



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2014 – 09:19 PM EDT

PDB ID : 4D11
Title : GalNAc-T2 crystal soaked with UDP-5SGalNAc, mEA2 peptide and manganese (Lower resolution dataset)
Authors : Lira-Navarrete, E.; Iglesias-Fernandez, J.; Zandberg, W.F.; Companon, I.; Kong, Y.; Corzana, F.; Pinto, B.M.; Clausen, H.; Peregrina, J.M.; Vocadlo, D.; Rovira, C.; Hurtado-Guerrero, R.
Deposited on : 2014-05-01
Resolution : 2.85 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

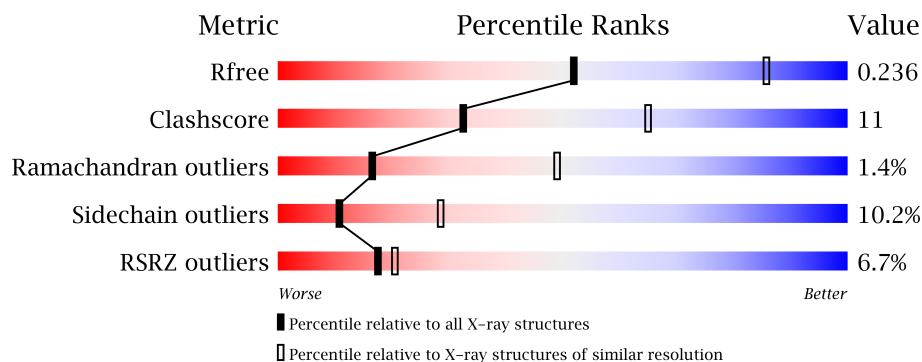
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.85 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}	66092	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (2.90-2.82)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	571	
1	B	571	
1	D	571	
1	E	571	
1	F	571	
2	C	571	
3	L	6	
3	O	6	
3	P	6	
3	X	6	
3	Z	6	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	BBK	B	1572	-	X
5	BBK	D	1572	-	X
5	BBK	E	1571	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21829 atoms, of which 0 are hydrogen and 0 are deuterium.

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 POLYPEPTIDE GALNAC-TRANSFERASE T2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	20	0	0
			3938	2477	715	722	24			
1	B	482	Total	C	N	O	S	20	1	0
			3877	2441	703	710	23			
1	D	487	Total	C	N	O	S	20	0	0
			3916	2465	711	716	24			
1	E	487	Total	C	N	O	S	20	0	0
			3917	2465	711	717	24			
1	F	276	Total	C	N	O	S	8	0	0
			2246	1419	406	407	14			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
B	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
D	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
E	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
F	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471

- Molecule 2 is a protein called POLYPEPTIDE GALNAC-TRANSFERASE T2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	436	Total	C	N	O	S	20	0	0
			3560	2249	646	644	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	74	SER	GLY	CONFLICT	UNP Q10471
C	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471

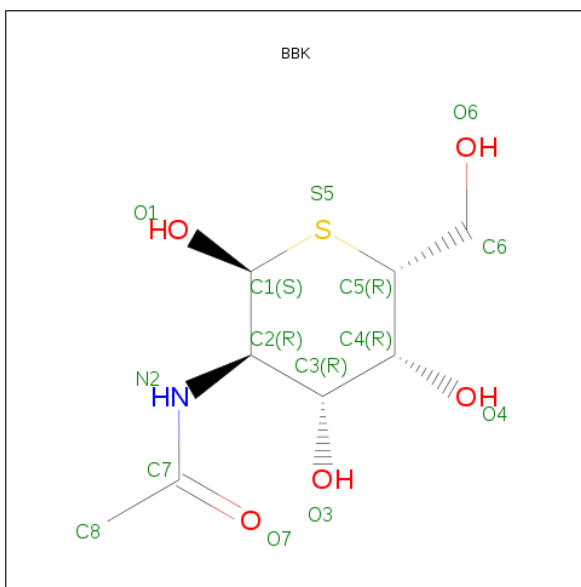
- Molecule 3 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
3	O	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
3	P	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
3	X	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
3	Z	5	Total	C	N	O	S	0	0	0
			31	18	5	7	1			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

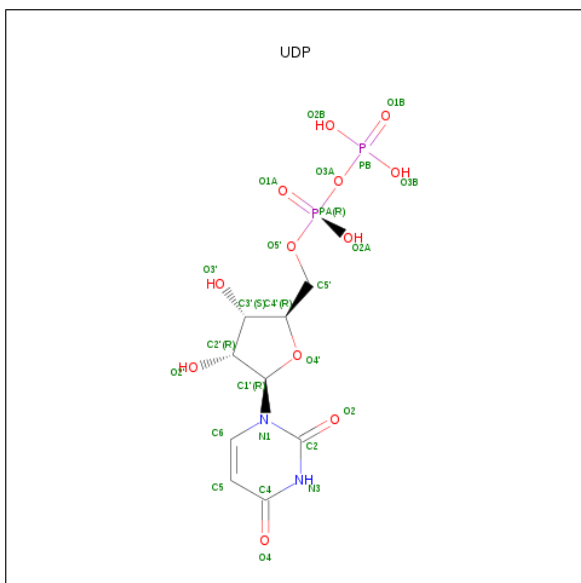
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mn	0	0
			1	1		
4	E	1	Total	Mn	0	0
			1	1		
4	B	1	Total	Mn	0	0
			1	1		
4	C	1	Total	Mn	0	0
			1	1		
4	A	1	Total	Mn	0	0
			1	1		
4	F	1	Total	Mn	0	0
			1	1		

- Molecule 5 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-5-THIO-ALPHA-D-GALACTOPYRANOSE) (three-letter code: BBK) (formula: C₈H₁₅NO₅S).

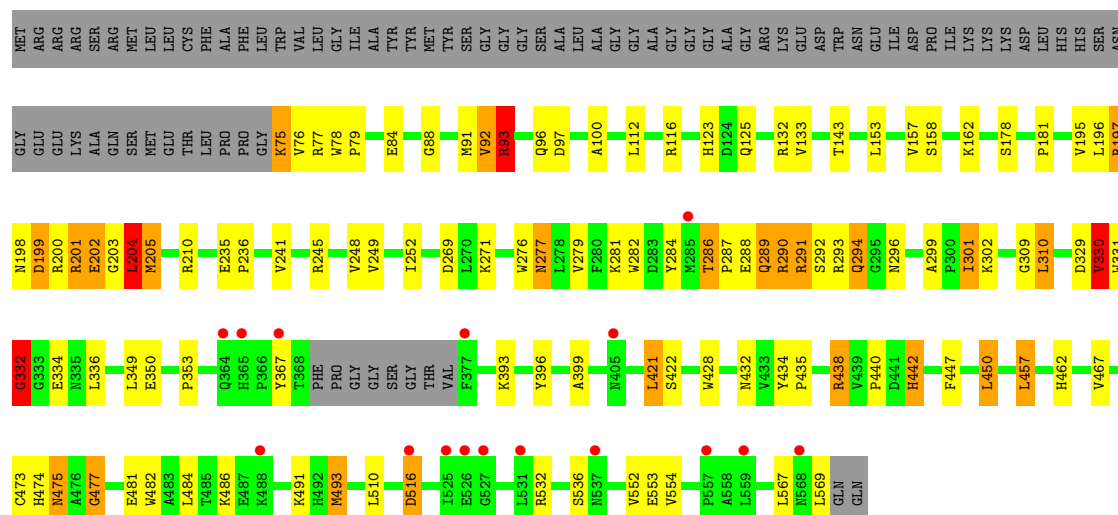


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	E	1	Total	C	N	O	S	0	0
			15	8	1	5	1		

- Molecule 6 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).

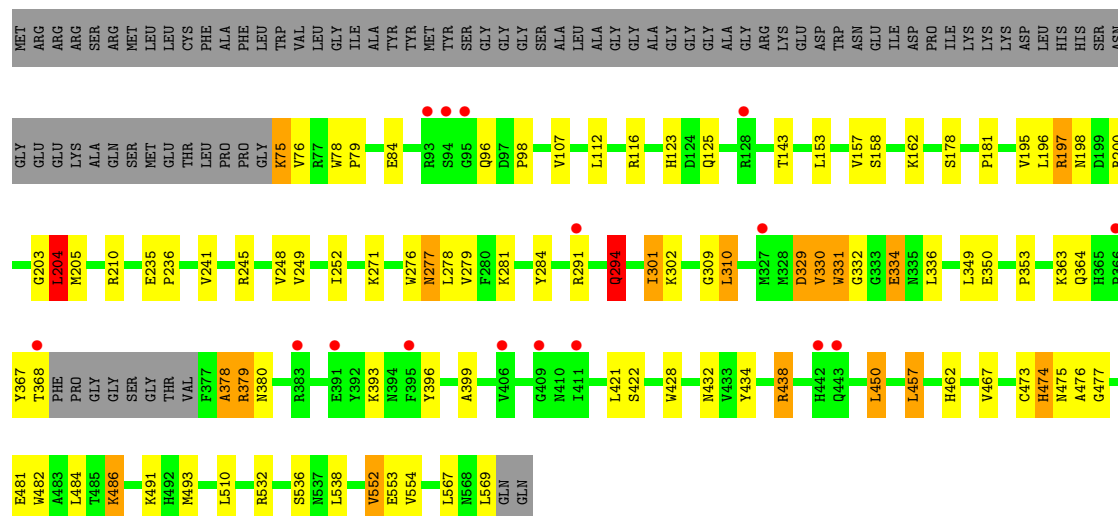


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	F	1	Total	C	N	O	P	0	0
			25	9	2	12	2		



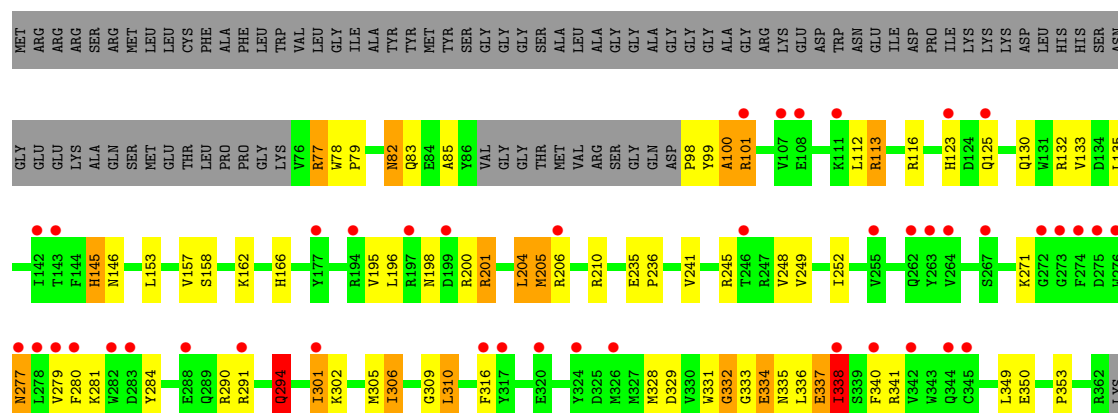
• Molecule 1: POLYPEPTIDE GALNAC-TRANSFERASE T2

Chain E:



• Molecule 1: POLYPEPTIDE GALNAC-TRANSFERASE T2

Chain F:



[illegible]

- Molecule 2: POLYPEPTIDE GALNAC-TRANSFERASE T2

Chain C:

[illegible]

- Molecule 3: PEPTIDE

Chain L:

Diagram illustrating a 10-slot bus system with 5 red LEDs. The slots are labeled S5, T6, C7, P8, A9, and A10. The LEDs are lit in slots S5, P8, A9, and A10, and are unlit in slot T6.

