HIS:CD2	3.08	0.44
1:E:152:HIS:HE1	4:E:324:PEG:C1	2.28	0.44
1:C:83:LEU:C	1:C:83:LEU:HD12	2.38	0.44
1:E:311:LYS:NZ	1:F:190:GLU:OE1	2.50	0.44
1:E:209:HIS:CE1	1:E:226:ILE:HG13	2.52	0.44
1:A:121:LEU:HD21	1:A:310:LEU:HD11	2.00	0.44
1:B:120:PRO:HD2	1:B:281:ALA:O	2.17	0.44
1:B:90:ILE:HD11	1:B:104:ILE:HG13	2.00	0.44
1:D:278:PRO:HG3	1:D:318:PHE:CE1	2.52	0.44
1:F:57:ALA:HB3	1:F:58:PRO:HD3	2.00	0.44
1:A:123:LEU:HD11	1:A:306:LEU:HD21	2.00	0.44
1:E:16:ASP:HB3	1:E:19:VAL:HG12	1.99	0.44
1:F:38:ALA:HB3	1:F:118:TRP:CD1	2.53	0.44
1:B:210:THR:CG2	1:B:213:MSE:HE3	2.48	0.43
1:F:152:HIS:HE1	4:F:328:PEG:H41	1.83	0.43
1:D:104:ILE:O	1:D:108:MSE:HB2	2.18	0.43
1:D:107:THR:HG22	1:D:111:LEU:HD22	2.00	0.43
1:D:-1:ASN:HA	1:D:2:ASP:HB2	2.00	0.43
1:B:206:VAL:HG13	1:B:208:ILE:HG13	2.01	0.43
1:E:39:LEU:O	1:E:87:LEU:HB2	2.18	0.43
1:B:148:GLN:O	1:B:148:GLN:HG3	2.18	0.43
1:B:136:ALA:O	1:B:140:THR:HB	2.17	0.43
1:E:220:ILE:HB	1:E:221:PRO:HD3	2.01	0.43
1:A:227:LEU:HB3	1:A:228:PRO:HD3	1.99	0.43
1:B:170:ARG:HD2	1:B:200:TYR:CZ	2.54	0.43
1:B:26:ILE:HA	1:B:84:LEU:O	2.19	0.43
1:E:167:THR:N	1:E:168:PRO:CD	2.82	0.43
1:C:87:LEU:HD23	1:C:111:LEU:HD13	2.01	0.43
1:A:308:HIS:HE1	6:A:328:HOH:O	2.01	0.43
1:B:182:HIS:CE1	1:B:233:LYS:O	2.54	0.43
1:D:112:LEU:HB3	1:D:140:THR:HG21	1.99	0.43
1:D:203:LYS:HE2	1:D:203:LYS:HB2	1.94	0.43
1:A:51:HIS:NE2	2:A:321:CL:CL	2.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:THR:CG2	1:F:213:MSE:HE3	2.49	0.43
1:A:173:LEU:CD1	1:A:178:ILE:HG22	2.48	0.43
1:D:227:LEU:HB3	1:D:228:PRO:HD3	2.01	0.43
1:E:189:ARG:NH1	4:E:324:PEG:H21	2.33	0.43
1:C:112:LEU:HD13	1:C:118:TRP:CZ3	2.54	0.43
1:A:40:ILE:HD13	1:A:108:MSE:HE3	1.99	0.43
1:A:141:LYS:O	1:A:236:PHE:CE1	2.72	0.43
1:A:92:ILE:HD13	1:A:92:ILE:N	2.28	0.42
1:C:21:LYS:HE3	1:C:67:HIS:HA	2.00	0.42
1:C:294:PHE:CG	5:C:320[A]:CAC:C1	3.02	0.42
1:C:248:GLN:HB3	1:C:257:ILE:HB	2.00	0.42
1:E:112:LEU:CB	1:E:140:THR:HG21	2.49	0.42
1:A:97:ILE:HA	1:A:97:ILE:HD12	1.78	0.42
1:D:72:SER:HB3	1:D:75:LEU:HB2	2.01	0.42
1:C:80:VAL:HG12	1:C:80:VAL:O	2.20	0.42
1:B:242:ASP:C	1:B:242:ASP:OD1	2.57	0.42
1:D:162:GLY:O	1:D:164:THR:N	2.52	0.42
1:A:278:PRO:HG3	1:A:318:PHE:CZ	2.54	0.42
