



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:46 AM UTC

PDB ID : 2X8J / pdb_00002x8j
Title : Intracellular subtilisin precursor from *B. clausii*
Authors : Vedodova, J.; Gamble, M.; Ariza, A.; Dodson, E.; Jones, D.D.; Wilson, K.S.
Deposited on : 2010-03-09
Resolution : 1.56 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

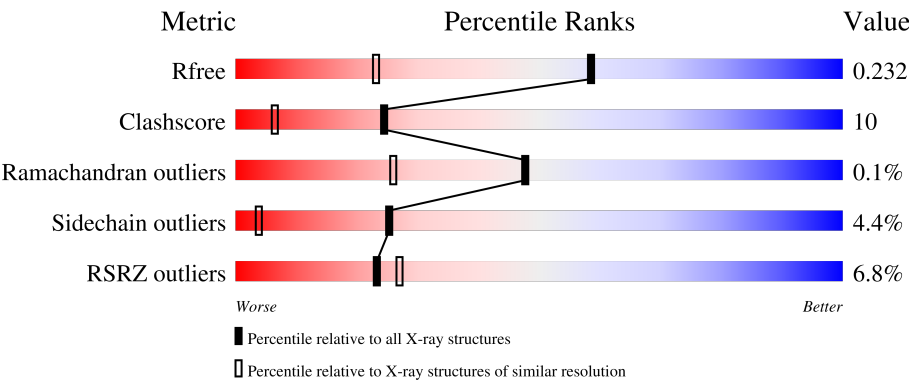
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 1.56 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}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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 $\leq 5\%$. 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	327	5% 75% 15% • 7%
1	C	327	3% 76% 14% • 7%
1	D	327	8% 78% 14% • 6%
1	E	327	5% 71% 17% 5% • 6%
1	F	327	3% 74% 17% • 6%

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Mol	Chain	Length	Quality of chain
2	B	327	14% 73% 17% 6%

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
5	GOL	D	1319	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15480 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 INTRACELLULAR SUBTILISIN PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	3	8	0
			2308	1447	398	455	8			
1	C	304	Total	C	N	O	S	3	7	0
			2316	1453	396	457	10			
1	D	308	Total	C	N	O	S	0	6	0
			2329	1461	396	461	11			
1	E	307	Total	C	N	O	S	3	5	0
			2312	1448	397	456	11			
1	F	307	Total	C	N	O	S	0	5	0
			2311	1449	396	458	8			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	322	HIS	-	expression tag	UNP D0AB41
A	323	HIS	-	expression tag	UNP D0AB41
A	324	HIS	-	expression tag	UNP D0AB41
A	325	HIS	-	expression tag	UNP D0AB41
A	326	HIS	-	expression tag	UNP D0AB41
A	327	HIS	-	expression tag	UNP D0AB41
C	322	HIS	-	expression tag	UNP D0AB41
C	323	HIS	-	expression tag	UNP D0AB41
C	324	HIS	-	expression tag	UNP D0AB41
C	325	HIS	-	expression tag	UNP D0AB41
C	326	HIS	-	expression tag	UNP D0AB41
C	327	HIS	-	expression tag	UNP D0AB41
D	322	HIS	-	expression tag	UNP D0AB41
D	323	HIS	-	expression tag	UNP D0AB41
D	324	HIS	-	expression tag	UNP D0AB41
D	325	HIS	-	expression tag	UNP D0AB41
D	326	HIS	-	expression tag	UNP D0AB41
D	327	HIS	-	expression tag	UNP D0AB41
E	322	HIS	-	expression tag	UNP D0AB41

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Chain	Residue	Modelled	Actual	Comment	Reference
E	323	HIS	-	expression tag	UNP D0AB41
E	324	HIS	-	expression tag	UNP D0AB41
E	325	HIS	-	expression tag	UNP D0AB41
E	326	HIS	-	expression tag	UNP D0AB41
E	327	HIS	-	expression tag	UNP D0AB41
F	322	HIS	-	expression tag	UNP D0AB41
F	323	HIS	-	expression tag	UNP D0AB41
F	324	HIS	-	expression tag	UNP D0AB41
F	325	HIS	-	expression tag	UNP D0AB41
F	326	HIS	-	expression tag	UNP D0AB41
F	327	HIS	-	expression tag	UNP D0AB41
A	250	ALA	SER	engineered mutation	UNP D0AB41
C	250	ALA	SER	engineered mutation	UNP D0AB41
D	250	ALA	SER	engineered mutation	UNP D0AB41
E	250	ALA	SER	engineered mutation	UNP D0AB41
F	250	ALA	SER	engineered mutation	UNP D0AB41

- Molecule 2 is a protein called INTRACELLULAR SUBTILISIN PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	307	Total	C	N	O	S	0	7	0
			2325	1455	398	463	9			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	322	HIS	-	expression tag	UNP D0AB41
B	323	HIS	-	expression tag	UNP D0AB41
B	324	HIS	-	expression tag	UNP D0AB41
B	325	HIS	-	expression tag	UNP D0AB41
B	326	HIS	-	expression tag	UNP D0AB41
B	327	HIS	-	expression tag	UNP D0AB41
B	250	ALA	SER	engineered mutation	UNP D0AB41

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

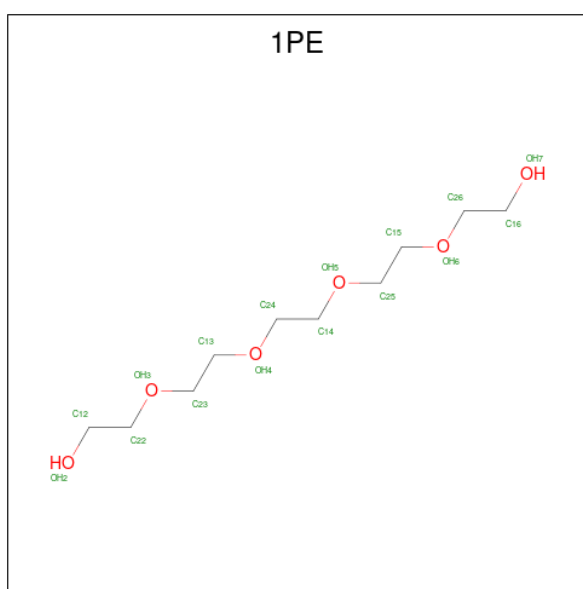
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

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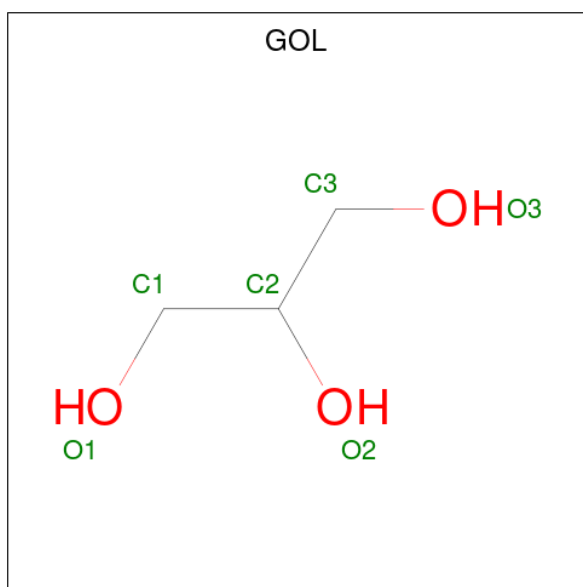
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		
3	F	1	Total	Na	0	0
			1	1		

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			10	6	4		
4	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



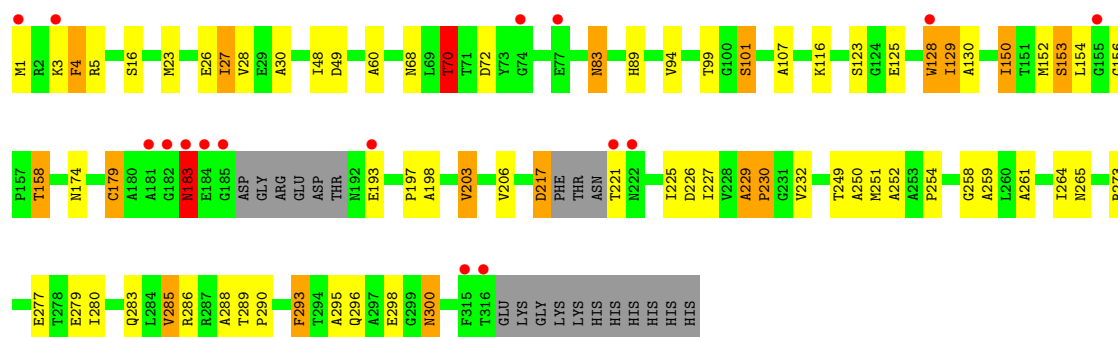
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