- Molecule 3: PEPTIDE

Chain 0: 

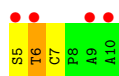
- Molecule 3: PEPTIDE

Chain P: 



● Molecule 3: PEPTIDE

Chain X: 



● Molecule 3: PEPTIDE

Chain Z: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.77Å 120.90Å 249.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	249.61 – 2.85 46.14 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (249.61-2.85) 100.0 (46.14-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.216 , 0.235 0.219 , 0.236	Depositor DCC
R_{free} test set	2285 reflections (2.83%)	DCC
Wilson B-factor (Å ²)	64.9	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.0	EDS
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 83232 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21829	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, MN, BBK

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	0.95	4/4027 (0.1%)	1.03	4/5443 (0.1%)
1	B	1.19	5/3967 (0.1%)	1.05	6/5361 (0.1%)
1	D	1.18	4/4005 (0.1%)	1.05	8/5413 (0.1%)
1	E	1.12	3/4006 (0.1%)	1.05	7/5415 (0.1%)
1	F	0.84	1/2297 (0.0%)	1.03	2/3104 (0.1%)
2	C	0.90	2/3639 (0.1%)	1.03	3/4909 (0.1%)
3	L	0.64	0/32	0.65	0/44
3	O	0.87	0/32	1.25	0/44
3	P	0.94	0/32	1.33	0/44
3	X	0.68	0/32	0.89	0/44
3	Z	0.90	0/31	0.93	0/42
All	All	1.05	19/22100 (0.1%)	1.04	30/29863 (0.1%)