1:D:147:ILE:HD11	1:D:227:LEU:HD13	2.01	0.42
1:A:75:LEU:HD11	1:A:315:LEU:HD13	2.01	0.42
1:D:252:PRO:HB2	1:F:294:PHE:HE1	1.84	0.42
1:B:155:VAL:O	1:B:170:ARG:HD3	2.20	0.42
1:E:316:SER:HA	1:E:317:PRO:HD3	1.80	0.42
1:B:37:PRO:HA	1:B:119:VAL:O	2.20	0.42
1:C:218:GLY:O	1:C:222:THR:HG22	2.20	0.42
1:F:163:PRO:HB3	1:F:171:ARG:NH2	2.35	0.42
1:B:82:GLU:HG3	1:B:83:LEU:O	2.19	0.42
1:A:46:LYS:HG3	1:D:46:LYS:HG2	2.02	0.42
1:D:99:LYS:HE2	1:D:99:LYS:HB2	1.88	0.41
1:F:96:ASP:OD2	1:F:99:LYS:HG3	2.20	0.41
1:E:242:ASP:OD1	1:E:242:ASP:C	2.58	0.41
1:E:29:TRP:HA	1:E:85:TYR:CD1	2.55	0.41
1:A:159:GLU:O	1:A:160:ASP:C	2.59	0.41
1:B:105:PHE:CE2	1:B:135:LYS:CD	3.03	0.41
1:A:83:LEU:C	1:A:83:LEU:CD1	2.88	0.41
1:D:200:TYR:CD2	1:D:200:TYR:C	2.94	0.41
1:A:0:ALA:O	1:A:1:MSE:HE3	2.20	0.41
1:E:108:MSE:HE1	1:E:120:PRO:HB3	2.02	0.41
1:B:181:GLN:CD	1:B:181:GLN:H	2.24	0.41
4:A:325:PEG:H22	1:B:268:LEU:HD23	2.01	0.41
1:E:227:LEU:HB3	1:E:228:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ILE:HD11	1:D:306:LEU:HD13	2.02	0.41
1:A:285:ILE:CD1	1:A:306:LEU:HD13	2.50	0.41
1:F:47:SER:HB2	1:F:126:ASP:OD2	2.20	0.41
1:A:222:THR:O	1:A:226:ILE:HG22	2.21	0.41
1:B:316:SER:HA	1:B:317:PRO:HD3	1.91	0.41
1:B:311:LYS:O	1:B:315:LEU:HB2	2.20	0.41
1:A:95:THR:HB	1:D:161:GLY:O	2.20	0.41
1:B:131:TYR:CE1	1:B:171:ARG:HB3	2.56	0.41
1:D:37:PRO:HG3	1:D:313:MSE:HE1	2.03	0.41
1:F:19:VAL:HG12	1:F:21:LYS:HG3	2.01	0.41
1:A:49:ILE:H	1:A:165:ASN:HB2	1.85	0.41
1:F:83:LEU:C	1:F:83:LEU:CD1	2.89	0.41
1:D:180:GLY:HA3	1:D:204:HIS:O	2.20	0.41
1:C:9:GLU:O	1:C:10:ALA:C	2.58	0.41
1:A:252:PRO:HB2	1:B:294:PHE:CE1	2.56	0.41
1:F:35:LYS:HG2	1:F:35:LYS:H	1.74	0.41
1:E:26:ILE:HA	1:E:84:LEU:O	2.20	0.41
1:B:285:ILE:HD12	1:B:306:LEU:HD13	2.01	0.40
1:B:275:ALA:HA	1:B:280:VAL:HG21	2.03	0.40
1:B:258:GLY:HA3	6:B:334:HOH:O	2.21	0.40
1:E:225:GLU:HG2	1:E:226:ILE:HD13	2.03	0.40
1:C:37:PRO:HA	1:C:119:VAL:O	2.21	0.40
1:C:268:LEU:HG	1:C:308:HIS:CD2	2.56	0.40
1:B:90:ILE:HG12	1:B:104:ILE:HG12	2.02	0.40
1:B:111:LEU:HD13	1:D:4:TYR:CE2	2.57	0.40
1:A:14:PHE:CD1	1:F:94:VAL:HG21	2.57	0.40
1:A:278:PRO:HG3	1:A:318:PHE:CE2	2.56	0.40
1:B:131:TYR:OH	1:B:175:GLU:OE1	2.34	0.40