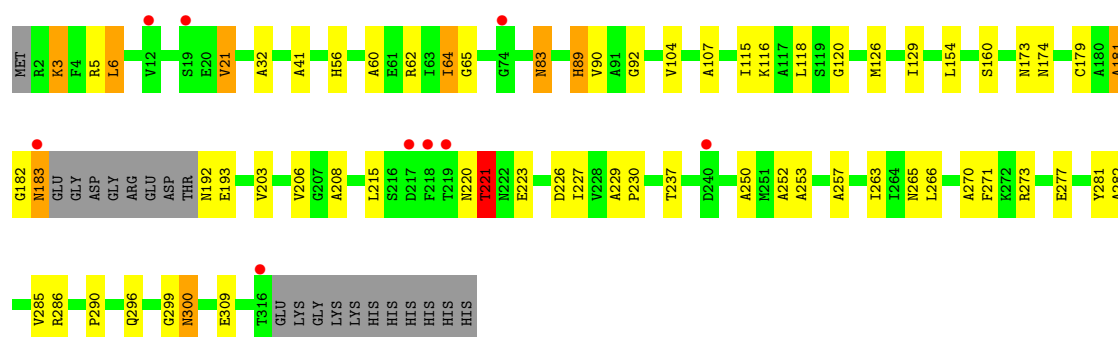
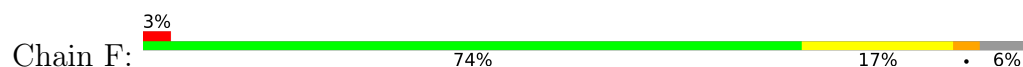
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	241	Total	O	0	0
			241	241		
6	B	208	Total	O	0	0
			208	208		
6	C	264	Total	O	0	0
			264	264		
6	D	213	Total	O	0	0
			213	213		
6	E	265	Total	O	0	0
			265	265		
6	F	310	Total	O	0	0
			310	310		



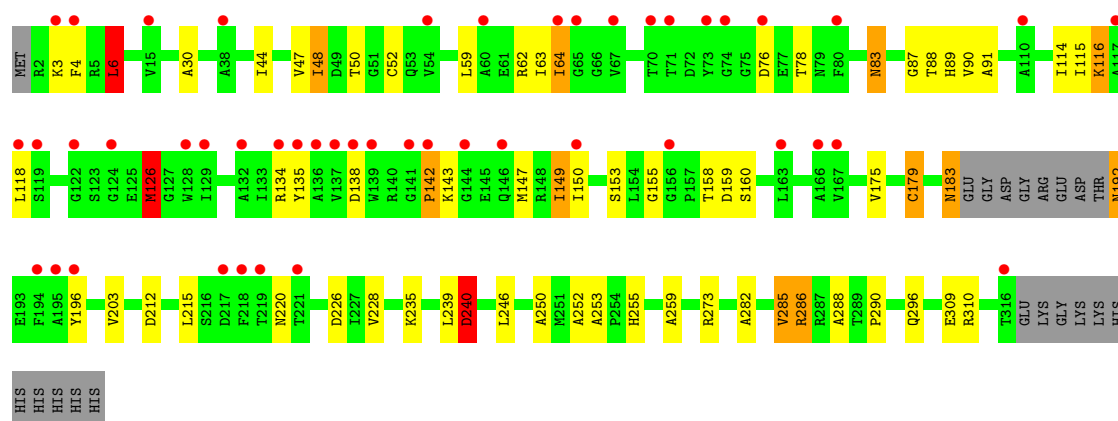
• Molecule 1: INTRACELLULAR SUBTILISIN PROTEASE



• Molecule 1: INTRACELLULAR SUBTILISIN PROTEASE



• Molecule 2: INTRACELLULAR SUBTILISIN PROTEASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	125.66Å 125.66Å 106.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.98 – 1.56 75.98 – 1.56	Depositor EDS
% Data completeness (in resolution range)	100.0 (75.98-1.56) 99.7 (75.98-1.56)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.187 , 0.230 0.192 , 0.232	Depositor DCC
R_{free} test set	16527 reflections (6.16%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.019 for h,-h-k,-l 0.013 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15480	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, GOL, NA, CSX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.56	15/2332 (0.6%)	1.22	7/3162 (0.2%)
1	C	1.68	18/2339 (0.8%)	1.37	9/3172 (0.3%)
1	D	1.50	10/2354 (0.4%)	1.32	7/3194 (0.2%)
1	E	28.50	38/2335 (1.6%)	2.46	25/3165 (0.8%)
1	F	1.60	19/2336 (0.8%)	1.37	9/3173 (0.3%)
2	B	1.61	19/2342 (0.8%)	1.32	10/3178 (0.3%)
All	All	11.72	119/14038 (0.8%)	1.57	67/19044 (0.4%)