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	D	0	1
2	C	0	1
All	All	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	LYS	CB-CG	-34.06	0.60	1.52
1	D	202	GLU	C-N	-33.06	0.73	1.33
1	B	84	GLU	CB-CG	-32.47	0.90	1.52
1	E	84	GLU	CB-CG	-30.61	0.94	1.52
1	D	486	LYS	CB-CG	-25.67	0.83	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	75	LYS	CB-CG	-25.50	0.83	1.52
2	C	75	LYS	CB-CG	-25.45	0.83	1.52
1	D	75	LYS	CB-CG	-23.67	0.88	1.52
1	E	486	LYS	CB-CG	-21.82	0.93	1.52
1	A	294	GLN	CB-CG	-19.74	0.99	1.52
1	D	84	GLU	CB-CG	-19.63	1.14	1.52
1	B	486	LYS	CB-CG	-19.11	1.00	1.52
1	B	294	GLN	CB-CG	-14.55	1.13	1.52
1	F	294	GLN	CB-CG	-14.29	1.14	1.52
1	A	75	LYS	CB-CG	-12.67	1.18	1.52
1	B	515	GLU	CB-CG	9.37	1.70	1.52
1	A	486	LYS	CB-CG	-7.99	1.30	1.52
1	A	78	TRP	CB-CG	-6.17	1.39	1.50
2	C	84	GLU	CB-CG	-5.95	1.40	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	75	LYS	CB-CG-CD	18.38	159.39	111.60
1	B	84	GLU	CA-CB-CG	13.47	143.04	113.40
1	A	294	GLN	CA-CB-CG	11.16	137.95	113.40
1	B	75	LYS	CA-CB-CG	11.01	137.63	113.40
2	C	75	LYS	CB-CG-CD	10.64	139.28	111.60
1	F	294	GLN	CA-CB-CG	10.56	136.64	113.40
1	E	75	LYS	CA-CB-CG	9.63	134.59	113.40
1	B	294	GLN	CA-CB-CG	8.86	132.90	113.40
1	A	486	LYS	CB-CG-CD	-7.42	92.30	111.60
1	B	84	GLU	CB-CG-CD	7.17	133.57	114.20
1	B	473	CYS	CA-CB-SG	6.85	126.33	114.00
1	A	75	LYS	CA-CB-CG	6.65	128.04	113.40
2	C	294	GLN	CA-CB-CG	-6.62	98.85	113.40
1	E	84	GLU	CA-CB-CG	6.49	127.68	113.40
1	E	75	LYS	CB-CG-CD	6.33	128.06	111.60
1	E	473	CYS	CA-CB-SG	6.21	125.17	114.00
1	D	75	LYS	CA-CB-CG	-6.07	100.05	113.40
1	D	516	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	D	493	MET	CG-SD-CE	5.51	109.02	100.20
1	D	286	THR	C-N-CD	5.42	139.77	128.40
1	E	204	LEU	CA-CB-CG	5.42	127.76	115.30
1	E	294	GLN	CA-CB-CG	5.41	125.30	113.40
1	D	77	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	D	204	LEU	CA-CB-CG	5.33	127.55	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	204	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	204	LEU	CA-CB-CG	5.29	127.46	115.30
1	B	204	LEU	CA-CB-CG	5.23	127.33	115.30
1	E	486	LYS	CA-CB-CG	5.23	124.90	113.40
1	F	204	LEU	CA-CB-CG	5.14	127.12	115.30
1	D	473	CYS	CA-CB-SG	5.04	123.08	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	127	GLN	Peptide
1	D	332	GLY	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3938	0	3863	38	0
1	B	3877	0	3804	96	0
1	D	3916	0	3842	82	0
1	E	3917	0	3843	75	0
1	F	2246	0	2214	88	0
2	C	3560	0	3495	106	0
3	L	32	0	28	3	0
3	O	32	0	28	1	0
3	P	32	0	28	0	0
3	X	32	0	28	7	0
3	Z	31	0	28	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	15	0	0	0	0
5	B	15	0	0	1	0
5	D	15	0	0	0	0
5	E	15	0	0	0	0
6	A	25	0	11	0	0
6	B	25	0	11	0	0
6	C	25	0	11	0	0
6	D	25	0	11	0	0
6	E	25	0	11	1	0
6	F	25	0	11	0	0
All	All	21829	0	21267	483	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (483) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:328:MET:SD	1:F:334:GLU:CB	2.07	1.42
1:D:202:GLU:C	1:D:203:GLY:CA	1.92	1.36
1:D:202:GLU:CA	1:D:203:GLY:N	1.92	1.30
1:F:328:MET:SD	1:F:334:GLU:HB2	1.68	1.29
1:B:329:ASP:HB2	1:B:379:ARG:NH2	1.47	1.28
1:D:202:GLU:O	1:D:203:GLY:N	1.73	1.19
2:C:258:MET:HE3	2:C:363:LYS:HE3	1.22	1.16
1:F:328:MET:SD	1:F:334:GLU:HB3	1.79	1.14
1:B:332:GLY:HA2	1:B:334:GLU:OE1	1.48	1.11
2:C:258:MET:CE	2:C:363:LYS:CE	2.35	1.03
1:B:330:VAL:HG23	1:B:331:TRP:N	1.76	1.01
2:C:457:LEU:HD12	2:C:458:ASP:N	1.76	1.00
2:C:258:MET:CE	2:C:363:LYS:HE2	1.91	1.00
1:F:145:HIS:HE1	1:F:146:ASN:ND2	1.61	0.99
2:C:258:MET:HE3	2:C:363:LYS:CE	1.92	0.98
1:E:205:MET:SD	1:E:330:VAL:HG22	2.05	0.96
2:C:525:ILE:CG1	2:C:530:LYS:HB2	1.94	0.96
1:F:145:HIS:HE1	1:F:146:ASN:HD22	1.13	0.96
1:F:331:TRP:HD1	1:F:332:GLY:H	1.10	0.95
2:C:258:MET:HE1	2:C:363:LYS:HE2	1.46	0.95
2:C:514:ARG:HH11	2:C:514:ARG:HG3	1.31	0.94
1:B:329:ASP:CB	1:B:379:ARG:HH21	1.81	0.93
1:B:329:ASP:CB	1:B:379:ARG:NH2	2.31	0.93
1:F:145:HIS:CE1	1:F:146:ASN:ND2	2.35	0.93
1:B:329:ASP:HB2	1:B:379:ARG:HH21	1.16	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:98:PRO:HG2	1:F:99:TYR:HA	1.51	0.92
2:C:258:MET:CE	2:C:363:LYS:HE3	1.97	0.92
1:D:329:ASP:O	1:D:330:VAL:HG23	1.70	0.90
1:B:132:ARG:HG2	1:B:134:ASP:OD1	1.71	0.90
2:C:459:THR:HG23	2:C:460:LEU:HB3	1.54	0.89
1:D:202:GLU:O	1:D:203:GLY:CA	2.13	0.88
2:C:525:ILE:HD11	2:C:530:LYS:HB2	1.54	0.88
1:B:330:VAL:HG23	1:B:331:TRP:H	1.33	0.86
1:F:133:VAL:CG1	1:F:166:HIS:CE1	2.57	0.86
2:C:517:ASP:OD1	2:C:518:SER:N	2.08	0.86
2:C:525:ILE:CD1	2:C:530:LYS:HB2	2.05	0.86
2:C:131:TRP:HB3	2:C:239:GLU:OE1	1.76	0.85
1:B:379:ARG:HH11	1:B:379:ARG:HG3	1.42	0.85
1:E:277:ASN:CG	1:E:279:VAL:HG12	1.97	0.85
2:C:411:ILE:HD12	2:C:415:LEU:HD12	1.56	0.85
1:B:330:VAL:HG21	1:B:331:TRP:CE3	2.12	0.85
2:C:411:ILE:HD12	2:C:415:LEU:CD1	2.07	0.85
1:B:329:ASP:O	1:B:376:VAL:HG11	1.78	0.83
1:D:286:THR:OG1	1:D:289:GLN:HB2	1.78	0.83
1:F:82:ASN:ND2	1:F:85:ALA:H	1.76	0.82
1:B:330:VAL:CG2	1:B:331:TRP:H	1.91	0.82
2:C:411:ILE:CD1	2:C:415:LEU:CD1	2.56	0.82
1:F:98:PRO:CG	1:F:99:TYR:HA	2.09	0.82
1:B:329:ASP:HB2	1:B:379:ARG:HH22	1.40	0.81
2:C:459:THR:HA	2:C:460:LEU:HB2	1.60	0.81
2:C:410:ASN:OD1	2:C:411:ILE:N	2.13	0.81
1:E:204:LEU:N	1:E:330:VAL:HG21	1.96	0.81
1:E:204:LEU:H	1:E:330:VAL:HG21	1.44	0.81
2:C:478:GLY:O	2:C:479:ASN:HB2	1.80	0.80
1:F:98:PRO:HB2	1:F:100:ALA:N	1.96	0.80
1:B:331:TRP:CE3	1:B:376:VAL:HG21	2.17	0.79
1:E:205:MET:SD	1:E:330:VAL:CG2	2.70	0.79
2:C:525:ILE:HD11	2:C:530:LYS:HE3	1.64	0.79
1:F:133:VAL:CG1	1:F:166:HIS:HE1	1.93	0.79
1:B:331:TRP:CE3	1:B:376:VAL:CG2	2.65	0.79
1:F:334:GLU:O	1:F:337:GLU:N	2.16	0.78
1:B:331:TRP:HE3	1:B:376:VAL:CG2	1.97	0.78
1:D:202:GLU:C	1:D:203:GLY:N	0.73	0.78
2:C:401:PRO:HD2	2:C:402:SER:H	1.49	0.78
2:C:459:THR:CA	2:C:460:LEU:HB2	2.14	0.78
1:D:200:ARG:O	1:D:202:GLU:HG2	1.82	0.77
2:C:258:MET:HE1	2:C:363:LYS:CE	2.08	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:X:5:SER:O	3:X:6:THR:O	2.03	0.76
2:C:525:ILE:HD11	2:C:530:LYS:CB	2.15	0.76
1:B:245:ARG:HH12	1:B:316:PHE:HD2	1.29	0.76
3:X:6:THR:HG22	3:X:7:CYS:N	2.01	0.75
1:B:245:ARG:NH1	1:B:316:PHE:HD2	1.84	0.75
1:E:329:ASP:CG	1:E:379:ARG:NE	2.40	0.75
2:C:411:ILE:CD1	2:C:415:LEU:HD12	2.17	0.75
1:D:252:ILE:HD12	1:D:353:PRO:HA	1.68	0.74
3:X:6:THR:HG22	3:X:7:CYS:H	1.53	0.73
1:E:277:ASN:OD1	1:E:279:VAL:CG1	2.36	0.73
1:E:329:ASP:OD2	1:E:379:ARG:NE	2.22	0.73
1:B:331:TRP:HE3	1:B:376:VAL:CB	2.01	0.73
1:B:332:GLY:CA	1:B:334:GLU:OE1	2.33	0.72
2:C:411:ILE:HD11	2:C:415:LEU:HD11	1.69	0.72
1:E:329:ASP:OD2	1:E:379:ARG:NH2	2.22	0.72
1:F:334:GLU:OE1	1:F:335:ASN:N	2.22	0.72
2:C:252:ILE:HD12	2:C:353:PRO:HA	1.70	0.72
2:C:514:ARG:HG3	2:C:514:ARG:NH1	2.05	0.71
1:F:145:HIS:ND1	1:F:145:HIS:C	2.44	0.71
1:D:198:ASN:HD22	1:D:210:ARG:HH11	1.36	0.71
1:F:98:PRO:HG2	1:F:100:ALA:H	1.55	0.71
2:C:131:TRP:HD1	2:C:132:ARG:O	1.72	0.71
2:C:411:ILE:CD1	2:C:415:LEU:HD11	2.20	0.70
1:F:145:HIS:HD2	1:F:201:ARG:NE	1.89	0.70
2:C:459:THR:HG23	2:C:460:LEU:CB	2.21	0.70
1:F:133:VAL:HG13	1:F:166:HIS:CE1	2.23	0.70
1:E:329:ASP:OD1	1:E:379:ARG:CD	2.39	0.70
1:F:331:TRP:CD1	1:F:332:GLY:N	2.56	0.70
1:D:198:ASN:ND2	1:D:210:ARG:HH11	1.88	0.70
1:E:329:ASP:OD1	1:E:379:ARG:HD3	1.92	0.70
1:F:252:ILE:HD12	1:F:353:PRO:HA	1.74	0.69
1:D:329:ASP:C	1:D:330:VAL:CG2	2.61	0.69
1:E:277:ASN:ND2	1:E:279:VAL:HG12	2.06	0.69
2:C:325:ASP:HB2	2:C:414:ARG:NH1	2.07	0.69
1:B:334:GLU:HG2	1:B:335:ASN:H	1.56	0.69
1:F:145:HIS:CD2	1:F:201:ARG:CZ	2.76	0.69
1:F:98:PRO:HD2	1:F:99:TYR:CD1	2.28	0.69
1:E:123:HIS:HD2	1:E:125:GLN:H	1.40	0.69
1:E:329:ASP:OD1	1:E:379:ARG:NE	2.26	0.69
2:C:123:HIS:HD2	2:C:125:GLN:H	1.42	0.68
1:F:328:MET:SD	1:F:334:GLU:CG	2.81	0.68
1:B:131:TRP:O	1:B:132:ARG:O	2.11	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:330:VAL:CG2	1:B:331:TRP:CE3	2.76	0.68
1:B:331:TRP:HE3	1:B:376:VAL:HB	1.57	0.68
1:D:202:GLU:O	1:D:203:GLY:HA3	1.92	0.68
1:A:252:ILE:HD12	1:A:353:PRO:HA	1.75	0.68
1:E:329:ASP:OD2	1:E:379:ARG:CZ	2.42	0.68
1:E:252:ILE:HD12	1:E:353:PRO:HA	1.74	0.67
1:B:252:ILE:HD12	1:B:353:PRO:HA	1.76	0.67
1:F:337:GLU:OE2	1:F:341:ARG:NH2	2.27	0.67
2:C:178:SER:O	2:C:197:ARG:NH2	2.28	0.67
2:C:459:THR:CB	2:C:460:LEU:HB2	2.25	0.66
2:C:456:CYS:N	2:C:473:CYS:SG	2.69	0.66