1:B:263:TYR:O	1:B:266:GLU:HG3	2.21	0.40
1:B:268:LEU:HA	1:B:268:LEU:HD12	1.83	0.40
1:A:95:THR:HG21	1:D:163:PRO:HD2	2.03	0.40
1:B:116:PRO:O	1:B:141:LYS:NZ	2.54	0.40
1:A:99:LYS:HE2	1:A:103:HIS:NE2	2.36	0.40
1:A:156:ARG:HA	1:A:197:TYR:CE1	2.56	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	314/322 (98%)	297 (95%)	17 (5%)	0	100	100
1	B	315/322 (98%)	306 (97%)	7 (2%)	2 (1%)	30	29
1	C	314/322 (98%)	306 (98%)	7 (2%)	1 (0%)	46	50
1	D	319/322 (99%)	307 (96%)	12 (4%)	0	100	100
1	E	314/322 (98%)	301 (96%)	13 (4%)	0	100	100
1	F	314/322 (98%)	302 (96%)	11 (4%)	1 (0%)	46	50
All	All	1890/1932 (98%)	1819 (96%)	67 (4%)	4 (0%)	52	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	32	GLN
1	B	82	GLU
1	F	229	VAL
1	C	80	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	270/265 (102%)	243 (90%)	27 (10%)	9	8
1	B	269/265 (102%)	244 (91%)	25 (9%)	11	10
1	C	268/265 (101%)	245 (91%)	23 (9%)	13	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	272/265 (103%)	253 (93%)	19 (7%)	19 19
1	E	268/265 (101%)	251 (94%)	17 (6%)	22 24
1	F	268/265 (101%)	250 (93%)	18 (7%)	20 21
All	All	1615/1590 (102%)	1486 (92%)	129 (8%)	15 15

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	1	MSE
1	A	35	LYS
1	A	46	LYS
1	A	47	SER
1	A	63	GLN
1	A	80	VAL
1	A	82	GLU
1	A	92	ILE
1	A	94	VAL
1	A	95	THR
1	A	97	ILE
1	A	98	VAL
1	A	123	LEU
1	A	127	ASN
1	A	158	THR
1	A	172	LEU
1	A	173	LEU
1	A	178	ILE
1	A	190	GLU
1	A	206	VAL
1	A	212	ASP
1	A	216	GLU
1	A	232	ASP
1	A	306	LEU
1	A	310	LEU
1	A	315	LEU
1	B	1	MSE
1	B	9	GLU
1	B	14	PHE
1	B	17	ARG
1	B	25	LEU
1	B	30	ASP

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Mol	Chain	Res	Type
1	B	50	SER
1	B	90	ILE
1	B	95	THR
1	B	111	LEU
1	B	127	ASN
1	B	140	THR
1	B	172	LEU
1	B	181	GLN
1	B	183	LEU
1	B	189	ARG
1	B	234	THR
1	B	235	ASP
1	B	265	ASP
1	B	266	GLU
1	B	268	LEU
1	B	272	LYS
1	B	276	GLN
1	B	306	LEU
1	B	310	LEU
1	C	2	ASP
1	C	17	ARG
1	C	20	THR
1	C	28	THR
1	C	47	SER
1	C	80	VAL
1	C	82	GLU
1	C	94	VAL
1	C	95	THR
1	C	97	ILE
1	C	103	HIS
1	C	112	LEU
1	C	123	LEU
1	C	127	ASN
1	C	140	THR
1	C	172	LEU
1	C	173	LEU
1	C	183	LEU
1	C	222	THR
1	C	268	LEU
1	C	272	LYS