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	E	1	0

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	183	ASN	CA-CB	1129.32	20.62	1.53
1	E	183	ASN	CB-CG	783.59	21.11	1.52
1	A	3	LYS	CG-CD	-29.02	0.65	1.52
1	C	3	LYS	CG-CD	-23.66	0.81	1.52
1	E	101	SER	C-O	14.12	1.40	1.24
1	E	227	ILE	CA-CB	13.19	1.65	1.55
1	C	250	ALA	CA-CB	-10.04	1.35	1.53
1	D	285	VAL	CA-CB	8.74	1.67	1.54
2	B	91	ALA	N-CA	-8.20	1.36	1.46
1	F	300	ASN	N-CA	-8.02	1.35	1.46
1	F	250	ALA	CA-CB	-8.01	1.39	1.53
1	F	115	ILE	CA-CB	7.58	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	91	ALA	CA-CB	7.58	1.65	1.53
1	C	64	ILE	CG1-CD1	-7.49	1.22	1.51
1	A	114	ILE	CA-CB	7.46	1.62	1.54
1	F	60	ALA	CA-CB	7.41	1.65	1.53
1	E	129	ILE	CA-CB	-7.35	1.45	1.54
1	E	60	ALA	CA-CB	7.21	1.64	1.53
1	C	149	ILE	CA-CB	-7.12	1.44	1.54
2	B	285	VAL	CB-CG2	-7.11	1.29	1.52
2	B	48	ILE	CA-CB	7.08	1.61	1.53
2	B	149	ILE	CA-CB	7.03	1.63	1.54
1	C	133	ILE	N-CA	7.02	1.54	1.46
1	E	289	THR	C-O	-6.97	1.16	1.24
1	A	181	ALA	CA-CB	-6.95	1.42	1.53
1	E	251	MET	SD-CE	-6.72	1.62	1.79
1	E	225	ILE	CA-CB	-6.70	1.45	1.54
2	B	240	ASP	CB-CG	-6.66	1.35	1.52
1	C	111	ASP	C-O	6.64	1.31	1.23
2	B	115	ILE	CA-CB	6.61	1.62	1.53
1	D	286	ARG	CB-CG	-6.53	1.32	1.52
1	A	264	ILE	CA-CB	-6.50	1.46	1.54
2	B	259	ALA	CA-CB	6.49	1.63	1.53
1	F	290	PRO	C-O	-6.42	1.16	1.23
1	F	271	PHE	C-O	-6.37	1.15	1.24
1	E	229	ALA	C-O	6.35	1.30	1.24
1	E	296	GLN	CA-CB	6.32	1.63	1.53
2	B	252	ALA	CA-CB	6.29	1.63	1.53
1	E	254	PRO	C-O	6.28	1.31	1.24
1	E	49	ASP	CA-C	6.22	1.59	1.53
1	E	48	ILE	C-N	6.15	1.38	1.33
1	F	299	GLY	N-CA	6.15	1.54	1.45
1	E	94	VAL	CA-CB	-6.14	1.47	1.54
1	F	227	ILE	CA-CB	6.12	1.60	1.55
1	A	170	ALA	CA-CB	6.10	1.62	1.53
1	F	253	ALA	C-O	-6.09	1.18	1.24
1	C	110	ALA	CA-CB	6.07	1.63	1.53
2	B	30	ALA	CA-CB	-6.06	1.45	1.53
1	A	175	VAL	CA-CB	-6.03	1.46	1.54
2	B	228	VAL	CA-C	6.02	1.59	1.52
1	D	261	ALA	C-O	6.00	1.31	1.24
1	E	232	VAL	CA-CB	-5.97	1.46	1.54
1	E	28	VAL	CA-C	5.91	1.58	1.52
1	E	153	SER	C-O	5.89	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	114	ILE	CA-CB	5.87	1.60	1.54
1	F	181	ALA	CA-CB	-5.86	1.44	1.53
1	F	90	VAL	CA-CB	-5.85	1.47	1.54
1	E	27	ILE	CA-CB	5.83	1.61	1.54
1	E	261	ALA	C-O	5.83	1.31	1.24
2	B	286	ARG	CB-CG	-5.71	1.35	1.52
1	E	156	GLY	N-CA	5.70	1.52	1.44
1	F	270	ALA	CA-CB	5.70	1.62	1.53
1	D	207	GLY	N-CA	5.69	1.50	1.44
1	C	293	PHE	C-O	5.69	1.29	1.23
1	A	30	ALA	N-CA	-5.67	1.40	1.46
1	E	265	ASN	C-O	5.64	1.30	1.24
2	B	116	LYS	CA-CB	5.58	1.60	1.53
1	E	203	VAL	CA-CB	5.57	1.61	1.54
1	C	145	GLU	N-CA	5.56	1.52	1.46
1	A	30	ALA	C-O	-5.55	1.19	1.24
2	B	47	VAL	CA-CB	5.54	1.60	1.53
1	E	298	GLU	N-CA	5.50	1.52	1.46
1	E	285	VAL	CA-CB	5.46	1.61	1.54
1	E	4	PHE	N-CA	5.43	1.52	1.46
1	C	227	ILE	CA-CB	5.41	1.59	1.55
1	E	293	PHE	C-O	5.39	1.29	1.23
1	A	293	PHE	C-O	5.37	1.29	1.23
1	F	265	ASN	N-CA	5.36	1.52	1.46
1	E	101	SER	CA-C	5.34	1.60	1.53
1	A	136	ALA	N-CA	-5.32	1.40	1.46
1	C	107	ALA	CA-C	5.31	1.58	1.52
1	D	30	ALA	N-CA	-5.30	1.40	1.46
1	F	257	ALA	CA-CB	5.30	1.61	1.53
1	F	252	ALA	CA-CB	5.30	1.61	1.53
1	D	258	GLY	C-O	5.30	1.30	1.23
1	F	89	HIS	CA-C	5.29	1.59	1.52
2	B	253	ALA	CA-CB	5.27	1.60	1.53
1	D	71	THR	CA-C	5.27	1.59	1.52
1	D	27	ILE	CA-CB	5.26	1.61	1.54
1	C	158	THR	CA-CB	5.25	1.60	1.53
1	E	259	ALA	CA-CB	5.25	1.61	1.53
1	F	92	GLY	N-CA	-5.25	1.39	1.45
1	E	252	ALA	C-O	5.25	1.30	1.24
1	E	279	GLU	C-O	-5.23	1.17	1.24
2	B	240	ASP	CA-C	-5.22	1.46	1.53
1	E	129	ILE	N-CA	5.22	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	ALA	CA-CB	5.21	1.61	1.53
1	E	258	GLY	C-O	5.20	1.30	1.23
1	E	295	ALA	CA-C	-5.18	1.45	1.52
1	C	256	VAL	CA-CB	5.17	1.60	1.54
1	E	198	ALA	N-CA	5.17	1.52	1.46
1	C	253	ALA	N-CA	5.16	1.51	1.46
1	E	295	ALA	C-N	5.16	1.40	1.33
1	D	224	GLU	CA-C	5.15	1.59	1.52
1	F	206	VAL	CA-C	5.14	1.59	1.52
1	A	227	ILE	CA-CB	5.14	1.59	1.55
2	B	273	ARG	CB-CG	-5.13	1.37	1.52
2	B	253	ALA	C-N	5.13	1.40	1.33
1	C	288	ALA	N-CA	5.13	1.52	1.46
1	C	80	PHE	C-O	5.12	1.30	1.23
1	F	41	ALA	CA-CB	5.12	1.61	1.53
1	C	181	ALA	CA-C	-5.09	1.46	1.53
1	C	303	LEU	N-CA	5.09	1.52	1.46
1	E	300	ASN	N-CA	-5.09	1.39	1.46
1	E	288	ALA	N-CA	5.08	1.52	1.46
1	A	257	ALA	N-CA	5.04	1.52	1.46
1	A	27	ILE	N-CA	-5.03	1.39	1.46
1	D	94	VAL	CA-CB	-5.01	1.48	1.54
1	A	228	VAL	CA-CB	5.00	1.62	1.54

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	183	ASN	CA-CB-CG	-105.75	6.85	112.60
1	E	183	ASN	CB-CG-ND2	-27.68	74.89	116.40
1	E	183	ASN	CB-CG-OD1	20.26	161.31	120.80
1	C	3	LYS	CG-CD-CE	-11.52	84.80	111.30
1	E	183	ASN	CB-CA-C	8.97	128.27	110.42
1	E	249	THR	CA-C-N	8.34	132.56	120.38
1	E	249	THR	C-N-CA	8.34	132.56	120.38
1	F	221	THR	CB-CA-C	-7.94	93.52	109.79
1	D	28	VAL	CA-CB-CG1	7.62	123.36	110.40
2	B	252	ALA	N-CA-C	7.44	119.47	111.36
2	B	273	ARG	CB-CA-C	-7.38	94.22	109.94
1	F	120	GLY	N-CA-C	7.25	122.73	113.24
1	E	283	GLN	N-CA-C	7.16	120.12	111.82
1	E	101	SER	CA-C-O	7.01	129.59	121.32
1	A	199	ALA	N-CA-C	6.93	121.32	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	LYS	CB-CG-CD	6.70	126.71	111.30
1	E	70	THR	N-CA-CB	-6.60	100.86	110.70
1	C	283	GLN	N-CA-C	6.34	119.17	111.82
1	A	3	LYS	CB-CG-CD	6.26	125.71	111.30
1	E	295	ALA	CA-C-O	6.18	126.97	119.49
2	B	310	ARG	N-CA-C	6.14	118.77	111.71
1	F	263	ILE	N-CA-C	6.13	116.88	110.62
1	A	315	PHE	CA-C-N	5.91	132.34	121.70
1	A	315	PHE	C-N-CA	5.91	132.34	121.70
1	E	206	VAL	CA-C-O	-5.91	114.19	120.39
2	B	91	ALA	N-CA-C	5.85	117.66	111.28
2	B	212	ASP	N-CA-C	-5.79	105.98	113.16
2	B	6	LEU	CB-CG-CD1	5.77	128.00	110.70
1	E	249	THR	CA-C-O	-5.75	114.42	120.63
2	B	88	THR	O-C-N	5.75	128.21	122.12
1	E	130	ALA	CA-C-O	5.74	126.64	120.55
1	E	158	THR	CB-CA-C	-5.72	100.30	109.75
1	E	206	VAL	O-C-N	5.72	129.44	123.26
1	C	182	GLY	N-CA-C	5.70	119.42	111.10
1	C	174	ASN	N-CA-C	5.67	119.40	111.74
1	C	310	ARG	NE-CZ-NH2	-5.65	114.12	119.20
1	D	109	LYS	CA-C-O	5.63	126.02	119.32
1	E	5	ARG	N-CA-C	5.62	117.34	108.96
1	F	281	TYR	O-C-N	-5.59	116.19	122.12
1	E	107	ALA	O-C-N	5.53	126.34	121.37
1	A	174	ASN	N-CA-C	5.47	119.24	112.24
1	E	289	THR	CA-C-N	-5.46	114.14	119.76
1	E	289	THR	C-N-CA	-5.46	114.14	119.76
1	C	134	ARG	NE-CZ-NH2	-5.45	114.30	119.20
1	E	101	SER	N-CA-C	5.43	115.45	108.34
1	F	273	ARG	NE-CZ-NH2	5.43	124.09	119.20
2	B	255	HIS	CA-C-O	5.38	126.25	120.55
1	F	21	VAL	N-CA-C	-5.38	102.66	107.56
1	D	21	VAL	N-CA-C	-5.37	102.23	107.55
2	B	126	MET	CA-CB-CG	5.37	124.84	114.10
1	E	295	ALA	O-C-N	-5.37	115.41	122.39
1	D	286	ARG	CB-CG-CD	-5.36	98.97	111.30
1	C	120	GLY	N-CA-C	5.34	120.37	113.27
1	C	36	ALA	N-CA-C	5.31	117.82	111.71
1	D	286	ARG	NE-CZ-NH2	-5.28	114.44	119.20
1	E	30	ALA	O-C-N	5.21	125.12	120.48
1	A	228	VAL	N-CA-C	5.17	117.06	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	128	TRP	N-CA-C	-5.14	105.76	111.36
1	F	107	ALA	O-C-N	5.14	125.99	121.37
1	A	277	GLU	N-CA-C	-5.13	105.69	111.28
1	D	34	TRP	N-CA-C	5.12	116.86	111.28
1	E	264	ILE	N-CA-C	-5.08	105.54	110.42
2	B	90	VAL	CA-C-O	5.07	126.54	121.17
1	F	208	ALA	N-CA-C	5.06	117.81	109.72
1	F	32	ALA	N-CA-C	5.05	117.52	111.71
1	D	263	ILE	N-CA-C	5.00	115.22	110.42
1	E	230	PRO	O-C-N	-5.00	117.50	123.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	183	ASN	CA