2:C:478:GLY:N	2:C:481:GLU:HB2	2.10	0.66
1:F:123:HIS:HD2	1:F:125:GLN:H	1.43	0.66
2:C:461:GLY:O	2:C:462:HIS:CD2	2.49	0.66
1:D:92:VAL:HG12	1:D:93:ARG:N	2.11	0.66
1:D:290:ARG:HH11	1:D:290:ARG:CG	2.09	0.65
1:D:123:HIS:HD2	1:D:125:GLN:H	1.44	0.65
1:E:331:TRP:CH2	3:O:5:SER:HA	2.31	0.65
1:A:123:HIS:HD2	1:A:125:GLN:H	1.42	0.65
1:B:331:TRP:CE3	1:B:376:VAL:HB	2.31	0.65
1:D:329:ASP:C	1:D:330:VAL:HG23	2.16	0.65
1:B:123:HIS:HD2	1:B:125:GLN:H	1.45	0.65
2:C:411:ILE:HD11	2:C:415:LEU:CD1	2.25	0.65
1:F:328:MET:CE	1:F:334:GLU:HB2	2.27	0.65
1:F:145:HIS:CD2	1:F:201:ARG:NE	2.64	0.65
1:A:569:LEU:HD12	1:A:569:LEU:N	2.11	0.64
1:E:205:MET:HE1	1:E:332:GLY:H	1.62	0.64
2:C:525:ILE:HG13	2:C:530:LYS:HB2	1.78	0.64
1:E:178:SER:O	1:E:197:ARG:NH2	2.31	0.64
1:D:202:GLU:N	1:D:203:GLY:N	2.46	0.64
1:F:337:GLU:OE2	1:F:341:ARG:NE	2.31	0.64
1:F:334:GLU:O	1:F:337:GLU:HB3	1.98	0.63
2:C:401:PRO:CD	2:C:402:SER:H	2.10	0.63
1:E:277:ASN:CG	1:E:279:VAL:CG1	2.65	0.63
1:D:475:ASN:C	1:D:477:GLY:H	2.00	0.63
2:C:457:LEU:C	2:C:457:LEU:HD12	2.19	0.63
1:E:205:MET:CE	1:E:332:GLY:H	2.11	0.63
1:E:378:ALA:O	1:E:380:ASN:N	2.32	0.63
1:E:203:GLY:HA3	1:E:330:VAL:HG21	1.80	0.62
2:C:410:ASN:OD1	2:C:412:GLN:N	2.31	0.62
1:F:82:ASN:C	1:F:82:ASN:HD22	2.02	0.62
1:A:329:ASP:OD1	1:A:329:ASP:N	2.31	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:199:ASP:N	1:D:199:ASP:OD1	2.33	0.62
1:D:290:ARG:HH11	1:D:290:ARG:HG3	1.65	0.62
1:F:305:MET:HG2	1:F:306:ILE:N	2.14	0.62
1:F:335:ASN:O	1:F:338:ILE:HG23	2.00	0.62
1:F:336:LEU:HD23	1:F:336:LEU:O	1.99	0.61
1:B:330:VAL:CG2	1:B:331:TRP:N	2.45	0.61
1:B:374:GLY:C	1:B:377:PHE:HB2	2.21	0.61
1:B:379:ARG:CG	1:B:379:ARG:HH11	2.12	0.61
1:F:98:PRO:CD	1:F:99:TYR:HD1	2.13	0.61
1:A:178:SER:O	1:A:197:ARG:NH2	2.34	0.61
1:E:329:ASP:N	1:E:329:ASP:OD1	2.34	0.61
1:D:291:ARG:O	1:D:293:ARG:N	2.28	0.61
1:F:145:HIS:CD2	1:F:201:ARG:NH2	2.69	0.61
1:B:331:TRP:HE3	1:B:376:VAL:HG21	1.58	0.61
2:C:271:LYS:HG2	2:C:301:ILE:HD11	1.83	0.61
1:B:329:ASP:O	1:B:330:VAL:HG22	2.01	0.60
1:E:205:MET:HG3	1:E:334:GLU:HG3	1.83	0.60
1:E:205:MET:HE1	1:E:332:GLY:N	2.15	0.60
1:D:178:SER:O	1:D:197:ARG:NH2	2.35	0.60
1:F:98:PRO:CG	1:F:100:ALA:H	2.14	0.60
1:E:457:LEU:HD13	1:E:482:TRP:CE2	2.36	0.60
1:F:309:GLY:C	1:F:310:LEU:HD23	2.22	0.60
1:E:271:LYS:HG2	1:E:301:ILE:HD11	1.83	0.59
2:C:459:THR:OG1	2:C:460:LEU:HB2	2.01	0.59
1:D:291:ARG:O	1:D:292:SER:HB3	2.01	0.59
1:D:435:PRO:HB2	1:E:291:ARG:HE	1.67	0.59
1:F:331:TRP:HD1	1:F:332:GLY:N	1.92	0.59
1:D:198:ASN:HD22	1:D:210:ARG:NH1	2.01	0.59
1:F:271:LYS:HG2	1:F:301:ILE:HD11	1.85	0.59
1:B:329:ASP:O	1:B:376:VAL:CG1	2.48	0.59
1:E:329:ASP:O	1:E:330:VAL:HB	2.03	0.58
2:C:458:ASP:CG	2:C:459:THR:N	2.57	0.58
2:C:518:SER:C	2:C:520:GLN:H	2.07	0.58
1:D:271:LYS:HG2	1:D:301:ILE:HD11	1.85	0.58
2:C:525:ILE:CD1	2:C:530:LYS:HE3	2.32	0.57
2:C:309:GLY:C	2:C:310:LEU:HD23	2.25	0.57
1:D:201:ARG:HH22	1:D:367:TYR:HB2	1.68	0.57
1:A:457:LEU:HD13	1:A:482:TRP:CE2	2.40	0.57
1:B:335:ASN:HD22	1:B:335:ASN:N	2.02	0.57
1:E:309:GLY:C	1:E:310:LEU:HD23	2.25	0.57
1:E:399:ALA:HB2	1:E:567:LEU:HD22	1.86	0.57
1:A:330:VAL:HG22	1:A:331:TRP:N	2.19	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:198:ASN:HD22	1:E:210:ARG:HH11	1.52	0.56
1:E:205:MET:CG	1:E:334:GLU:HG3	2.35	0.56
1:E:277:ASN:OD1	1:E:279:VAL:HG11	2.05	0.56
1:B:131:TRP:C	1:B:132:ARG:O	2.42	0.56
1:A:329:ASP:OD1	1:A:380:ASN:ND2	2.29	0.56
1:E:249:VAL:HG12	1:E:350:GLU:HB2	1.88	0.56
1:E:205:MET:HE2	1:E:334:GLU:OE1	2.06	0.56
1:A:474:HIS:CE1	1:A:476:ALA:HB3	2.41	0.56
1:B:457:LEU:HD13	1:B:482:TRP:CE2	2.40	0.56
1:B:134:ASP:OD1	1:B:134:ASP:N	2.36	0.55
1:D:289:GLN:O	1:D:293:ARG:HG3	2.07	0.55
1:F:98:PRO:HB2	1:F:99:TYR:C	2.26	0.55
1:D:92:VAL:O	1:D:93:ARG:HB2	2.06	0.55
1:B:331:TRP:CZ3	1:B:376:VAL:CG2	2.89	0.55
2:C:198:ASN:HD22	2:C:210:ARG:HH11	1.55	0.55
1:F:133:VAL:HG12	1:F:166:HIS:CE1	2.38	0.55
1:F:82:ASN:HD21	1:F:85:ALA:H	1.53	0.55
1:E:203:GLY:CA	1:E:330:VAL:HG21	2.37	0.55
1:D:293:ARG:NH1	1:D:299:ALA:O	2.40	0.55
2:C:383:ARG:NH1	2:C:410:ASN:O	2.36	0.54
1:F:198:ASN:HD22	1:F:210:ARG:HH11	1.55	0.54
1:F:98:PRO:N	1:F:99:TYR:HD1	2.05	0.54
1:B:329:ASP:CG	1:B:379:ARG:HH21	2.11	0.54
1:A:198:ASN:HD22	1:A:210:ARG:HH11	1.53	0.54
1:B:458:ASP:OD1	5:B:1572:BBK:O3	2.25	0.54
1:B:198:ASN:HD22	1:B:210:ARG:HH11	1.56	0.54
1:B:399:ALA:HB2	1:B:567:LEU:HD22	1.89	0.54
2:C:325:ASP:CB	2:C:414:ARG:NH1	2.70	0.54
1:F:98:PRO:CD	1:F:99:TYR:CD1	2.90	0.54
1:B:330:VAL:HG22	1:B:376:VAL:HG11	1.89	0.54
1:F:98:PRO:CB	1:F:100:ALA:N	2.68	0.54
1:D:92:VAL:HG12	1:D:93:ARG:H	1.72	0.53
1:F:98:PRO:HG2	1:F:100:ALA:N	2.22	0.53
2:C:329:ASP:N	2:C:329:ASP:OD1	2.41	0.53
1:D:249:VAL:HG12	1:D:350:GLU:HB2	1.91	0.53
1:A:309:GLY:C	1:A:310:LEU:HD23	2.28	0.53
1:B:249:VAL:HG12	1:B:350:GLU:HB2	1.90	0.53
1:B:309:GLY:C	1:B:310:LEU:HD23	2.29	0.53
2:C:131:TRP:CD1	2:C:132:ARG:O	2.58	0.53
1:F:249:VAL:HG12	1:F:350:GLU:HB2	1.90	0.53
1:B:316:PHE:CE2	1:B:320:GLU:OE2	2.62	0.53
1:A:249:VAL:HG12	1:A:350:GLU:HB2	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:131:TRP:C	2:C:132:ARG:O	2.44	0.52
1:D:442:HIS:HD1	1:D:442:HIS:C	2.13	0.52
1:E:277:ASN:ND2	1:E:279:VAL:CG1	2.70	0.52
1:D:457:LEU:HD13	1:D:482:TRP:CE2	2.44	0.52
3:L:6:THR:HG22	3:L:7:CYS:N	2.24	0.52
2:C:249:VAL:HG12	2:C:350:GLU:HB2	1.90	0.52
2:C:524:GLN:OE1	2:C:528:ASN:HB3	2.10	0.52
2:C:158:SER:O	2:C:162:LYS:HB2	2.10	0.52
2:C:282:TRP:NE1	3:L:7:CYS:O	2.38	0.52
1:A:330:VAL:CG2	1:A:331:TRP:N	2.72	0.52
1:E:205:MET:HE1	1:E:330:VAL:HA	1.92	0.52
3:X:6:THR:CG2	3:X:7:CYS:N	2.70	0.52
1:B:170:GLU:OE1	1:B:194:ARG:NH1	2.38	0.51
1:B:327:MET:O	1:B:329:ASP:OD1	2.27	0.51
1:F:98:PRO:CB	1:F:99:TYR:HA	2.40	0.51
1:B:375:THR:C	1:B:377:PHE:N	2.62	0.51
2:C:181:PRO:HB3	2:C:197:ARG:NE	2.25	0.51
1:A:158:SER:O	1:A:162:LYS:HB2	2.11	0.51
2:C:364:GLN:O	2:C:365:HIS:ND1	2.44	0.51
1:D:158:SER:O	1:D:162:LYS:HB2	2.10	0.51
1:E:204:LEU:H	1:E:330:VAL:CG2	2.18	0.51
1:F:98:PRO:CG	1:F:100:ALA:N	2.74	0.51
1:A:399:ALA:HB2	1:A:567:LEU:HD22	1.93	0.51
1:D:329:ASP:O	1:D:330:VAL:CG2	2.50	0.51
1:D:288:GLU:O	1:D:288:GLU:HG3	2.11	0.50
1:B:316:PHE:HE2	1:B:320:GLU:OE2	1.94	0.50
1:B:334:GLU:HG2	1:B:335:ASN:N	2.23	0.50
1:D:309:GLY:C	1:D:310:LEU:HD23	2.32	0.50
2:C:458:ASP:O	2:C:459:THR:HB	2.11	0.50
1:E:158:SER:O	1:E:162:LYS:HB2	2.12	0.50
2:C:459:THR:CG2	2:C:460:LEU:HB3	2.34	0.50
1:D:331:TRP:O	1:D:332:GLY:O	2.30	0.50
1:F:336:LEU:HD21	1:F:340:PHE:CZ	2.46	0.50
3:X:6:THR:C	3:X:7:CYS:SG	2.89	0.50
1:B:331:TRP:CZ3	1:B:376:VAL:HG21	2.47	0.50
1:F:158:SER:O	1:F:162:LYS:HB2	2.12	0.50
2:C:271:LYS:HG2	2:C:301:ILE:CD1	2.42	0.50
2:C:461:GLY:O	2:C:462:HIS:CG	2.64	0.49
1:D:287:PRO:O	1:D:290:ARG:N	2.45	0.49
1:B:158:SER:O	1:B:162:LYS:HB2	2.12	0.49
2:C:401:PRO:CD	2:C:402:SER:N	2.74	0.49
1:B:194:ARG:NH2	1:D:97:ASP:OD2	2.40	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:379:ARG:CG	1:B:379:ARG:NH1	2.73	0.49
1:A:277:ASN:HD21	1:A:279:VAL:HG12	1.77	0.49
1:A:205:MET:HG3	1:A:334:GLU:HG2	1.95	0.49
1:F:334:GLU:OE1	1:F:334:GLU:N	2.46	0.49
1:A:181:PRO:HB3	1:A:197:ARG:NE	2.26	0.49
1:D:435:PRO:HB2	1:E:291:ARG:NE	2.27	0.49
1:D:93:ARG:HB3	1:D:96:GLN:HG3	1.95	0.49
2:C:459:THR:CB	2:C:460:LEU:CB	2.91	0.48
1:F:328:MET:SD	1:F:334:GLU:HG3	2.53	0.48
1:B:329:ASP:O	1:B:331:TRP:N	2.45	0.48
2:C:438:ARG:HG2	2:C:481:GLU:OE2	2.13	0.48
1:D:181:PRO:HB3	1:D:197:ARG:NE	2.28	0.48
1:D:462:HIS:HD2	1:D:467:VAL:O	1.96	0.48
1:E:331:TRP:HZ2	6:E:1572:UDP:O1B	1.95	0.48
1:B:462:HIS:HD2	1:B:467:VAL:O	1.97	0.48
1:D:293:ARG:O	1:D:296:ASN:N	2.47	0.48
1:F:331:TRP:O	1:F:332:GLY:O	2.32	0.48
1:F:337:GLU:O	1:F:340:PHE:N	2.46	0.48
1:F:98:PRO:CB	1:F:99:TYR:CA	2.90	0.48
2:C:414:ARG:HD2	2:C:414:ARG:N	2.28	0.48
1:F:77:ARG:HG2	1:F:79:PRO:HD2	1.96	0.48
1:E:277:ASN:OD1	1:E:279:VAL:HG12	2.08	0.48
1:E:78:TRP:CG	1:E:79:PRO:HD3	2.49	0.48
1:F:98:PRO:HG2	1:F:99:TYR:CA	2.34	0.48
1:D:438:ARG:HG2	1:D:481:GLU:OE2	2.14	0.48
1:D:532:ARG:HD3	1:D:536:SER:O	2.13	0.48
2:C:459:THR:CG2	2:C:460:LEU:CB	2.92	0.47
1:D:276:TRP:O	1:D:396:TYR:HA	2.14	0.47
2:C:493:MET:SD	1:F:290:ARG:NH1	2.87	0.47
1:A:329:ASP:O	1:A:331:TRP:N	2.47	0.47
1:B:205:MET:H	1:B:205:MET:HE2	1.80	0.47
2:C:364:GLN:O	2:C:365:HIS:CB	2.62	0.47