1	C	310	LEU
1	C	315	LEU

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Mol	Chain	Res	Type
1	D	3	LYS
1	D	30	ASP
1	D	33	ASP
1	D	82	GLU
1	D	97	ILE
1	D	111	LEU
1	D	112	LEU
1	D	123	LEU
1	D	127	ASN
1	D	173	LEU
1	D	183	LEU
1	D	212	ASP
1	D	231	GLN
1	D	277	GLN
1	D	292	LEU
1	D	306	LEU
1	D	310	LEU
1	D	315	LEU
1	D	316	SER
1	E	2	ASP
1	E	8	ARG
1	E	15	LYS
1	E	35	LYS
1	E	78	HIS
1	E	83	LEU
1	E	123	LEU
1	E	127	ASN
1	E	140	THR
1	E	172	LEU
1	E	173	LEU
1	E	181	GLN
1	E	189	ARG
1	E	203	LYS
1	E	212	ASP
1	E	306	LEU
1	E	310	LEU
1	F	9	GLU
1	F	17	ARG
1	F	33	ASP
1	F	35	LYS
1	F	81	SER
1	F	83	LEU

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Mol	Chain	Res	Type
1	F	95	THR
1	F	97	ILE
1	F	106	GLN
1	F	112	LEU
1	F	121	LEU
1	F	123	LEU
1	F	127	ASN
1	F	170	ARG
1	F	173	LEU
1	F	177	ILE
1	F	183	LEU
1	F	315	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	78	HIS
1	A	93	HIS
1	A	106	GLN
1	A	115	HIS
1	A	250	HIS
1	A	308	HIS
1	B	93	HIS
1	B	106	GLN
1	B	115	HIS
1	B	182	HIS
1	B	308	HIS
1	C	204	HIS
1	C	231	GLN
1	C	276	GLN
1	C	277	GLN
1	D	93	HIS
1	D	101	HIS
1	D	103	HIS
1	D	276	GLN
1	D	277	GLN
1	D	304	HIS
1	E	102	HIS
1	E	181	GLN
1	E	250	HIS
1	F	78	HIS

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Mol	Chain	Res	Type
1	F	93	HIS
1	F	231	GLN
1	F	277	GLN
1	F	304	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 48 ligands modelled in this entry, 21 are monoatomic - leaving 27 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	$\#\|Z\| > 2$
4	PEG	A	324	-	6,6,6	0.58	0	5,5,5	0.71	0
4	PEG	A	325	-	6,6,6	0.57	0	5,5,5	0.62	0
4	PEG	A	326	-	6,6,6	0.53	0	5,5,5	0.94	1 (20%)
4	PEG	B	324	-	6,6,6	0.56	0	5,5,5	0.81	0
4	PEG	B	325	-	6,6,6	0.57	0	5,5,5	0.71	0
5	CAC	C	320[A]	-	0,4,4	0.00	-	0,6,6	0.00	-
5	CAC	C	320[B]	-	0,4,4	0.00	-	0,6,6	0.00	-
4	PEG	C	325	-	6,6,6	0.53	0	5,5,5	0.79	0
4	PEG	C	326	-	6,6,6	0.55	0	5,5,5	0.73	0
4	PEG	C	327	-	6,6,6	0.60	0	5,5,5	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PEG	C	328	-	6,6,6	0.53	0	5,5,5	0.77	0
4	PEG	C	329	-	6,6,6	0.54	0	5,5,5	0.70	0
4	PEG	C	330	-	6,6,6	0.55	0	5,5,5	0.80	0
4	PEG	C	331	-	6,6,6	0.57	0	5,5,5	0.74	0
4	PEG	D	323	-	6,6,6	0.62	0	5,5,5	1.17	1 (20%)