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	2308	0	2254	38	0
1	C	2316	0	2274	42	0
1	D	2329	0	2280	50	0
1	E	2312	0	2268	57	0
1	F	2311	0	2260	62	0
2	B	2325	0	2266	52	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	10	0	13	3	0
4	B	10	0	13	3	0
4	C	10	0	13	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	10	0	13	3	0
4	E	10	0	13	2	0
4	F	10	0	13	4	0
5	C	6	0	8	0	0
5	D	6	0	8	7	0
6	A	241	0	0	3	0
6	B	208	0	0	10	0
6	C	264	0	0	7	0
6	D	213	0	0	5	0
6	E	265	0	0	10	0
6	F	310	0	0	8	0
All	All	15480	0	13696	274	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 (274) 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)
4:F:1318:1PE:C14	4:F:1318:1PE:OH5	1.65	1.42
1:E:273[A]:ARG:NH1	6:E:2234:HOH:O	1.58	1.28
1:E:129:ILE:HG12	6:E:2116:HOH:O	1.08	1.25
1:F:309:GLU:HG3	6:F:2296:HOH:O	1.43	1.18
1:A:309:GLU:HG3	6:A:2233:HOH:O	1.46	1.15
1:E:183:ASN:CG	1:E:183:ASN:HA	1.75	1.10
1:D:286:ARG:NE	5:D:1319:GOL:O3	1.86	1.08
2:B:149:ILE:O	2:B:150:ILE:HD12	1.54	1.07
1:D:286:ARG:NH2	5:D:1319:GOL:O3	1.89	1.04
1:F:309:GLU:HG2	6:F:2302:HOH:O	1.56	1.02
1:A:285:VAL:HG21	2:B:282:ALA:HB1	1.42	0.99
1:F:182:GLY:O	1:F:221:THR:HG23	1.64	0.98
2:B:149:ILE:C	2:B:150:ILE:HD12	1.89	0.97
1:E:286[B]:ARG:NH1	6:E:2245:HOH:O	1.84	0.96
1:E:125:GLU:HG2	6:E:2114:HOH:O	1.71	0.89
1:E:179[A]:CSX:SG	1:E:203:VAL:HG11	2.13	0.89
1:D:286:ARG:CZ	5:D:1319:GOL:O3	2.22	0.88
1:D:1:MET:HE3	1:D:121:ASP:O	1.76	0.85
1:A:282:ALA:HB1	2:B:285:VAL:HG21	1.57	0.85
1:A:272:LYS:HD2	2:B:296:GLN:HE22	1.41	0.85
1:F:3:LYS:CD	1:F:3:LYS:H	1.90	0.85
2:B:192:ASN:N	2:B:192:ASN:HD22	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:GLU:CD	1:C:310:ARG:HH22	1.85	0.84
1:D:226:ASP:OD1	4:D:1318:1PE:H132	1.77	0.84
1:D:248:GLY:N	1:D:251[B]:MET:HE1	1.92	0.84
1:D:247:SER:C	1:D:251[B]:MET:HE1	2.03	0.83
1:C:226:ASP:OD1	4:C:1319:1PE:H132	1.78	0.83
1:A:29:GLU:OE1	1:A:306[B]:ASP:OD2	1.94	0.83
1:F:181:ALA:HB1	1:F:221:THR:HG21	1.60	0.82
2:B:179[A]:CSX:SG	2:B:203:VAL:HG11	2.20	0.81
1:E:286[B]:ARG:CD	1:F:285[B]:VAL:HG23	2.10	0.81
2:B:226:ASP:OD1	4:B:1318:1PE:H132	1.80	0.81
1:F:3:LYS:HE2	1:F:126:MET:H	1.44	0.81
1:E:183:ASN:CG	1:E:183:ASN:CA	2.54	0.81
2:B:6:LEU:HD13	2:B:118:LEU:CD1	2.12	0.80
1:E:286[B]:ARG:HD2	1:F:285[B]:VAL:CG2	2.11	0.80
2:B:138:ASP:OD1	6:B:2095:HOH:O	2.01	0.78
2:B:192:ASN:N	2:B:192:ASN:ND2	2.29	0.78
1:E:70:THR:HG23	1:E:72:ASP:H	1.46	0.78
1:C:179[A]:CSX:SG	1:C:203[A]:VAL:HG11	2.23	0.78
1:A:226:ASP:OD1	4:A:1318:1PE:H132	1.85	0.77
1:C:11:GLN:HE22	1:C:14:LYS:HG3	1.51	0.76
1:E:286[B]:ARG:HD2	1:F:285[B]:VAL:HG23	1.69	0.75
1:F:3:LYS:H	1:F:3:LYS:HD2	1.51	0.74
2:B:215:LEU:HB3	2:B:220:ASN:HD21	1.52	0.74
1:F:83:ASN:HD21	1:F:116:LYS:HZ1	1.32	0.74
1:E:226:ASP:OD1	4:E:1318:1PE:H132	1.89	0.73
1:E:152[A]:MET:HE1	1:E:197:PRO:HG3	1.69	0.73
2:B:76:ASP:OD2	2:B:78:THR:OG1	2.07	0.72
1:E:285:VAL:CG1	1:F:286[A]:ARG:HD2	2.20	0.72
1:C:286[B]:ARG:NH1	6:C:2248:HOH:O	2.23	0.72
1:A:153:SER:HB3	1:A:250:ALA:HB1	1.70	0.72
1:A:272:LYS:HD2	2:B:296:GLN:NE2	2.04	0.71
1:F:226:ASP:OD1	4:F:1318:1PE:H132	1.91	0.71
2:B:6:LEU:HD13	2:B:118:LEU:HD13	1.74	0.70
1:F:179[A]:CSX:SG	1:F:203:VAL:HG11	2.33	0.69
1:A:179[B]:CSX:SG	1:A:203:VAL:HG11	2.32	0.69
1:C:203[A]:VAL:O	4:C:1319:1PE:H131	1.92	0.68
1:F:215:LEU:HB3	1:F:220:ASN:HD21	1.58	0.68
1:A:306[B]:ASP:OD2	1:A:310:ARG:NH2	2.27	0.68
1:F:83:ASN:HD21	1:F:116:LYS:NZ	1.92	0.68
1:D:248:GLY:CA	1:D:251[B]:MET:HE1	2.24	0.68
1:D:283:GLN:OE1	5:D:1319:GOL:H31	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:VAL:HG22	1:C:104:VAL:HG11	1.76	0.68
1:E:152[A]:MET:HE1	1:E:197:PRO:CG	2.24	0.68
2:B:52:CSX:OD	2:B:63:ILE:HD11	1.94	0.67
2:B:309:GLU:HG2	6:B:2200:HOH:O	1.92	0.67
1:D:173:ASN:O	1:D:174[A]:ASN:ND2	2.28	0.66
1:C:217:ASP:C	6:C:2217:HOH:O	2.38	0.66
1:F:5:ARG:NH1	1:F:193:GLU:OE2	2.28	0.66
1:E:293:PHE:O	6:E:2249:HOH:O	2.14	0.66
1:F:64:ILE:HD12	1:F:64:ILE:C	2.21	0.66
1:D:83:ASN:H	1:D:83:ASN:HD22	1.44	0.66
1:A:203:VAL:O	4:A:1318:1PE:H131	1.96	0.65
2:B:203:VAL:O	4:B:1318:1PE:H131	1.97	0.64
1:C:203[B]:VAL:O	4:C:1319:1PE:H131	1.97	0.64
2:B:149:ILE:C	2:B:150:ILE:CD1	2.67	0.64
1:D:248:GLY:N	1:D:251[B]:MET:CE	2.60	0.64
1:F:3:LYS:CE	1:F:126:MET:H	2.11	0.64
1:D:6:LEU:HD13	1:D:118:LEU:CD1	2.27	0.64
1:C:286[A]:ARG:HD2	1:D:285:VAL:CG1	2.27	0.64
1:A:83:ASN:H	1:A:83:ASN:HD22	1.46	0.63
1:D:286:ARG:HE	5:D:1319:GOL:C3	2.12	0.63
2:B:153:SER:HB3	2:B:250:ALA:HB1	1.80	0.62
1:C:286[A]:ARG:CG	1:D:285:VAL:HG12	2.29	0.62
1:C:153:SER:HB3	1:C:250:ALA:HB1	1.82	0.61
1:E:70:THR:CG2	1:E:72:ASP:H	2.14	0.61
1:E:179[A]:CSX:SG	1:E:203:VAL:CG1	2.89	0.60
1:C:21:VAL:HA	1:C:104:VAL:HG12	1.83	0.60
2:B:179[A]:CSX:SG	2:B:203:VAL:CG1	2.89	0.60
1:F:203:VAL:O	4:F:1318:1PE:H131	2.02	0.60
2:B:83:ASN:HD21	2:B:116:LYS:HZ1	1.50	0.59
1:D:247:SER:C	1:D:251[B]:MET:CE	2.74	0.59
4:F:1318:1PE:OH5	4:F:1318:1PE:C24	2.47	0.59
1:D:215:LEU:HB3	1:D:220:ASN:HD21	1.67	0.59
1:E:217:ASP:OD1	1:E:217:ASP:C	2.46	0.59
1:E:203:VAL:O	4:E:1318:1PE:H131	2.02	0.59
1:C:179[A]:CSX:SG	1:C:203[A]:VAL:CG1	2.91	0.59
1:C:286[A]:ARG:HG3	1:D:285:VAL:HG12	1.85	0.58
1:A:192:ASN:N	1:A:192:ASN:OD1	2.36	0.58
1:C:83:ASN:HD21	1:C:116:LYS:HZ1	1.51	0.58
1:D:173:ASN:C	1:D:174[A]:ASN:HD22	2.11	0.58
1:C:64:ILE:C	1:C:64:ILE:HD12	2.28	0.58
1:D:286:ARG:NH1	6:D:2187:HOH:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:VAL:O	4:D:1318:1PE:H131	2.03	0.57
1:A:286[B]:ARG:NH1	2:B:288:ALA:O	2.37	0.57
1:C:89:HIS:HD2	6:C:2099:HOH:O	1.87	0.57
1:E:129:ILE:HD13	1:E:154:LEU:HD11	1.87	0.57
1:E:23[B]:MET:CE	1:E:26:GLU:OE1	2.53	0.56
1:F:6:LEU:HD13	1:F:118:LEU:CD1	2.34	0.56
1:C:83:ASN:HD21	1:C:116:LYS:NZ	2.04	0.56
1:A:23:MET:HA	1:A:23:MET:HE2	1.88	0.56
1:C:286[B]:ARG:NH2	6:C:2247:HOH:O	2.16	0.56
1:E:83:ASN:HD22	1:E:83:ASN:H	1.52	0.56
1:F:83:ASN:H	1:F:83:ASN:HD22	1.54	0.55
1:D:286:ARG:NH2	5:D:1319:GOL:HO3	1.98	0.55
1:E:286[B]:ARG:HD2	1:F:285[B]:VAL:HG21	1.86	0.55
1:D:18:LEU:HD22	1:D:20:GLU:HG2	1.89	0.55
1:A:48:ILE:HD12	1:A:150:ILE:CG2	2.37	0.55
1:C:21:VAL:HG13	1:C:104:VAL:CG1	2.37	0.55
1:D:83:ASN:HD22	1:D:83:ASN:N	2.03	0.55
1:D:153:SER:HB3	1:D:250:ALA:HB1	1.89	0.54
1:E:286[B]:ARG:CD	1:F:285[B]:VAL:CG2	2.75	0.54
1:A:83:ASN:H	1:A:83:ASN:ND2	2.06	0.54
1:D:5:ARG:NH1	1:D:193:GLU:HG2	2.23	0.54
1:E:129:ILE:HD13	1:E:154:LEU:CD1	2.37	0.54
2:B:83:ASN:HD21	2:B:116:LYS:NZ	2.06	0.54
1:E:290:PRO:HG3	1:F:286[A]:ARG:HH22	1.73	0.53
2:B:239:LEU:O	2:B:240:ASP:HB2	2.09	0.53
1:E:286[B]:ARG:CG	1:F:285[B]:VAL:HG23	2.38	0.53
2:B:235:LYS:NZ	6:B:2156:HOH:O	2.41	0.53
1:F:3:LYS:HE2	1:F:126:MET:N	2.19	0.53
2:B:226:ASP:CG	4:B:1318:1PE:H132	2.34	0.52
1:F:3:LYS:H	1:F:3:LYS:HD3	1.73	0.52
1:D:248:GLY:HA3	1:D:251[B]:MET:HE1	1.90	0.52
1:F:64:ILE:C	1:F:64:ILE:CD1	2.83	0.52
1:A:83:ASN:HD21	1:A:116:LYS:NZ	2.08	0.52
1:C:64:ILE:HD12	1:C:65:GLY:N	2.24	0.52