2:C:457:LEU:HD12	2:C:458:ASP:H	1.70	0.47
2:C:525:ILE:HG12	2:C:530:LYS:HB2	1.86	0.47
1:D:284:TYR:CE1	1:E:493:MET:HG3	2.48	0.47
1:A:438:ARG:HG2	1:A:481:GLU:OE2	2.15	0.47
2:C:266:ALA:HB1	3:L:9:ALA:O	2.15	0.47
3:X:6:THR:O	3:X:7:CYS:SG	2.70	0.47
2:C:518:SER:C	2:C:520:GLN:N	2.68	0.47
1:D:277:ASN:HD21	1:D:279:VAL:HG12	1.78	0.47
1:D:291:ARG:C	1:D:293:ARG:H	2.15	0.47
1:A:78:TRP:CG	1:A:79:PRO:HD3	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:178:SER:O	1:B:197:ARG:NH2	2.47	0.47
1:F:133:VAL:HG13	1:F:166:HIS:HE1	1.66	0.47
1:A:393:LYS:O	1:A:396:TYR:HB3	2.15	0.47
1:E:271:LYS:HG2	1:E:301:ILE:CD1	2.44	0.47
1:F:277:ASN:HD21	1:F:279:VAL:HG12	1.80	0.47
1:A:198:ASN:ND2	1:A:210:ARG:HH11	2.13	0.47
1:F:337:GLU:OE2	1:F:341:ARG:CZ	2.63	0.47
2:C:277:ASN:HD21	2:C:279:VAL:HG12	1.80	0.46
1:D:271:LYS:HG2	1:D:301:ILE:CD1	2.44	0.46
1:E:98:PRO:HB3	1:E:107:VAL:HG23	1.98	0.46
1:E:532:ARG:HD3	1:E:536:SER:O	2.14	0.46
2:C:460:LEU:HD22	2:C:471:TYR:HE2	1.80	0.46
1:B:532:ARG:HD3	1:B:536:SER:O	2.15	0.46
1:D:399:ALA:HB2	1:D:567:LEU:HD22	1.98	0.46
1:E:181:PRO:HB3	1:E:197:ARG:NE	2.30	0.46
1:F:271:LYS:HG2	1:F:301:ILE:CD1	2.45	0.46
1:D:393:LYS:O	1:D:396:TYR:HB3	2.16	0.46
1:E:367:TYR:HD1	1:E:368:THR:HG23	1.81	0.46
1:E:428:TRP:CD1	1:E:432:ASN:ND2	2.84	0.46
1:F:83:GLN:HE22	1:F:113:ARG:HG3	1.80	0.46
1:F:145:HIS:CE1	1:F:146:ASN:HD22	2.04	0.46
2:C:133:VAL:CG1	2:C:134:ASP:N	2.78	0.46
2:C:276:TRP:O	2:C:396:TYR:HA	2.16	0.46
2:C:514:ARG:CG	2:C:514:ARG:NH1	2.76	0.46
1:A:532:ARG:HD3	1:A:536:SER:O	2.15	0.46
2:C:457:LEU:HD11	2:C:482:TRP:CZ2	2.51	0.46
1:B:277:ASN:HD21	1:B:279:VAL:HG12	1.81	0.46
2:C:364:GLN:O	2:C:365:HIS:CG	2.69	0.46
1:D:88:GLY:HA2	1:D:91:MET:HG3	1.97	0.46
1:B:329:ASP:C	1:B:330:VAL:HG22	2.35	0.45
1:E:393:LYS:O	1:E:396:TYR:HB3	2.16	0.45
1:B:330:VAL:HG23	1:B:331:TRP:CB	2.46	0.45
1:A:462:HIS:HD2	1:A:467:VAL:O	1.99	0.45
1:D:235:GLU:HB2	1:D:236:PRO:HD3	1.98	0.45
1:A:277:ASN:ND2	1:A:279:VAL:HG12	2.32	0.45
1:D:277:ASN:ND2	1:D:279:VAL:HG12	2.32	0.45
1:F:305:MET:HG2	1:F:306:ILE:H	1.81	0.45
1:B:235:GLU:HB2	1:B:236:PRO:HD3	1.99	0.45
1:B:379:ARG:HG3	1:B:379:ARG:NH1	2.20	0.45
2:C:399:ALA:HB2	2:C:567:LEU:HD22	1.98	0.45
2:C:527:GLY:C	2:C:529:SER:N	2.69	0.45
1:F:332:GLY:HA2	1:F:333:GLY:HA2	1.60	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:78:TRP:CG	2:C:79:PRO:HD3	2.52	0.45
1:D:205:MET:H	1:D:205:MET:HE2	1.82	0.45
1:F:235:GLU:HB2	1:F:236:PRO:HD3	1.98	0.45
1:F:78:TRP:CG	1:F:79:PRO:HD3	2.52	0.45
2:C:397:TYR:O	2:C:400:VAL:O	2.35	0.45
1:E:277:ASN:HD22	1:E:277:ASN:N	2.15	0.45
1:E:203:GLY:C	1:E:330:VAL:HG21	2.37	0.45
1:E:205:MET:SD	1:E:330:VAL:HG23	2.55	0.45
1:F:291:ARG:O	1:F:294:GLN:HB2	2.16	0.45
1:B:331:TRP:CZ3	1:B:376:VAL:HG23	2.52	0.44
1:B:78:TRP:CG	1:B:79:PRO:HD3	2.52	0.44
1:D:143:THR:HG21	1:D:204:LEU:HD23	1.99	0.44
1:B:276:TRP:O	1:B:396:TYR:HA	2.16	0.44
2:C:393:LYS:O	2:C:396:TYR:HB3	2.17	0.44
1:D:290:ARG:C	1:D:291:ARG:O	2.53	0.44
1:E:329:ASP:CG	1:E:379:ARG:HE	2.16	0.44
1:E:438:ARG:HG2	1:E:481:GLU:OE2	2.17	0.44
1:E:474:HIS:O	1:E:476:ALA:N	2.51	0.44
1:B:143:THR:HG21	1:B:204:LEU:HD23	1.99	0.44
1:B:363:LYS:HD2	1:B:363:LYS:HA	1.61	0.44
1:E:291:ARG:O	1:E:294:GLN:HB2	2.17	0.44
1:B:133:VAL:C	1:B:135:LEU:H	2.21	0.44
1:B:375:THR:O	1:B:376:VAL:C	2.55	0.44
1:B:438:ARG:HG2	1:B:481:GLU:OE2	2.18	0.44
1:B:474:HIS:C	1:B:476:ALA:H	2.21	0.44
1:A:276:TRP:O	1:A:396:TYR:HA	2.18	0.44
1:B:329:ASP:CG	1:B:379:ARG:NH2	2.69	0.44
1:B:474:HIS:O	1:B:476:ALA:N	2.50	0.44
1:D:450:LEU:HD23	1:D:450:LEU:HA	1.93	0.44
1:F:100:ALA:HB1	1:F:101:ARG:HE	1.83	0.44
2:C:457:LEU:CD1	2:C:457:LEU:C	2.82	0.43
1:A:291:ARG:NH1	1:B:435:PRO:HB2	2.33	0.43
1:A:235:GLU:HB2	1:A:236:PRO:HD3	2.01	0.43
1:D:421:LEU:HA	1:D:421:LEU:HD12	1.93	0.43
1:F:153:LEU:O	1:F:157:VAL:HG13	2.18	0.43
1:D:282:TRP:NE1	3:X:7:CYS:O	2.41	0.43
2:C:205:MET:HE2	2:C:205:MET:HB2	1.84	0.43
1:F:133:VAL:HG12	1:F:166:HIS:NE2	2.33	0.43
1:B:379:ARG:O	1:B:382:ARG:HB2	2.18	0.43
1:D:442:HIS:ND1	1:D:442:HIS:C	2.72	0.43
1:D:78:TRP:CG	1:D:79:PRO:HD3	2.54	0.43
1:B:491:LYS:HD3	1:B:493:MET:O	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:153:LEU:O	1:D:157:VAL:HG13	2.18	0.43
1:A:474:HIS:ND1	1:A:476:ALA:HB3	2.34	0.43
1:E:462:HIS:HD2	1:E:467:VAL:O	2.02	0.43
1:B:334:GLU:CG	1:B:335:ASN:H	2.26	0.43
1:B:393:LYS:O	1:B:396:TYR:HB3	2.19	0.42
2:C:277:ASN:ND2	2:C:279:VAL:HG12	2.34	0.42
1:D:248:VAL:HB	1:D:349:LEU:HD12	2.01	0.42
1:E:143:THR:HG21	1:E:204:LEU:HD23	2.01	0.42
2:C:143:THR:HG21	2:C:204:LEU:HD23	2.00	0.42
2:C:198:ASN:ND2	2:C:210:ARG:HH11	2.15	0.42
2:C:131:TRP:CB	2:C:239:GLU:OE1	2.57	0.42
1:D:92:VAL:O	1:D:93:ARG:CB	2.67	0.42
1:E:276:TRP:O	1:E:396:TYR:HA	2.19	0.42
2:C:414:ARG:HH11	2:C:414:ARG:CG	2.32	0.42
1:E:198:ASN:ND2	1:E:210:ARG:HH11	2.14	0.42
1:E:276:TRP:C	1:E:278:LEU:H	2.23	0.42
1:A:284:TYR:CZ	1:B:493:MET:HG3	2.54	0.42
2:C:153:LEU:O	2:C:157:VAL:HG13	2.18	0.42
2:C:235:GLU:HB2	2:C:236:PRO:HD3	2.00	0.42
1:E:205:MET:CE	1:E:334:GLU:OE1	2.68	0.42
1:A:153:LEU:O	1:A:157:VAL:HG13	2.19	0.42
2:C:322:GLY:O	2:C:414:ARG:NH2	2.52	0.42
1:D:331:TRP:C	1:D:332:GLY:O	2.56	0.42
1:E:235:GLU:HB2	1:E:236:PRO:HD3	2.01	0.42
1:F:336:LEU:CD2	1:F:340:PHE:CZ	3.03	0.42
1:A:257:ASN:O	1:A:261:PHE:HA	2.20	0.42
1:B:248:VAL:HB	1:B:349:LEU:HD12	2.02	0.42
1:D:290:ARG:NH1	1:D:290:ARG:CG	2.73	0.42
1:E:491:LYS:HD3	1:E:493:MET:O	2.19	0.42
1:F:336:LEU:HD22	1:F:340:PHE:CE2	2.55	0.42
2:C:450:LEU:HD23	2:C:450:LEU:HA	1.96	0.42
2:C:455:ASN:C	2:C:473:CYS:SG	2.99	0.42
1:B:196:LEU:HD11	1:D:100:ALA:HB2	2.01	0.42
1:E:153:LEU:O	1:E:157:VAL:HG13	2.20	0.42
1:E:248:VAL:HB	1:E:349:LEU:HD12	2.02	0.42
1:A:143:THR:HG21	1:A:204:LEU:HD23	2.01	0.42
1:D:440:PRO:HG3	1:D:447:PHE:CD2	2.54	0.42
1:B:330:VAL:CG2	1:B:376:VAL:HG11	2.50	0.41
1:D:200:ARG:O	1:D:201:ARG:C	2.58	0.41
1:D:428:TRP:CD1	1:D:432:ASN:ND2	2.87	0.41
1:E:329:ASP:O	1:E:330:VAL:CB	2.68	0.41
2:C:325:ASP:CA	2:C:414:ARG:NH1	2.83	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:461:GLY:C	2:C:462:HIS:CD2	2.93	0.41
1:B:277:ASN:HD22	1:B:277:ASN:N	2.17	0.41
1:B:377:PHE:HA	1:B:377:PHE:HD1	1.70	0.41
1:F:334:GLU:C	1:F:336:LEU:N	2.73	0.41
1:B:198:ASN:ND2	1:B:210:ARG:HH11	2.17	0.41
1:E:538:LEU:HB3	1:E:552:VAL:HG22	2.03	0.41
1:F:145:HIS:ND1	1:F:146:ASN:N	2.69	0.41
1:F:277:ASN:ND2	1:F:279:VAL:HG12	2.35	0.41
1:F:280:PHE:HD1	1:F:305:MET:SD	2.43	0.41
1:F:333:GLY:C	1:F:335:ASN:N	2.73	0.41
1:B:440:PRO:HG3	1:B:447:PHE:CD2	2.55	0.41
1:B:153:LEU:O	1:B:157:VAL:HG13	2.20	0.41
2:C:248:VAL:HB	2:C:349:LEU:HD12	2.02	0.41
1:D:200:ARG:HB3	1:D:200:ARG:HE	1.70	0.41
1:F:248:VAL:HB	1:F:349:LEU:HD12	2.03	0.41
1:D:277:ASN:HD22	1:D:277:ASN:N	2.18	0.41
1:D:252:ILE:CD1	1:D:353:PRO:HA	2.43	0.41
1:F:277:ASN:HD22	1:F:277:ASN:N	2.19	0.41
1:B:375:THR:O	1:B:378:ALA:N	2.54	0.41
1:D:269:ASP:OD2	1:E:493:MET:HB3	2.21	0.41
1:D:491:LYS:HD3	1:D:493:MET:O	2.21	0.41
1:A:93:ARG:HG3	1:A:94:SER:N	2.35	0.41
1:F:198:ASN:ND2	1:F:210:ARG:HH11	2.16	0.41
1:B:131:TRP:CZ2	1:B:236:PRO:HG3	2.57	0.40
1:B:321:LEU:O	1:B:341:ARG:HD2	2.21	0.40
1:B:428:TRP:CD1	1:B:432:ASN:ND2	2.89	0.40
2:C:411:ILE:HD12	2:C:411:ILE:O	2.21	0.40
1:D:200:ARG:O	1:D:202:GLU:CG	2.62	0.40
1:F:205:MET:O	1:F:206:ARG:C	2.60	0.40
1:A:94:SER:HB3	1:A:95:GLY:H	1.50	0.40
2:C:457:LEU:HA	2:C:470:VAL:HG12	2.02	0.40
1:F:133:VAL:CG1	1:F:166:HIS:NE2	2.83	0.40
1:E:450:LEU:HA	1:E:450:LEU:HD23	2.00	0.40
1:F:98:PRO:HB2	1:F:99:TYR:CA	2.51	0.40
1:A:421:LEU:HA	1:A:421:LEU:HD12	1.92	0.40
1:A:93:ARG:HG3	1:A:94:SER:H	1.86	0.40
1:B:277:ASN:ND2	1:B:279:VAL:HG12	2.36	0.40
1:B:442:HIS:O	1:B:442:HIS:CD2	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	487/571 (85%)	461 (95%)	24 (5%)	2 (0%)	43	80
1	B	477/571 (84%)	445 (93%)	26 (6%)	6 (1%)	18	51
1	D	483/571 (85%)	449 (93%)	28 (6%)	6 (1%)	19	54
1	E	483/571 (85%)	457 (95%)	21 (4%)	5 (1%)	22	59
1	F	272/571 (48%)	252 (93%)	15 (6%)	5 (2%)	13	41
2	C	422/571 (74%)	387 (92%)	27 (6%)	8 (2%)	12	39
3	L	4/6 (67%)	1 (25%)	1 (25%)	2 (50%)	0	0
3	O	4/6 (67%)	2 (50%)	2 (50%)	0	100	100
3	P	4/6 (67%)	3 (75%)	0	1 (25%)	0	0
3	X	4/6 (67%)	1 (25%)	2 (50%)	1 (25%)	0	0
3	Z	3/6 (50%)	3 (100%)	0	0	100	100
All	All	2643/3456 (76%)	2461 (93%)	146 (6%)	36 (1%)	16	49