4	PEG	D	324	-	6,6,6	0.55	0	5,5,5	0.62	0
5	CAC	E	320[A]	-	0,4,4	0.00	-	0,6,6	0.00	-
5	CAC	E	320[B]	-	0,4,4	0.00	-	0,6,6	0.00	-
4	PEG	E	324	-	6,6,6	0.58	0	5,5,5	0.69	0
4	PEG	E	325	-	6,6,6	0.60	0	5,5,5	0.83	0
4	PEG	E	326	-	6,6,6	0.51	0	5,5,5	0.80	0
4	PEG	F	323	-	6,6,6	0.53	0	5,5,5	0.83	0
4	PEG	F	324	-	6,6,6	0.53	0	5,5,5	0.62	0
4	PEG	F	325	-	6,6,6	0.55	0	5,5,5	0.76	0
4	PEG	F	326	-	6,6,6	0.58	0	5,5,5	0.92	0
4	PEG	F	327	-	6,6,6	0.54	0	5,5,5	0.75	0
4	PEG	F	328	-	6,6,6	0.55	0	5,5,5	0.58	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	PEG	A	324	-	-	0/4/4/4	0/0/0/0
4	PEG	A	325	-	-	0/4/4/4	0/0/0/0
4	PEG	A	326	-	-	0/4/4/4	0/0/0/0
4	PEG	B	324	-	-	0/4/4/4	0/0/0/0
4	PEG	B	325	-	-	0/4/4/4	0/0/0/0
5	CAC	C	320[A]	-	-	0/0/0/0	0/0/0/0
5	CAC	C	320[B]	-	-	0/0/0/0	0/0/0/0
4	PEG	C	325	-	-	0/4/4/4	0/0/0/0
4	PEG	C	326	-	-	0/4/4/4	0/0/0/0
4	PEG	C	327	-	-	0/4/4/4	0/0/0/0
4	PEG	C	328	-	-	0/4/4/4	0/0/0/0
4	PEG	C	329	-	-	0/4/4/4	0/0/0/0
4	PEG	C	330	-	-	0/4/4/4	0/0/0/0
4	PEG	C	331	-	-	0/4/4/4	0/0/0/0
4	PEG	D	323	-	-	0/4/4/4	0/0/0/0
4	PEG	D	324	-	-	0/4/4/4	0/0/0/0
5	CAC	E	320[A]	-	-	0/0/0/0	0/0/0/0
5	CAC	E	320[B]	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	E	324	-	-	0/4/4/4	0/0/0/0
4	PEG	E	325	-	-	0/4/4/4	0/0/0/0
4	PEG	E	326	-	-	0/4/4/4	0/0/0/0
4	PEG	F	323	-	-	0/4/4/4	0/0/0/0
4	PEG	F	324	-	-	0/4/4/4	0/0/0/0
4	PEG	F	325	-	-	0/4/4/4	0/0/0/0
4	PEG	F	326	-	-	0/4/4/4	0/0/0/0
4	PEG	F	327	-	-	0/4/4/4	0/0/0/0
4	PEG	F	328	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	326	PEG	C3-O2-C2	2.03	122.03	113.31
4	D	323	PEG	C3-O2-C2	2.50	124.04	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	324	PEG	3	0
4	A	325	PEG	8	0
4	A	326	PEG	5	0
4	B	324	PEG	4	0
5	C	320[A]	CAC	2	0
5	C	320[B]	CAC	1	0
4	C	327	PEG	1	0
4	C	328	PEG	3	0
4	C	329	PEG	1	0
4	D	323	PEG	4	0
4	D	324	PEG	1	0
5	E	320[A]	CAC	1	0
4	E	324	PEG	5	0
4	E	325	PEG	2	0
4	F	323	PEG	2	0
4	F	328	PEG	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	310/322 (96%)	0.62	39 (12%)	5 5	27, 52, 85, 148	0
1	B	309/322 (95%)	0.74	45 (14%)	3 3	25, 55, 92, 108	0
1	C	309/322 (95%)	0.48	33 (10%)	8 7	25, 44, 71, 105	0