1:A:272:LYS:CD	2:B:296:GLN:HE22	2.18	0.52
1:F:89:HIS:HD2	6:F:2107:HOH:O	1.92	0.52
2:B:64:ILE:CD1	2:B:64:ILE:C	2.83	0.51
1:E:26:GLU:HG2	6:E:2027:HOH:O	2.10	0.51
1:C:285:VAL:HG12	1:D:286:ARG:HD2	1.92	0.51
1:E:89:HIS:HD2	6:E:2085:HOH:O	1.94	0.51
1:C:29:GLU:HG2	6:D:2208:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ASN:HD22	1:C:83:ASN:H	1.57	0.51
1:E:23[B]:MET:HE1	1:E:26:GLU:OE1	2.10	0.51
1:E:286[B]:ARG:CG	1:F:285[B]:VAL:CG2	2.88	0.51
2:B:83:ASN:H	2:B:83:ASN:HD22	1.58	0.50
1:C:216:SER:O	1:C:217:ASP:HB2	2.10	0.50
1:E:285:VAL:HG12	1:F:286[A]:ARG:HD2	1.93	0.50
1:D:56:HIS:CE1	1:D:237:THR:HG22	2.46	0.50
1:F:179[A]:CSX:SG	1:F:203:VAL:CG1	2.99	0.50
1:A:174:ASN:HA	1:A:277:GLU:HB2	1.94	0.50
1:D:83:ASN:H	1:D:83:ASN:ND2	2.09	0.50
1:A:179[B]:CSX:SG	1:A:203:VAL:CG1	2.99	0.50
1:F:173:ASN:O	1:F:174[B]:ASN:CB	2.55	0.50
1:E:125:GLU:HG3	1:E:128:TRP:CE2	2.47	0.50
1:A:89:HIS:HD2	6:A:2087:HOH:O	1.95	0.50
2:B:64:ILE:C	2:B:64:ILE:HD12	2.37	0.49
1:E:1:MET:HG2	1:E:123:SER:HB3	1.92	0.49
1:A:315:PHE:O	1:A:316:THR:HG23	2.11	0.49
1:E:285:VAL:HG13	1:F:286[A]:ARG:HD2	1.95	0.49
1:E:4:PHE:HB3	1:E:129:ILE:HD11	1.95	0.49
1:F:192:ASN:HB3	6:F:2205:HOH:O	2.11	0.49
1:D:286:ARG:HH21	5:D:1319:GOL:HO3	1.47	0.49
1:D:192:ASN:HB2	1:D:195:ALA:HB2	1.94	0.48
1:F:282:ALA:O	1:F:286[A]:ARG:HB2	2.13	0.48
2:B:44:ILE:HG22	2:B:147:MET:HG2	1.94	0.48
2:B:89:HIS:HD2	6:B:2071:HOH:O	1.96	0.48
1:D:83:ASN:HD21	1:D:116:LYS:HZ1	1.62	0.48
1:D:154:LEU:HD12	1:D:154:LEU:C	2.37	0.48
1:F:286[A]:ARG:NH2	6:F:2281:HOH:O	2.35	0.48
1:F:183:ASN:ND2	6:F:2201:HOH:O	2.46	0.48
1:E:174:ASN:HA	1:E:277:GLU:HB2	1.94	0.47
2:B:50:THR:C	6:B:2048:HOH:O	2.56	0.47
1:D:179[A]:CSX:SG	1:D:203:VAL:HG11	2.54	0.47
1:A:315:PHE:C	1:A:316:THR:HG23	2.40	0.47
1:E:83:ASN:HD21	1:E:116:LYS:NZ	2.12	0.47
1:A:282:ALA:HA	1:A:285:VAL:HG22	1.96	0.47
1:C:226:ASP:CG	4:C:1319:1PE:H132	2.38	0.47
1:E:23[B]:MET:HE2	1:E:26:GLU:OE1	2.15	0.47
1:A:155:GLY:HA2	1:A:196:TYR:O	2.16	0.46
2:B:155:GLY:HA2	2:B:196:TYR:O	2.15	0.46
1:F:266:LEU:C	1:F:266:LEU:HD12	2.40	0.46
2:B:4:PHE:CE1	2:B:126:MET:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:THR:HG21	6:B:2102:HOH:O	2.14	0.46
1:A:23:MET:HA	1:A:23:MET:CE	2.45	0.46
1:E:300:ASN:O	1:F:286[B]:ARG:NH2	2.48	0.46
2:B:150:ILE:HD13	2:B:175:VAL:CG1	2.46	0.46
1:D:6:LEU:HD13	1:D:118:LEU:HD13	1.97	0.46
1:F:183:ASN:HB2	6:F:2199:HOH:O	2.16	0.46
2:B:309:GLU:CG	6:B:2200:HOH:O	2.59	0.46
1:D:226:ASP:CG	4:D:1318:1PE:H132	2.40	0.46
1:D:251[B]:MET:HB2	1:D:251[B]:MET:HE2	1.52	0.46
2:B:134[A]:ARG:NH1	6:B:2106:HOH:O	2.48	0.46
1:A:226:ASP:CG	4:A:1318:1PE:H132	2.39	0.45
1:C:21:VAL:HG13	1:C:104:VAL:HG13	1.98	0.45
1:C:64:ILE:C	1:C:64:ILE:CD1	2.89	0.45
1:F:229:ALA:HB1	1:F:230:PRO:CD	2.46	0.45
1:C:6:LEU:HD13	1:C:118:LEU:CD1	2.46	0.45
1:C:285:VAL:CG1	1:D:286:ARG:HD2	2.46	0.45
1:E:26:GLU:CG	6:E:2027:HOH:O	2.64	0.45
1:A:21:VAL:HG22	1:A:104:VAL:HG11	1.98	0.45
1:E:68:ASN:OD1	1:E:70:THR:HB	2.16	0.45
1:C:29:GLU:OE2	1:C:310:ARG:NH2	2.48	0.45
1:D:57:PRO:HG2	6:D:2159:HOH:O	2.16	0.45
2:B:48:ILE:HD12	2:B:150:ILE:CG2	2.47	0.45
1:F:221:THR:CG2	1:F:223:GLU:H	2.30	0.45
1:C:163:LEU:HD23	6:C:2176:HOH:O	2.17	0.44
2:B:150:ILE:CD1	2:B:150:ILE:N	2.78	0.44
1:E:150:ILE:HG21	1:E:150:ILE:HD13	1.30	0.44
1:E:83:ASN:HD22	1:E:83:ASN:N	2.12	0.44
2:B:89:HIS:CD2	2:B:246:LEU:HD12	2.53	0.44
1:C:273[A]:ARG:NH2	6:C:2233:HOH:O	2.37	0.44
1:C:174:ASN:HA	1:C:277:GLU:HB2	1.99	0.44
1:A:290:PRO:HG3	2:B:286:ARG:HH22	1.82	0.44
2:B:59:LEU:O	2:B:63:ILE:HG13	2.17	0.44
1:E:152[A]:MET:HB2	1:E:152[A]:MET:HE2	1.37	0.44
1:A:14:LYS:NZ	6:A:2019:HOH:O	2.51	0.44
1:D:183:ASN:C	6:D:2123:HOH:O	2.61	0.44
2:B:87:GLY:HA3	6:B:2048:HOH:O	2.18	0.43
1:E:286[B]:ARG:HG3	1:F:285[B]:VAL:HG22	2.01	0.43
1:E:286[B]:ARG:HG3	1:F:285[B]:VAL:CG2	2.47	0.43
1:A:83:ASN:HD21	1:A:116:LYS:HZ1	1.64	0.43
1:E:286[B]:ARG:NH1	1:F:300:ASN:O	2.52	0.43
1:C:192:ASN:N	6:C:2172:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:ASN:ND2	1:F:116:LYS:NZ	2.62	0.43
1:E:83:ASN:HD21	1:E:116:LYS:HZ1	1.67	0.43
1:D:89:HIS:HA	1:D:237:THR:O	2.18	0.43
2:B:159:ASP:HB2	2:B:196:TYR:CZ	2.54	0.43
1:D:45:ILE:HD11	1:D:261:ALA:HB2	2.01	0.43
1:D:179[A]:CSX:SG	1:D:203:VAL:CG1	3.06	0.43
1:F:129:ILE:HD13	1:F:154:LEU:HD13	2.01	0.43
1:F:64:ILE:HD12	1:F:65:GLY:N	2.34	0.43
1:A:48:ILE:HD12	1:A:150:ILE:HG21	2.01	0.42
1:F:183:ASN:ND2	1:F:183:ASN:C	2.77	0.42
2:B:78:THR:HA	6:B:2062:HOH:O	2.18	0.42
1:F:83:ASN:H	1:F:83:ASN:ND2	2.16	0.42
1:D:1:MET:HE1	6:D:2005:HOH:O	2.20	0.42
1:E:153:SER:HB3	1:E:250:ALA:HB1	2.01	0.42
1:E:229:ALA:HB1	1:E:230:PRO:CD	2.50	0.42
1:F:173:ASN:O	1:F:174[B]:ASN:HB3	2.19	0.42
1:A:181:ALA:O	1:A:249:THR:HG21	2.20	0.42
1:C:21:VAL:HG22	1:C:104:VAL:CG1	2.46	0.42
2:B:135:TYR:CD1	2:B:135:TYR:C	2.97	0.41
1:C:83:ASN:HD22	1:C:83:ASN:N	2.15	0.41
1:F:174[A]:ASN:HA	1:F:277:GLU:HB2	2.01	0.41
1:A:44:ILE:HD11	1:A:145:GLU:HB3	2.02	0.41
1:C:83:ASN:H	1:C:83:ASN:ND2	2.18	0.41
1:A:259:ALA:HB2	1:A:303:LEU:HD21	2.03	0.41
1:C:1:MET:HE2	1:C:121:ASP:O	2.21	0.41
1:A:286[B]:ARG:NH1	2:B:290:PRO:HD3	2.36	0.41
1:D:83:ASN:HD21	1:D:116:LYS:NZ	2.17	0.41
1:E:193:GLU:HG2	6:E:2171:HOH:O	2.21	0.41
1:E:280:ILE:HD13	1:E:280:ILE:HA	1.91	0.41
1:E:286[B]:ARG:CZ	6:E:2245:HOH:O	2.50	0.41
1:F:3:LYS:CD	1:F:3:LYS:N	2.70	0.41
1:F:174[B]:ASN:ND2	6:F:2193:HOH:O	2.54	0.41
1:F:221:THR:HG22	1:F:223:GLU:H	1.85	0.41
1:A:222:ASN:ND2	1:A:223:GLU:OE2	2.54	0.40
1:E:99:THR:OG1	1:E:101:SER:O	2.39	0.40
1:F:56:HIS:CE1	1:F:237:THR:HG22	2.57	0.40
1:C:7:ILE:HD12	1:C:180:ALA:HB3	2.02	0.40
1:C:273[A]:ARG:NH1	1:C:279:GLU:OE2	2.54	0.40
1:D:296:GLN:CD	1:D:296:GLN:H	2.29	0.40
1:F:21:VAL:HA	1:F:104:VAL:HG12	2.02	0.40
1:F:182:GLY:O	1:F:221:THR:CG2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:ASN:H	2:B:83:ASN:ND2	2.20	0.40
2:B:183:ASN:HD22	2:B:183:ASN:H	1.69	0.40
1:F:6:LEU:HD13	1:F:118:LEU:HD13	2.02	0.40
1:D:23[B]:MET:O	1:D:23[B]:MET:HG3	2.21	0.40
1:D:253:ALA:HB3	1:D:254:PRO:HD3	2.04	0.40
1:E:286[B]:ARG:NE	1:F:285[B]:VAL:HG23	2.36	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	303/327 (93%)	294 (97%)	9 (3%)	0	100	100
1	C	304/327 (93%)	295 (97%)	9 (3%)	0	100	100
1	D	308/327 (94%)	300 (97%)	8 (3%)	0	100	100
1	E	304/327 (93%)	295 (97%)	9 (3%)	0	100	100
1	F	306/327 (94%)	293 (96%)	13 (4%)	0	100	100
2	B	307/327 (94%)	295 (96%)	11 (4%)	1 (0%)	36	18
All	All	1832/1962 (93%)	1772 (97%)	59 (3%)	1 (0%)	48	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	142	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	234/249 (94%)	220 (94%)	14 (6%)	17	2
1	C	236/249 (95%)	229 (97%)	7 (3%)	36	9
1	D	238/249 (96%)	227 (95%)	11 (5%)	24	3
1	E	235/249 (94%)	225 (96%)	10 (4%)	26	4
1	F	236/249 (95%)	226 (96%)	10 (4%)	26	4
2	B	237/248 (96%)	225 (95%)	12 (5%)	21	2
All	All	1416/1493 (95%)	1352 (96%)	64 (4%)	25	3