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	VAL
1	A	477	GLY
1	B	132	ARG
1	B	477	GLY
2	C	365	HIS
2	C	460	LEU
1	D	92	VAL
1	D	93	ARG
1	D	477	GLY
1	E	378	ALA
1	E	477	GLY
1	F	329	ASP
1	F	332	GLY

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Mol	Chain	Res	Type
3	L	7	CYS
3	X	6	THR
1	B	330	VAL
1	B	332	GLY
2	C	132	ARG
1	D	332	GLY
1	E	379	ARG
1	F	100	ALA
2	C	330	VAL
2	C	332	GLY
2	C	479	ASN
1	B	133	VAL
2	C	401	PRO
2	C	517	ASP
1	E	330	VAL
1	F	337	GLU
3	L	6	THR
3	P	9	ALA
1	D	294	GLN
1	D	330	VAL
1	E	475	ASN
1	B	475	ASN
1	F	338	ILE

5.3.2 Protein sidechains ⓘ

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	425/485 (88%)	386 (91%)	39 (9%)	13	35
1	B	418/485 (86%)	379 (91%)	39 (9%)	13	35
1	D	423/485 (87%)	379 (90%)	44 (10%)	10	27
1	E	423/485 (87%)	384 (91%)	39 (9%)	13	35
1	F	244/485 (50%)	215 (88%)	29 (12%)	8	19
2	C	385/486 (79%)	340 (88%)	45 (12%)	8	20
3	L	4/4 (100%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O	4/4 (100%)	2 (50%)	2 (50%)	0	0
3	P	4/4 (100%)	3 (75%)	1 (25%)	1	2
3	X	4/4 (100%)	4 (100%)	0	100	100
3	Z	4/4 (100%)	3 (75%)	1 (25%)	1	2
All	All	2338/2931 (80%)	2099 (90%)	239 (10%)	11	28

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LYS
1	A	94	SER
1	A	96	GLN
1	A	112	LEU
1	A	116	ARG
1	A	130	GLN
1	A	132	ARG
1	A	133	VAL
1	A	195	VAL
1	A	196	LEU
1	A	197	ARG
1	A	200	ARG
1	A	204	LEU
1	A	205	MET
1	A	241	VAL
1	A	245	ARG
1	A	277	ASN
1	A	281	LYS
1	A	284	TYR
1	A	294	GLN
1	A	302	LYS
1	A	310	LEU
1	A	329	ASP
1	A	334	GLU
1	A	336	LEU
1	A	349	LEU
1	A	421	LEU
1	A	422	SER
1	A	434	TYR
1	A	438	ARG
1	A	450	LEU
1	A	457	LEU

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Mol	Chain	Res	Type
1	A	484	LEU
1	A	486	LYS
1	A	510	LEU
1	A	552	VAL
1	A	553	GLU
1	A	554	VAL
1	A	569	LEU
1	B	76	VAL
1	B	112	LEU
1	B	116	ARG
1	B	127	GLN
1	B	130	GLN
1	B	131	TRP
1	B	132	ARG
1	B	133	VAL
1	B	195	VAL
1	B	196	LEU
1	B	200	ARG
1	B	204	LEU
1	B	205	MET
1	B	241	VAL
1	B	245	ARG
1	B	277	ASN
1	B	281	LYS
1	B	302	LYS
1	B	306	ILE
1	B	310	LEU
1	B	329	ASP
1	B	335	ASN
1	B	336	LEU
1	B	375	THR
1	B	377	PHE
1	B	379	ARG
1	B	421	LEU
1	B	422	SER
1	B	434	TYR
1	B	438	ARG
1	B	450	LEU
1	B	457	LEU
1	B	474	HIS
1	B	484	LEU
1	B	510	LEU

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Mol	Chain	Res	Type
1	B	552	VAL
1	B	553	GLU
1	B	554	VAL
1	B	569	LEU
2	C	75	LYS
2	C	76	VAL
2	C	112	LEU
2	C	116	ARG
2	C	128	ARG
2	C	131	TRP
2	C	132	ARG
2	C	195	VAL
2	C	196	LEU
2	C	197	ARG
2	C	199	ASP
2	C	200	ARG
2	C	204	LEU
2	C	205	MET
2	C	241	VAL
2	C	245	ARG
2	C	277	ASN
2	C	281	LYS
2	C	294	GLN
2	C	301	ILE
2	C	306	ILE
2	C	310	LEU
2	C	329	ASP
2	C	335	ASN
2	C	336	LEU
2	C	365	HIS
2	C	402	SER
2	C	414	ARG
2	C	421	LEU
2	C	422	SER
2	C	434	TYR
2	C	438	ARG
2	C	450	LEU
2	C	457	LEU
2	C	458	ASP
2	C	459	THR
2	C	472	GLU
2	C	480	GLN