1	D	313/322 (97%)	0.60	36 (11%)	6 6	24, 50, 81, 105	0
1	E	309/322 (95%)	0.57	34 (11%)	7 7	24, 46, 81, 112	0
1	F	309/322 (95%)	0.61	36 (11%)	6 6	25, 50, 83, 113	0
All	All	1859/1932 (96%)	0.61	223 (11%)	6 5	24, 50, 84, 148	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	0	ALA	7.1
1	D	162	GLY	7.1
1	F	14	PHE	6.8
1	E	14	PHE	6.0
1	B	14	PHE	5.9
1	C	81	SER	5.9
1	A	160	ASP	5.7
1	E	317	PRO	5.6
1	A	-1	ASN	5.5
1	D	161	GLY	5.5
1	D	160	ASP	5.5
1	A	283	ILE	5.3
1	A	0	ALA	5.2
1	C	286	VAL	5.2
1	E	241	VAL	5.1
1	C	283	ILE	5.1
1	B	241	VAL	5.0
1	F	241	VAL	5.0
1	B	240	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	241	VAL	4.9
1	A	240	SER	4.9
1	B	285	ILE	4.8
1	F	162	GLY	4.8
1	D	241	VAL	4.8
1	A	239	ILE	4.8
1	E	239	ILE	4.8
1	B	317	PRO	4.7
1	D	158	THR	4.5
1	C	241	VAL	4.4
1	E	17	ARG	4.4
1	B	122	ILE	4.4
1	E	286	VAL	4.4
1	E	283	ILE	4.4
1	A	286	VAL	4.4
1	A	17	ARG	4.4
1	B	239	ILE	4.3
1	D	239	ILE	4.3
1	E	285	ILE	4.3
1	D	286	VAL	4.0
1	F	8	ARG	4.0
1	A	285	ILE	4.0
1	D	283	ILE	3.9
1	E	240	SER	3.9
1	A	14	PHE	3.9
1	B	283	ILE	3.8
1	E	82	GLU	3.8
1	B	30	ASP	3.8
1	F	239	ILE	3.8
1	F	161	GLY	3.8
1	E	147	ILE	3.8
1	C	122	ILE	3.7
1	F	285	ILE	3.7
1	B	149	PHE	3.6
1	A	122	ILE	3.6
1	C	240	SER	3.6
1	F	17	ARG	3.6
1	F	160	ASP	3.6
1	B	286	VAL	3.6
1	F	158	THR	3.6
1	B	245	VAL	3.5
1	E	15	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	122	ILE	3.5
1	D	130	SER	3.5
1	B	315	LEU	3.5
1	C	285	ILE	3.5
1	D	285	ILE	3.5
1	E	81	SER	3.5
1	A	238	PHE	3.5
1	B	238	PHE	3.5
1	D	-2	SER	3.4
1	C	306	LEU	3.4
1	C	121	LEU	3.4
1	A	134	ILE	3.4
1	B	143	THR	3.4
1	F	318	PHE	3.4
1	D	122	ILE	3.4
1	A	30	ASP	3.3
1	A	93	HIS	3.3
1	A	129	ILE	3.2
1	F	286	VAL	3.2
1	D	240	SER	3.2
1	D	121	LEU	3.2
1	C	239	ILE	3.2
1	C	216	GLU	3.2
1	E	146	VAL	3.2
1	E	122	ILE	3.1
1	A	164	THR	3.1
1	A	161	GLY	3.1
1	B	282	GLY	3.1
1	F	3	LYS	3.0
1	E	216	GLU	3.0
1	F	305	VAL	3.0
1	D	30	ASP	3.0
1	D	159	GLU	3.0
1	F	12	SER	3.0
1	D	282	GLY	3.0
1	B	77	GLU	3.0
1	B	160	ASP	3.0
1	D	95	THR	2.9
1	D	134	ILE	2.9
1	B	83	LEU	2.9
1	D	17	ARG	2.9
1	D	94	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	-1	ASN	2.9
1	C	159	GLU	2.9
1	F	149	PHE	2.9
1	B	158	THR	2.9
1	F	13	SER	2.9
1	C	2	ASP	2.9