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	3	LYS
1	A	15	VAL
1	A	16	SER
1	A	23	MET
1	A	27	ILE
1	A	35	ARG
1	A	83	ASN
1	A	171	VAL
1	A	192	ASN
1	A	193	GLU
1	A	274[A]	SER
1	A	274[B]	SER
1	A	316	THR
2	B	3	LYS
2	B	6	LEU
2	B	62	ARG
2	B	64	ILE
2	B	83	ASN
2	B	126	MET
2	B	142	PRO
2	B	143	LYS
2	B	160	SER
2	B	183	ASN
2	B	192	ASN
2	B	240	ASP

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Mol	Chain	Res	Type
1	C	3	LYS
1	C	6	LEU
1	C	10	LYS
1	C	11	GLN
1	C	62	ARG
1	C	83	ASN
1	C	307	LEU
1	D	6	LEU
1	D	18	LEU
1	D	28	VAL
1	D	62	ARG
1	D	83	ASN
1	D	143	LYS
1	D	158	THR
1	D	174[A]	ASN
1	D	174[B]	ASN
1	D	192	ASN
1	D	286	ARG
1	E	3	LYS
1	E	16	SER
1	E	27	ILE
1	E	70	THR
1	E	83	ASN
1	E	150	ILE
1	E	158	THR
1	E	183	ASN
1	E	217	ASP
1	E	221	THR
1	F	3	LYS
1	F	6	LEU
1	F	62	ARG
1	F	64	ILE
1	F	83	ASN
1	F	160[A]	SER
1	F	160[B]	SER
1	F	183	ASN
1	F	221	THR
1	F	296	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	89	HIS
1	A	192	ASN
1	A	222	ASN
1	A	314	GLN
2	B	43	GLN
2	B	83	ASN
2	B	89	HIS
2	B	183	ASN
2	B	220	ASN
1	C	11	GLN
1	C	83	ASN
1	C	89	HIS
1	C	192	ASN
1	D	83	ASN
1	D	89	HIS
1	D	220	ASN
1	E	43	GLN
1	E	83	ASN
1	E	89	HIS
1	F	83	ASN
1	F	89	HIS
1	F	146	GLN
1	F	183	ASN
1	F	220	ASN
1	F	296	GLN
1	F	314	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