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Mol	Chain	Res	Type
2	C	484	LEU
2	C	486	LYS
2	C	510	LEU
2	C	514	ARG
2	C	526	GLU
2	C	528	ASN
2	C	569	LEU
1	D	75	LYS
1	D	76	VAL
1	D	93	ARG
1	D	112	LEU
1	D	116	ARG
1	D	132	ARG
1	D	133	VAL
1	D	195	VAL
1	D	196	LEU
1	D	197	ARG
1	D	199	ASP
1	D	201	ARG
1	D	204	LEU
1	D	205	MET
1	D	241	VAL
1	D	245	ARG
1	D	277	ASN
1	D	281	LYS
1	D	289	GLN
1	D	290	ARG
1	D	291	ARG
1	D	294	GLN
1	D	301	ILE
1	D	302	LYS
1	D	310	LEU
1	D	330	VAL
1	D	334	GLU
1	D	336	LEU
1	D	421	LEU
1	D	422	SER
1	D	434	TYR
1	D	438	ARG
1	D	442	HIS
1	D	450	LEU
1	D	457	LEU

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Mol	Chain	Res	Type
1	D	474	HIS
1	D	475	ASN
1	D	484	LEU
1	D	510	LEU
1	D	516	ASP
1	D	552	VAL
1	D	553	GLU
1	D	554	VAL
1	D	569	LEU
1	E	75	LYS
1	E	76	VAL
1	E	96	GLN
1	E	112	LEU
1	E	116	ARG
1	E	195	VAL
1	E	196	LEU
1	E	197	ARG
1	E	200	ARG
1	E	204	LEU
1	E	241	VAL
1	E	245	ARG
1	E	277	ASN
1	E	281	LYS
1	E	284	TYR
1	E	294	GLN
1	E	301	ILE
1	E	302	LYS
1	E	310	LEU
1	E	329	ASP
1	E	331	TRP
1	E	334	GLU
1	E	336	LEU
1	E	363	LYS
1	E	364	GLN
1	E	421	LEU
1	E	422	SER
1	E	434	TYR
1	E	438	ARG
1	E	450	LEU
1	E	457	LEU
1	E	474	HIS
1	E	484	LEU

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Mol	Chain	Res	Type
1	E	486	LYS
1	E	510	LEU
1	E	552	VAL
1	E	553	GLU
1	E	554	VAL
1	E	569	LEU
1	F	77	ARG
1	F	82	ASN
1	F	101	ARG
1	F	112	LEU
1	F	113	ARG
1	F	116	ARG
1	F	130	GLN
1	F	132	ARG
1	F	135	LEU
1	F	145	HIS
1	F	195	VAL
1	F	196	LEU
1	F	200	ARG
1	F	201	ARG
1	F	204	LEU
1	F	205	MET
1	F	241	VAL
1	F	245	ARG
1	F	277	ASN
1	F	281	LYS
1	F	284	TYR
1	F	294	GLN
1	F	301	ILE
1	F	302	LYS
1	F	306	ILE
1	F	310	LEU
1	F	316	PHE
1	F	334	GLU
1	F	338	ILE
3	O	5	SER
3	O	7	CYS
3	P	7	CYS
3	Z	7	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	198	ASN
1	A	277	ASN
1	A	296	ASN
1	A	344	GLN
1	A	405	ASN
1	A	432	ASN
1	A	452	GLN
1	A	462	HIS
1	B	123	HIS
1	B	198	ASN
1	B	277	ASN
1	B	296	ASN
1	B	335	ASN
1	B	344	GLN
1	B	380	ASN
1	B	405	ASN
1	B	432	ASN
1	B	442	HIS
1	B	452	GLN
1	B	462	HIS
2	C	123	HIS
2	C	198	ASN
2	C	277	ASN
2	C	296	ASN
2	C	335	ASN
2	C	344	GLN
2	C	380	ASN
2	C	405	ASN
2	C	432	ASN
2	C	462	HIS
2	C	528	ASN
1	D	123	HIS
1	D	198	ASN
1	D	277	ASN
1	D	296	ASN
1	D	344	GLN
1	D	380	ASN
1	D	405	ASN
1	D	432	ASN
1	D	452	GLN
1	D	462	HIS
1	E	123	HIS

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Mol	Chain	Res	Type
1	E	198	ASN
1	E	277	ASN
1	E	296	ASN
1	E	335	ASN
1	E	344	GLN
1	E	364	GLN
1	E	405	ASN
1	E	432	ASN
1	E	452	GLN
1	E	462	HIS
1	E	537	ASN
1	F	82	ASN
1	F	123	HIS
1	F	145	HIS
1	F	146	ASN
1	F	198	ASN
1	F	277	ASN
1	F	296	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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$
5	BBK	A	1571	-	15,15,15	8.32	3 (20%)	21,21,21	2.50	4 (19%)
6	UDP	A	1572	4	26,26,26	1.33	4 (15%)	36,40,40	1.57	5 (13%)
5	BBK	B	1572	-	15,15,15	8.22	4 (26%)	21,21,21	2.53	3 (14%)
6	UDP	B	1573	4	26,26,26	1.45	5 (19%)	36,40,40	1.65	4 (11%)
6	UDP	C	1571	4	26,26,26	1.34	4 (15%)	36,40,40	1.49	5 (13%)
6	UDP	D	1571	4	26,26,26	1.41	4 (15%)	36,40,40	1.54	3 (8%)
5	BBK	D	1572	-	15,15,15	8.36	4 (26%)	21,21,21	2.14	8 (38%)
5	BBK	E	1571	-	15,15,15	8.59	4 (26%)	21,21,21	1.86	4 (19%)
6	UDP	E	1572	4	26,26,26	1.32	4 (15%)	36,40,40	1.62	3 (8%)
6	UDP	F	1364	4	26,26,26	1.25	4 (15%)	36,40,40	1.58	3 (8%)

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
5	BBK	A	1571	-	-	0/6/26/26	0/1/1/1
6	UDP	A	1572	4	-	0/14/32/32	0/2/2/2
5	BBK	B	1572	-	-	0/6/26/26	0/1/1/1
6	UDP	B	1573	4	-	0/14/32/32	0/2/2/2
6	UDP	C	1571	4	-	0/14/32/32	0/2/2/2
6	UDP	D	1571	4	-	0/14/32/32	0/2/2/2
5	BBK	D	1572	-	-	0/6/26/26	0/1/1/1
5	BBK	E	1571	-	-	0/6/26/26	0/1/1/1
6	UDP	E	1572	4	-	0/14/32/32	0/2/2/2
6	UDP	F	1364	4	-	0/14/32/32	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1571	BBK	C5-S5	-26.28	1.43	1.82
5	A	1571	BBK	C5-S5	-25.58	1.44	1.82
5	D	1572	BBK	C5-S5	-25.45	1.44	1.82
5	B	1572	BBK	C5-S5	-24.98	1.45	1.82
5	E	1571	BBK	C1-S5	-19.94	1.43	1.83
5	A	1571	BBK	C1-S5	-19.36	1.44	1.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1572	BBK	C1-S5	-19.22	1.44	1.83
5	B	1572	BBK	C1-S5	-18.97	1.44	1.83
5	D	1572	BBK	C6-C5	4.37	1.56	1.52
5	B	1572	BBK	C6-C5	3.89	1.55	1.52
6	D	1571	UDP	PB-O1B	3.82	1.63	1.51
6	E	1572	UDP	PB-O1B	3.82	1.63	1.51
6	B	1573	UDP	C2-N1	-3.74	1.34	1.38
6	C	1571	UDP	PB-O1B	3.62	1.63	1.51
6	B	1573	UDP	PB-O1B	3.32	1.62	1.51
5	D	1572	BBK	C4-C5	3.26	1.56	1.53
6	A	1572	UDP	O2-C2	3.18	1.25	1.21
6	B	1573	UDP	O2-C2	3.08	1.25	1.21
6	A	1572	UDP	PB-O1B	3.06	1.61	1.51
6	F	1364	UDP	PB-O1B	3.02	1.61	1.51
5	B	1572	BBK	C4-C5	2.97	1.55	1.53
6	F	1364	UDP	O2-C2	2.95	1.25	1.21
6	B	1573	UDP	O4'-C1'	2.93	1.44	1.41
6	F	1364	UDP	O4'-C1'	2.92	1.44	1.41
6	C	1571	UDP	O2-C2	2.86	1.25	1.21
6	D	1571	UDP	O4'-C1'	2.86	1.44	1.41
6	F	1364	UDP	C2-N1	-2.84	1.35	1.38
6	A	1572	UDP	O4'-C1'	2.77	1.44	1.41
5	E	1571	BBK	C6-C5	2.70	1.54	1.52
6	D	1571	UDP	C2-N1	-2.67	1.35	1.38
6	E	1572	UDP	O2-C2	2.65	1.25	1.21
5	E	1571	BBK	C4-C5	2.63	1.55	1.53
6	A	1572	UDP	C2-N1	-2.45	1.35	1.38
6	C	1571	UDP	O4'-C1'	2.41	1.44	1.41
6	C	1571	UDP	PA-O3A	2.28	1.63	1.59
6	E	1572	UDP	C2-N1	-2.17	1.36	1.38
6	E	1572	UDP	O3'-C3'	2.16	1.48	1.43
5	A	1571	BBK	C4-C5	2.14	1.55	1.53
6	B	1573	UDP	C5-C4	2.03	1.40	1.37
6	D	1571	UDP	PB-O3A	2.02	1.63	1.60