1	B	123	LEU	2.9
1	F	123	LEU	2.9
1	A	123	LEU	2.9
1	B	17	ARG	2.9
1	C	129	ILE	2.8
1	E	238	PHE	2.8
1	B	19	VAL	2.8
1	F	163	PRO	2.8
1	A	147	ILE	2.8
1	B	40	ILE	2.8
1	B	2	ASP	2.8
1	F	283	ILE	2.8
1	C	317	PRO	2.7
1	B	129	ILE	2.7
1	B	267	LEU	2.7
1	A	318	PHE	2.7
1	C	134	ILE	2.7
1	E	83	LEU	2.7
1	A	81	SER	2.7
1	E	305	VAL	2.7
1	F	157	ASN	2.7
1	A	94	VAL	2.7
1	C	17	ARG	2.7
1	C	302	ALA	2.7
1	D	133	THR	2.7
1	E	6	PHE	2.7
1	F	240	SER	2.7
1	A	83	LEU	2.6
1	D	33	ASP	2.6
1	E	302	ALA	2.6
1	A	306	LEU	2.6
1	E	123	LEU	2.6
1	E	129	ILE	2.6
1	D	163	PRO	2.6
1	B	31	GLY	2.6
1	B	216	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	284	GLU	2.6
1	E	149	PHE	2.6
1	B	186	LEU	2.6
1	E	315	LEU	2.6
1	C	120	PRO	2.5
1	B	146	VAL	2.5
1	B	131	TYR	2.5
1	B	305	VAL	2.5
1	D	129	ILE	2.5
1	A	203	LYS	2.5
1	B	147	ILE	2.5
1	D	147	ILE	2.5
1	D	305	VAL	2.5
1	B	117	ASP	2.5
1	F	302	ALA	2.4
1	A	173	LEU	2.4
1	C	14	PHE	2.4
1	B	284	GLU	2.4
1	E	29	TRP	2.4
1	A	176	GLU	2.4
1	F	246	LEU	2.4
1	C	282	GLY	2.4
1	E	282	GLY	2.4
1	A	159	GLU	2.4
1	C	15	LYS	2.4
1	A	133	THR	2.4
1	B	130	SER	2.4
1	F	95	THR	2.4
1	C	33	ASP	2.3
1	F	271	VAL	2.3
1	F	82	GLU	2.3
1	C	94	VAL	2.3
1	C	245	VAL	2.3
1	D	5	PRO	2.3
1	B	81	SER	2.3
1	F	216	GLU	2.3
1	D	217	LYS	2.3
1	E	32	GLN	2.3
1	E	306	LEU	2.3
1	E	169	PHE	2.2
1	F	6	PHE	2.2
1	A	96	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	18	ASP	2.2
1	D	157	ASN	2.2
1	B	306	LEU	2.2
1	F	143	THR	2.2
1	F	147	ILE	2.2
1	D	238	PHE	2.2
1	C	238	PHE	2.2
1	D	6	PHE	2.2
1	B	205	ASN	2.2
1	C	163	PRO	2.2
1	A	103	HIS	2.2
1	F	182	HIS	2.1
1	C	13	SER	2.1
1	E	20	THR	2.1
1	F	232	ASP	2.1
1	E	127	ASN	2.1
1	C	82	GLU	2.1
1	A	15	LYS	2.1
1	A	305	VAL	2.1
1	F	5	PRO	2.1
1	B	33	ASP	2.1
1	B	15	LYS	2.1
1	C	162	GLY	2.1
1	C	316	SER	2.1
1	D	174	ASP	2.1
1	D	245	VAL	2.1
1	A	2	ASP	2.1
1	B	176	GLU	2.1
1	E	18	ASP	2.1
1	F	30	ASP	2.1
1	E	75	LEU	2.0
1	B	76	GLY	2.0
1	A	82	GLU	2.0
1	C	149	PHE	2.0
1	C	146	VAL	2.0
1	A	130	SER	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
4	PEG	E	325	7/7	0.66	0.28	8.24	67,70,74,76	0
4	PEG	C	329	7/7	0.65	0.28	7.64	86,87,89,90	0
4	PEG	A	324	7/7	0.85	0.29	7.11	37,56,62,62	0
4	PEG	F	325	7/7	0.88	0.40	6.64	76,78,82,84	0