13 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	CSX	F	179[A]	1	3,6,7	0.96	0	1,6,8	0.29	0
2	CSX	B	179[B]	2	3,6,7	1.22	0	1,6,8	1.61	0
1	CSX	C	179[B]	1	3,6,7	0.88	0	1,6,8	1.33	0
1	CSX	A	179[B]	1	4,5,7	2.37	1 (25%)	1,5,8	2.81	1 (100%)
1	CSX	D	179[A]	1	3,6,7	1.35	0	1,6,8	0.33	0
1	CSX	E	179[A]	1	3,6,7	0.94	0	1,6,8	0.01	0
1	CSX	F	179[B]	1	3,6,7	1.01	0	1,6,8	0.08	0
1	CSX	D	179[B]	1	3,6,7	0.63	0	1,6,8	0.69	0
2	CSX	B	52	2	3,6,7	1.15	0	1,6,8	0.47	0
1	CSX	E	179[B]	1	3,6,7	1.66	1 (33%)	1,6,8	0.96	0
2	CSX	B	179[A]	2	4,5,7	1.79	2 (50%)	1,5,8	1.83	0
1	CSX	C	179[A]	1	4,5,7	2.33	3 (75%)	1,5,8	2.79	1 (100%)
1	CSX	A	179[A]	1	3,6,7	1.09	0	1,6,8	0.87	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	CSX	F	179[A]	1	-	0/2/5/7	-
2	CSX	B	179[B]	2	-	0/2/5/7	-
1	CSX	C	179[B]	1	-	0/2/5/7	-
1	CSX	A	179[B]	1	-	0/1/4/7	-
1	CSX	D	179[A]	1	-	0/2/5/7	-
1	CSX	E	179[A]	1	-	0/2/5/7	-
1	CSX	F	179[B]	1	-	0/2/5/7	-
1	CSX	D	179[B]	1	-	0/2/5/7	-
2	CSX	B	52	2	-	1/2/5/7	-
1	CSX	E	179[B]	1	-	0/2/5/7	-
2	CSX	B	179[A]	2	-	0/1/4/7	-
1	CSX	C	179[A]	1	-	0/1/4/7	-
1	CSX	A	179[A]	1	-	0/2/5/7	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179[B]	CSX	CB-CA	-4.43	1.48	1.53
1	C	179[A]	CSX	CB-CA	3.18	1.56	1.53
1	C	179[A]	CSX	O-C	2.67	1.30	1.20
1	E	179[B]	CSX	CB-CA	-2.65	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	179[A]	CSX	CB-CA	2.48	1.55	1.53
2	B	179[A]	CSX	CA-N	-2.06	1.42	1.48
1	C	179[A]	CSX	CB-SG	2.04	1.85	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179[B]	CSX	CA-CB-SG	-2.81	108.40	114.40
1	C	179[A]	CSX	CA-CB-SG	2.79	120.35	114.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	52	CSX	N-CA-CB-SG

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	179[A]	CSX	2	0
1	A	179[B]	CSX	2	0
1	D	179[A]	CSX	2	0
1	E	179[A]	CSX	2	0
2	B	52	CSX	1	0
2	B	179[A]	CSX	2	0
1	C	179[A]	CSX	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	1PE	C	1319	-	9,9,15	2.32	5 (55%)	8,8,14	0.56	0
4	1PE	E	1318	-	9,9,15	2.43	4 (44%)	8,8,14	0.59	0
4	1PE	D	1318	-	9,9,15	1.87	4 (44%)	8,8,14	1.07	0
4	1PE	F	1318	-	9,9,15	2.53	4 (44%)	8,8,14	0.66	0
4	1PE	B	1318	-	9,9,15	1.53	3 (33%)	8,8,14	1.35	2 (25%)
5	GOL	D	1319	-	5,5,5	0.24	0	5,5,5	0.50	0
5	GOL	C	1320	-	5,5,5	0.30	0	5,5,5	0.44	0
4	1PE	A	1318	-	9,9,15	1.37	2 (22%)	8,8,14	1.12	1 (12%)

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	1PE	C	1319	-	-	3/7/7/13	-
4	1PE	E	1318	-	-	3/7/7/13	-
4	1PE	D	1318	-	-	3/7/7/13	-
4	1PE	F	1318	-	-	3/7/7/13	-
4	1PE	B	1318	-	-	3/7/7/13	-
5	GOL	D	1319	-	-	1/4/4/4	-
5	GOL	C	1320	-	-	2/4/4/4	-
4	1PE	A	1318	-	-	3/7/7/13	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1318	1PE	OH5-C14	4.50	1.65	1.42
4	E	1318	1PE	OH5-C14	4.07	1.62	1.42
4	E	1318	1PE	OH4-C24	3.93	1.59	1.42
4	F	1318	1PE	OH4-C24	3.55	1.57	1.42
4	C	1319	1PE	OH3-C23	3.47	1.57	1.42
4	C	1319	1PE	OH5-C14	3.44	1.59	1.42
4	D	1318	1PE	OH4-C24	3.38	1.56	1.42
4	E	1318	1PE	OH3-C22	3.36	1.56	1.42
4	F	1318	1PE	OH3-C22	3.25	1.56	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1318	1PE	OH3-C23	3.10	1.55	1.42
4	A	1318	1PE	OH3-C23	2.71	1.53	1.42
4	C	1319	1PE	OH4-C13	2.64	1.53	1.42
4	C	1319	1PE	OH4-C24	2.62	1.53	1.42
4	D	1318	1PE	OH3-C22	2.56	1.53	1.42
4	D	1318	1PE	OH5-C14	2.44	1.54	1.42
4	C	1319	1PE	OH3-C22	2.31	1.52	1.42
4	E	1318	1PE	OH3-C23	2.27	1.51	1.42
4	B	1318	1PE	OH5-C14	2.25	1.53	1.42
4	B	1318	1PE	OH4-C24	2.22	1.51	1.42
4	D	1318	1PE	OH3-C23	2.16	1.51	1.42
4	A	1318	1PE	OH4-C13	2.10	1.51	1.42
4	B	1318	1PE	OH3-C23	2.00	1.50	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1318	1PE	OH3-C22-C12	2.52	121.22	110.11
4	A	1318	1PE	OH3-C22-C12	2.17	119.66	110.11
4	B	1318	1PE	OH3-C23-C13	2.07	119.80	110.35