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1571	BBK	C1-S5-C5	9.78	118.98	96.41
5	B	1572	BBK	C1-S5-C5	9.46	118.25	96.41
6	D	1571	UDP	N3-C2-N1	6.57	121.45	115.97
6	B	1573	UDP	N3-C2-N1	6.20	121.15	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1572	UDP	N3-C2-N1	6.15	121.11	115.97
5	D	1572	BBK	C1-S5-C5	5.99	110.23	96.41
6	E	1572	UDP	N3-C2-N1	5.97	120.95	115.97
5	E	1571	BBK	C1-S5-C5	5.48	109.07	96.41
6	C	1571	UDP	N3-C2-N1	5.46	120.53	115.97
6	F	1364	UDP	N3-C2-N1	5.39	120.47	115.97
6	F	1364	UDP	PA-O3A-PB	-4.87	118.44	131.93
6	E	1572	UDP	PA-O3A-PB	-4.53	119.39	131.93
5	E	1571	BBK	C4-C3-C2	4.36	116.72	110.51
6	B	1573	UDP	O3B-PB-O2B	4.09	122.72	107.38
6	D	1571	UDP	PA-O3A-PB	-3.76	121.51	131.93
6	F	1364	UDP	O3B-PB-O2B	3.72	121.35	107.38
5	D	1572	BBK	O4-C4-C5	3.49	116.68	108.72
6	C	1571	UDP	O3B-PB-O2B	3.38	120.07	107.38
6	A	1572	UDP	PA-O3A-PB	-3.36	122.63	131.93
6	C	1571	UDP	C2-N1-C1'	3.33	120.30	118.21
5	B	1572	BBK	O4-C4-C5	3.21	116.04	108.72
6	B	1573	UDP	C2-N1-C1'	-3.05	116.29	118.21
5	D	1572	BBK	C1-C2-C3	3.01	114.88	110.07
5	B	1572	BBK	O6-C6-C5	2.96	117.36	110.65
6	E	1572	UDP	O3B-PB-O2B	2.93	118.37	107.38
5	D	1572	BBK	C6-C5-S5	2.91	115.86	109.02
6	A	1572	UDP	O3B-PB-O2B	2.83	117.98	107.38
6	D	1571	UDP	O3B-PB-O2B	2.70	117.51	107.38
6	A	1572	UDP	C2'-C1'-N1	2.58	120.41	113.34
5	A	1571	BBK	O1-C1-C2	-2.56	103.57	109.27
5	D	1572	BBK	C3-C2-N2	-2.55	105.19	110.60
5	D	1572	BBK	O6-C6-C5	2.43	116.17	110.65
6	A	1572	UDP	O3B-PB-O3A	2.39	116.49	105.14
6	B	1573	UDP	C2'-C3'-C4'	2.35	107.33	102.64
6	C	1571	UDP	PA-O3A-PB	-2.31	125.55	131.93
5	D	1572	BBK	C3-C4-C5	-2.28	106.95	110.95
5	E	1571	BBK	C3-C4-C5	2.23	114.86	110.95
5	D	1572	BBK	C4-C5-S5	-2.20	105.57	110.12
6	C	1571	UDP	O2B-PB-O1B	-2.16	103.30	110.36
5	A	1571	BBK	C1-C2-N2	-2.09	107.55	111.53
5	A	1571	BBK	O4-C4-C5	2.07	113.44	108.72
5	E	1571	BBK	O1-C1-S5	-2.04	101.17	109.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	491/571 (85%)	0.02	14 (2%)	49	59	28, 56, 96, 129	5 (1%)
1	B	482/571 (84%)	0.12	15 (3%)	47	56	32, 65, 115, 151	5 (1%)
1	D	487/571 (85%)	0.16	16 (3%)	44	53	29, 64, 110, 144	5 (1%)
1	E	487/571 (85%)	0.15	16 (3%)	44	53	31, 58, 105, 159	5 (1%)
1	F	276/571 (48%)	0.98	43 (15%)	3	3	59, 112, 167, 187	2 (0%)
2	C	436/571 (76%)	0.70	67 (15%)	3	3	35, 89, 149, 182	5 (1%)
3	L	6/6 (100%)	2.22	4 (66%)	0	0	86, 109, 116, 126	0
3	O	6/6 (100%)	0.70	0	100	100	72, 94, 105, 110	0
3	P	6/6 (100%)	0.52	0	100	100	44, 72, 78, 90	0
3	X	6/6 (100%)	2.88	4 (66%)	0	0	91, 106, 118, 123	0
3	Z	5/6 (83%)	0.54	0	100	100	72, 73, 88, 92	0
All	All	2688/3456 (77%)	0.31	179 (6%)	17	20	28, 67, 136, 187	27 (1%)

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	10	ALA	7.3
1	F	276	TRP	6.9
2	C	500	VAL	6.7
1	F	264	VAL	6.5
2	C	511	GLN	6.1
1	F	274	PHE	6.0
2	C	454	THR	5.6
1	B	364	GLN	5.6
1	F	340	PHE	5.3
2	C	497	LEU	5.3
1	A	372	GLY	5.2
1	E	391	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
2	C	128	ARG	5.0
2	C	446	ALA	5.0
2	C	531	LEU	5.0
1	E	442	HIS	4.9
2	C	563	TRP	4.9
2	C	526	GLU	4.9
1	F	197	ARG	4.9
2	C	496	CYS	4.8
1	A	373	SER	4.7
2	C	534	VAL	4.6
2	C	533	HIS	4.6
2	C	509	LYS	4.5
3	L	10	ALA	4.5
1	F	324	TYR	4.5
2	C	100	ALA	4.5
2	C	525	ILE	4.5
2	C	524	GLN	4.5
1	F	278	LEU	4.4
1	B	101	ARG	4.4
2	C	501	ASP	4.4
1	A	442	HIS	4.4
1	F	273	GLY	4.4
1	F	272	GLY	4.3
2	C	470	VAL	4.3
2	C	523	GLU	4.3
2	C	403	ALA	4.2
1	B	97	ASP	4.1
1	F	342	VAL	4.1
2	C	565	PHE	4.0
2	C	510	LEU	3.9
1	B	103	LYS	3.8
2	C	530	LYS	3.8
1	E	95	GLY	3.7
1	F	277	ASN	3.7
1	A	95	GLY	3.6
1	F	267	SER	3.6
2	C	498	THR	3.6
2	C	490	VAL	3.6
1	F	101	ARG	3.5
2	C	462	HIS	3.5
2	C	502	ARG	3.5
2	C	527	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	525	ILE	3.4
2	C	374	GLY	3.4
2	C	522	TRP	3.4
1	F	246	THR	3.4
1	B	366	PRO	3.4
2	C	568	ASN	3.4
1	D	364	GLN	3.3
2	C	291	ARG	3.3
1	D	377	PHE	3.3
2	C	488	LYS	3.3
1	A	96	GLN	3.3
1	F	177	TYR	3.3
1	E	443	GLN	3.2
1	F	338	ILE	3.2
1	F	316	PHE	3.2
1	B	98	PRO	3.2
2	C	104	PHE	3.2
1	D	527	GLY	3.2
2	C	484	LEU	3.2
1	B	99	TYR	3.1
1	D	405	ASN	3.1
1	D	557	PRO	3.1
2	C	483	ALA	3.1
1	B	102	ASN	3.1
2	C	532	ARG	3.0
1	B	100	ALA	3.0
1	F	326	MET	3.0
1	F	262	GLN	3.0
1	F	199	ASP	3.0
2	C	482	TRP	3.0
1	A	94	SER	2.9
1	A	377	PHE	2.9
2	C	451	GLN	2.9
1	E	94	SER	2.9
1	E	366	PRO	2.9
1	D	568	ASN	2.9
1	A	375	THR	2.8
1	F	279	VAL	2.8
2	C	131	TRP	2.8
2	C	450	LEU	2.8
2	C	442	HIS	2.8
2	C	284	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	283	ASP	2.8
1	F	282	TRP	2.8
1	F	123	HIS	2.7
2	C	438	ARG	2.7
1	D	526	GLU	2.7
2	C	461	GLY	2.7
2	C	125	GLN	2.7
2	C	445	ILE	2.7
2	C	529	SER	2.7
1	E	93	ARG	2.7
1	E	406	VAL	2.6
2	C	74	SER	2.6
2	C	395	PHE	2.6
1	D	365	HIS	2.6
1	F	255	VAL	2.6
2	C	564	LYS	2.6
1	A	405	ASN	2.6
1	D	537	ASN	2.6
1	F	280	PHE	2.6
3	L	8	PRO	2.6
3	X	9	ALA	2.6
1	F	206	ARG	2.6
1	F	142	ILE	2.5
1	E	409	GLY	2.5
1	F	111	LYS	2.5
1	B	200	ARG	2.5
1	F	291	ARG	2.5
1	E	291	ARG	2.5
2	C	471	TYR	2.5
1	B	365	HIS	2.4
1	B	213	ASP	2.4
3	X	6	THR	2.4
1	F	194	ARG	2.4
2	C	472	GLU	2.4
2	C	516	ASP	2.4
1	F	108	GLU	2.4
2	C	455	ASN	2.4
3	X	5	SER	2.4
1	D	516	ASP	2.4
1	B	291	ARG	2.4
1	E	411	ILE	2.4
1	A	392	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	127	GLN	2.3
2	C	566	THR	2.3
1	A	401	PRO	2.3
1	D	488	LYS	2.3
2	C	293	ARG	2.3
1	E	368	THR	2.3
1	E	128	ARG	2.2
1	F	107	VAL	2.2
1	F	288	GLU	2.2
1	E	383	ARG	2.2
3	L	5	SER	2.2
1	F	143	THR	2.2
1	F	125	GLN	2.2
1	F	320	GLU	2.2
2	C	456	CYS	2.2
1	B	179	ASN	2.2
2	C	521	LYS	2.2
1	F	263	TYR	2.1
2	C	569	LEU	2.1
1	F	275	ASP	2.1
1	E	327	MET	2.1
1	F	301	ILE	2.1
1	A	391	GLU	2.1
1	A	443	GLN	2.1
2	C	447	PHE	2.1
1	F	317	TYR	2.1
1	B	104	PHE	2.1
2	C	457	LEU	2.1
3	L	9	ALA	2.1
1	D	559	LEU	2.1
1	F	344	GLN	2.1
1	F	345	CYS	2.0
2	C	375	THR	2.0
1	D	367	TYR	2.0
1	E	395	PHE	2.0
2	C	105	ASN	2.0
1	D	531	LEU	2.0
2	C	264	VAL	2.0
1	A	376	VAL	2.0
1	D	285	MET	2.0
2	C	485	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	BBK	E	1571	15/15	0.30	4.50	67,86,120,144	0
5	BBK	D	1572	15/15	0.28	3.34	97,106,117,122	0
5	BBK	B	1572	15/15	0.23	2.65	66,81,110,110	0
5	BBK	A	1571	15/15	0.21	1.42	52,76,82,88	0
6	UDP	C	1571	25/25	0.19	-0.30	83,96,111,114	0
6	UDP	D	1571	25/25	0.19	-0.32	64,98,118,128	0
6	UDP	B	1573	25/25	0.17	-0.57	77,89,97,106	0
4	MN	D	1570	1/1	0.14	-0.60	58,58,58,58	0
6	UDP	A	1572	25/25	0.14	-0.90	54,74,89,97	0
6	UDP	E	1572	25/25	0.15	-1.06	69,78,89,97	0
4	MN	B	1571	1/1	0.16	-1.19	63,63,63,63	0
6	UDP	F	1364	25/25	0.17	-1.27	107,134,151,177	0
4	MN	F	1363	1/1	0.10	-1.51	93,93,93,93	0
4	MN	C	1570	1/1	0.14	-1.59	67,67,67,67	0
4	MN	E	1570	1/1	0.13	-1.84	46,46,46,46	0
4	MN	A	1570	1/1	0.09	-2.33	46,46,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.