5	CAC	C	320[A]	5/5	0.92	0.20	5.82	15,30,57,125	5
5	CAC	E	320[A]	5/5	0.92	0.23	5.68	26,31,59,106	5
5	CAC	C	320[B]	5/5	0.92	0.20	5.37	12,16,72,128	5
2	CL	B	320	1/1	0.94	0.30	5.30	35,35,35,35	0
4	PEG	C	326	7/7	0.89	0.24	5.15	57,68,76,77	0
5	CAC	E	320[B]	5/5	0.92	0.23	5.04	15,20,48,134	5
4	PEG	A	326	7/7	0.81	0.36	4.35	69,70,76,77	0
2	CL	C	321	1/1	0.95	0.27	3.98	42,42,42,42	0
4	PEG	F	326	7/7	0.62	0.24	3.70	71,77,78,78	0
4	PEG	C	330	7/7	0.73	0.19	3.64	69,75,86,87	0
4	PEG	D	323	7/7	0.71	0.24	3.41	43,51,63,66	0
4	PEG	C	331	7/7	0.66	0.19	3.15	86,89,91,92	0
4	PEG	C	327	7/7	0.80	0.25	2.87	39,51,55,57	0
2	CL	A	320	1/1	0.92	0.23	2.52	49,49,49,49	0
2	CL	D	320	1/1	0.93	0.29	2.33	53,53,53,53	0
2	CL	E	321	1/1	0.95	0.29	2.29	34,34,34,34	0
4	PEG	E	326	7/7	0.94	0.17	2.29	50,60,71,72	0
3	CA	B	323	1/1	0.92	0.23	2.24	59,59,59,59	0
4	PEG	F	327	7/7	0.76	0.32	1.89	91,93,95,95	0
2	CL	F	320	1/1	0.98	0.24	1.85	48,48,48,48	0
4	PEG	B	324	7/7	0.81	0.26	1.77	37,46,59,59	0
4	PEG	F	328	7/7	0.89	0.22	1.73	50,62,66,67	0
4	PEG	C	328	7/7	0.89	0.23	1.59	43,57,67,68	0
3	CA	A	322	1/1	0.99	0.20	1.59	35,35,35,35	0
4	PEG	A	325	7/7	0.82	0.21	1.45	52,61,66,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CA	C	323	1/1	0.97	0.20	1.34	33,33,33,33	0
4	PEG	D	324	7/7	0.90	0.18	1.31	52,62,77,80	0
4	PEG	E	324	7/7	0.86	0.20	1.24	41,44,53,56	0
3	CA	A	323	1/1	0.90	0.26	1.17	69,69,69,69	0
3	CA	D	321	1/1	0.99	0.20	0.68	37,37,37,37	0
3	CA	D	322	1/1	0.88	0.21	0.62	84,84,84,84	0
3	CA	E	322	1/1	0.98	0.19	0.15	34,34,34,34	0
3	CA	B	322	1/1	0.98	0.18	0.14	39,39,39,39	0
3	CA	F	321	1/1	0.99	0.18	0.13	39,39,39,39	0
3	CA	F	322	1/1	0.66	0.17	-0.11	77,77,77,77	0
3	CA	E	323	1/1	0.93	0.14	-0.49	61,61,61,61	0
3	CA	C	324	1/1	0.94	0.15	-0.58	62,62,62,62	0
4	PEG	F	324	7/7	0.95	0.12	-0.72	48,59,71,77	0
4	PEG	C	325	7/7	0.92	0.10	-0.89	62,63,64,68	0
2	CL	A	321	1/1	0.85	0.08	-1.25	75,75,75,75	0
2	CL	C	322	1/1	0.78	0.11	-	89,89,89,89	0
4	PEG	B	325	7/7	0.59	0.33	-	76,81,86,87	0
2	CL	B	321	1/1	0.82	0.13	-	58,58,58,58	0
4	PEG	F	323	7/7	0.87	0.25	-	46,55,61,67	0

6.5 Other polymers (i)

There are no such residues in this entry.