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1318	1PE	C14-C24-OH4-C13
4	F	1318	1PE	C14-C24-OH4-C13
4	E	1318	1PE	C14-C24-OH4-C13
5	C	1320	GOL	C1-C2-C3-O3
4	B	1318	1PE	OH4-C13-C23-OH3
4	A	1318	1PE	C14-C24-OH4-C13
4	C	1319	1PE	OH5-C14-C24-OH4
4	B	1318	1PE	OH5-C14-C24-OH4
4	A	1318	1PE	OH4-C13-C23-OH3
4	C	1319	1PE	C14-C24-OH4-C13
4	F	1318	1PE	OH5-C14-C24-OH4
4	E	1318	1PE	OH5-C14-C24-OH4
4	B	1318	1PE	C14-C24-OH4-C13
4	E	1318	1PE	OH4-C13-C23-OH3
4	D	1318	1PE	OH4-C13-C23-OH3
4	F	1318	1PE	OH4-C13-C23-OH3
4	C	1319	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
5	D	1319	GOL	O1-C1-C2-C3
4	D	1318	1PE	OH5-C14-C24-OH4
4	A	1318	1PE	OH5-C14-C24-OH4
5	C	1320	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1319	1PE	4	0
4	E	1318	1PE	2	0
4	D	1318	1PE	3	0
4	F	1318	1PE	4	0
4	B	1318	1PE	3	0
5	D	1319	GOL	7	0
4	A	1318	1PE	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	179[A]:CSX	C	180:ALA	N	1.15
1	A	179[B]:CSX	C	180:ALA	N	1.14

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, 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	302/327 (92%)	0.57	17 (5%)	30 36	10, 26, 41, 60	8 (2%)
1	C	303/327 (92%)	0.17	10 (3%)	49 57	6, 20, 38, 55	7 (2%)
1	D	307/327 (93%)	0.63	25 (8%)	18 21	9, 25, 43, 54	5 (1%)
1	E	306/327 (93%)	0.26	16 (5%)	33 39	7, 20, 37, 60	5 (1%)
1	F	306/327 (93%)	0.26	9 (2%)	53 62	5, 21, 37, 46	4 (1%)
2	B	305/327 (93%)	1.00	47 (15%)	5 6	11, 27, 44, 62	6 (1%)
All	All	1829/1962 (93%)	0.48	124 (6%)	23 27	5, 23, 41, 62	35 (1%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	185	GLY	6.0
1	A	218	PHE	5.2
2	B	142	PRO	4.9
2	B	73	TYR	4.4
2	B	218	PHE	4.4
1	C	316	THR	4.4
1	D	218	PHE	4.4
2	B	128	TRP	4.1
1	A	181	ALA	4.0
2	B	74	GLY	3.9
1	D	1	MET	3.8
1	E	316	THR	3.8
1	E	221	THR	3.8
1	C	315	PHE	3.7
2	B	129	ILE	3.7
1	E	183	ASN	3.7
1	A	182	GLY	3.7
1	C	222	THR	3.6
1	D	14[A]	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	183	ASN	3.4
2	B	139	TRP	3.4
1	E	182	GLY	3.3
2	B	67	VAL	3.3
2	B	134[A]	ARG	3.2
1	D	99	THR	3.2
2	B	316	THR	3.2
1	D	15	VAL	3.2
2	B	4	PHE	3.1
1	A	316	THR	3.0
1	E	315	PHE	3.0
2	B	60	ALA	3.0
2	B	117	ALA	2.9
2	B	64	ILE	2.9
2	B	141	GLY	2.9
2	B	3	LYS	2.9
1	F	240	ASP	2.8
2	B	15	VAL	2.8
2	B	132	ALA	2.8
1	E	222	ASN	2.8
1	F	183	ASN	2.8
2	B	217	ASP	2.8
1	D	4	PHE	2.8
2	B	135	TYR	2.8
2	B	118	LEU	2.8
2	B	144	GLY	2.7
2	B	219	THR	2.7
2	B	163	LEU	2.7
1	F	219	THR	2.7
1	A	4	PHE	2.7
2	B	138	ASP	2.7
1	F	316	THR	2.7
2	B	76	ASP	2.7
1	D	18	LEU	2.6
1	A	3	LYS	2.6
2	B	122	GLY	2.6
2	B	156	GLY	2.6
1	F	218	PHE	2.6
1	D	217	ASP	2.6
2	B	124	GLY	2.6
1	D	2	ARG	2.5
2	B	137	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	17	ALA	2.5
1	A	142	PRO	2.5
1	D	74	GLY	2.5
1	A	128	TRP	2.5
2	B	80	PHE	2.5
2	B	136	ALA	2.4
1	E	155	GLY	2.4
2	B	167	VAL	2.4
2	B	70	THR	2.4
2	B	221	THR	2.4
1	A	15	VAL	2.4
2	B	196	TYR	2.4
1	A	222	ASN	2.4
1	A	285	VAL	2.3
1	D	11	GLN	2.3
1	F	74	GLY	2.3
1	A	2	ARG	2.3
1	E	128	TRP	2.3
1	D	174[A]	ASN	2.3
1	D	291	ILE	2.3
1	C	181	ALA	2.3
1	F	19	SER	2.3
2	B	119	SER	2.3
1	D	183	ASN	2.3
1	A	134[A]	ARG	2.3
1	E	74	GLY	2.3
1	D	316	THR	2.2
2	B	150	ILE	2.2
1	A	158	THR	2.2
1	D	21	VAL	2.2
1	D	54	VAL	2.2
1	F	12	VAL	2.2
2	B	71	THR	2.1
1	E	3	LYS	2.1
2	B	194	PHE	2.1
2	B	54	VAL	2.1
1	D	100	GLY	2.1
2	B	195	ALA	2.1
1	C	193	GLU	2.1
1	A	217	ASP	2.1
1	E	77	GLU	2.1
1	E	184	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	217	ASP	2.1
1	D	142	PRO	2.1
2	B	38	ALA	2.1
2	B	146	GLN	2.1
1	E	193	GLU	2.1
1	D	139	TRP	2.1
1	C	182	GLY	2.1
1	C	313	GLY	2.1
1	D	222	ASN	2.1
2	B	65	GLY	2.1
1	C	10	LYS	2.0
1	D	80	PHE	2.0
1	E	181	ALA	2.0
2	B	166	ALA	2.0
1	A	71	THR	2.0
1	D	71	THR	2.0
1	D	97	ALA	2.0
2	B	110	ALA	2.0
1	D	137	VAL	2.0
1	E	1	MET	2.0
1	F	217	ASP	2.0

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

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	CSX	B	52	7/8	0.93	0.12	27,29,31,31	0
2	CSX	B	179[A]	6/8	0.93	0.11	22,22,23,23	6
2	CSX	B	179[B]	7/8	0.93	0.11	20,22,23,26	7
1	CSX	D	179[A]	7/8	0.94	0.08	15,15,19,24	7
1	CSX	D	179[B]	7/8	0.94	0.08	15,16,20,24	7
1	CSX	F	179[A]	7/8	0.94	0.08	10,14,21,23	7
1	CSX	F	179[B]	7/8	0.94	0.08	12,13,15,23	7
1	CSX	A	179[B]	6/8	0.96	0.06	19,20,21,25	6
1	CSX	A	179[A]	7/8	0.96	0.06	19,19,21,22	7
1	CSX	E	179[A]	7/8	0.96	0.07	7,11,16,18	7
1	CSX	E	179[B]	7/8	0.96	0.07	11,12,16,17	7
1	CSX	C	179[A]	6/8	0.96	0.06	11,12,13,18	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CSX	C	179[B]	7/8	0.96	0.06	11,13,18,19	7

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	GOL	C	1320	6/6	0.82	0.16	53,57,57,58	0
5	GOL	D	1319	6/6	0.88	0.13	27,34,40,42	0
3	NA	B	1317	1/1	0.91	0.09	26,26,26,26	0
3	NA	D	1317	1/1	0.91	0.12	30,30,30,30	0
3	NA	A	1317	1/1	0.92	0.11	30,30,30,30	0
4	1PE	C	1319	10/16	0.95	0.06	10,15,20,20	0
3	NA	C	1317	1/1	0.95	0.07	23,23,23,23	0
4	1PE	B	1318	10/16	0.95	0.07	15,20,24,27	0
4	1PE	E	1318	10/16	0.96	0.05	8,13,20,21	0
4	1PE	F	1318	10/16	0.96	0.06	9,14,19,19	0
4	1PE	A	1318	10/16	0.96	0.06	11,19,23,23	0
4	1PE	D	1318	10/16	0.96	0.06	7,16,20,22	0
3	NA	E	1317	1/1	0.97	0.05	19,19,19,19	0
3	NA	F	1317	1/1	0.97	0.05	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.