



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:17 AM UTC

PDB ID : 3V83 / pdb_00003v83
Title : The 2.1 angstrom crystal structure of diferric human transferrin
Authors : Noinaj, N.; Steere, A.; Mason, A.B.; Buchanan, S.K.
Deposited on : 2011-12-22
Resolution : 2.10 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:

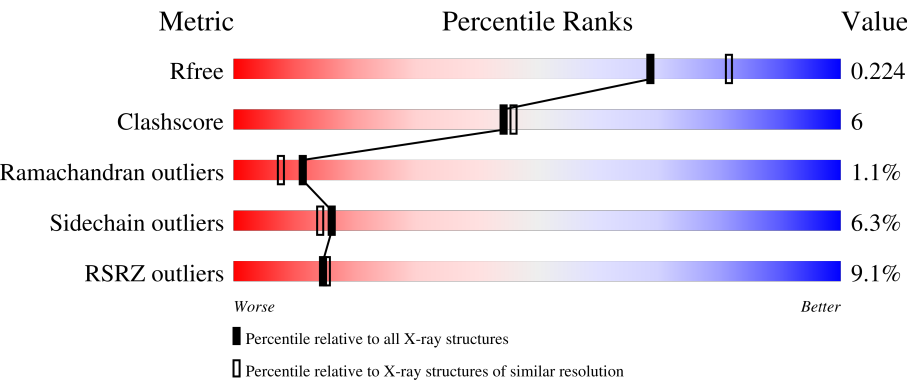
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	698	4% 81% 13% ..
1	B	698	4% 83% 12% ...
1	C	698	28% 77% 17% ..
1	D	698	5% 81% 14% ..
1	E	698	6% 81% 12% ..

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Mol	Chain	Length	Quality of chain
1	F	698	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BCT	C	702	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33928 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 Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	0	0
			5160	3247	892	974	47			
1	B	677	Total	C	N	O	S	0	0	0
			5179	3260	898	974	47			
1	C	674	Total	C	N	O	S	0	0	0
			5124	3221	888	968	47			
1	D	675	Total	C	N	O	S	0	0	0
			5193	3263	897	986	47			
1	E	674	Total	C	N	O	S	0	0	0
			5202	3267	898	990	47			
1	F	676	Total	C	N	O	S	0	0	0
			5191	3263	900	981	47			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	429	VAL	ILE	variant	UNP P02787
B	429	VAL	ILE	variant	UNP P02787
C	429	VAL	ILE	variant	UNP P02787
D	429	VAL	ILE	variant	UNP P02787
E	429	VAL	ILE	variant	UNP P02787
F	429	VAL	ILE	variant	UNP P02787

- Molecule 2 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

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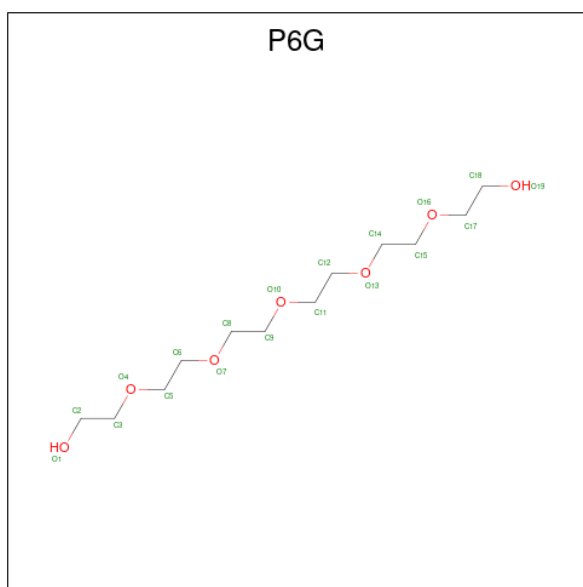
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 19	C 12	O 7	0	0
5	A	1	Total 19	C 12	O 7	0	0
5	A	1	Total 19	C 12	O 7	0	0
5	B	1	Total 19	C 12	O 7	0	0
5	B	1	Total 19	C 12	O 7	0	0
5	C	1	Total 19	C 12	O 7	0	0
5	C	1	Total 19	C 12	O 7	0	0
5	C	1	Total 19	C 12	O 7	0	0
5	D	1	Total 19	C 12	O 7	0	0
5	D	1	Total 19	C 12	O 7	0	0
5	E	1	Total 19	C 12	O 7	0	0
5	E	1	Total 19	C 12	O 7	0	0
5	F	1	Total 19	C 12	O 7	0	0
5	F	1	Total 19	C 12	O 7	0	0

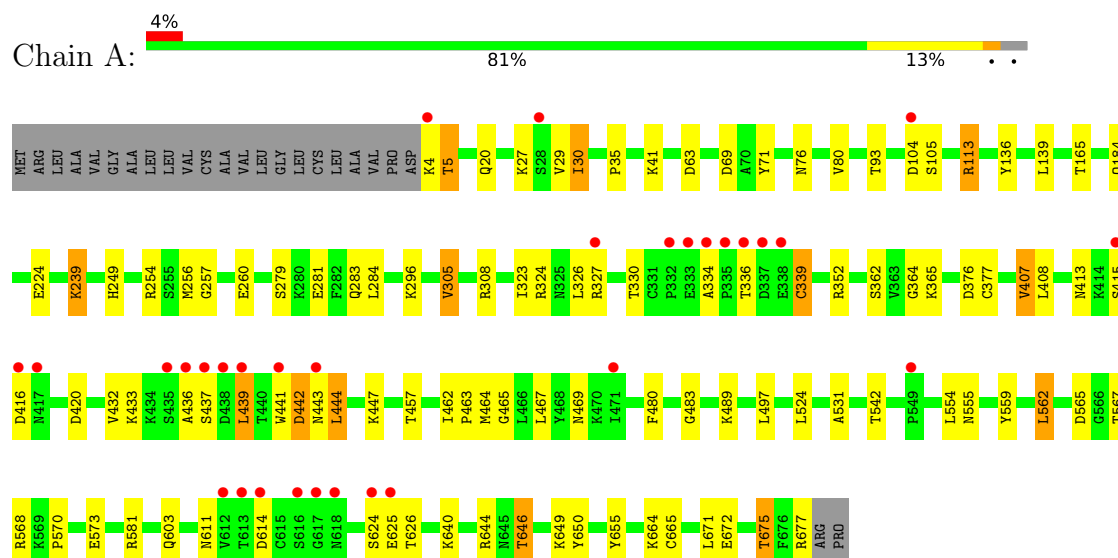
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	352	Total 352	O 352	0	0
6	B	454	Total 454	O 454	0	0
6	C	305	Total 305	O 305	0	0
6	D	398	Total 398	O 398	0	0
6	E	431	Total 431	O 431	0	0
6	F	393	Total 393	O 393	0	0

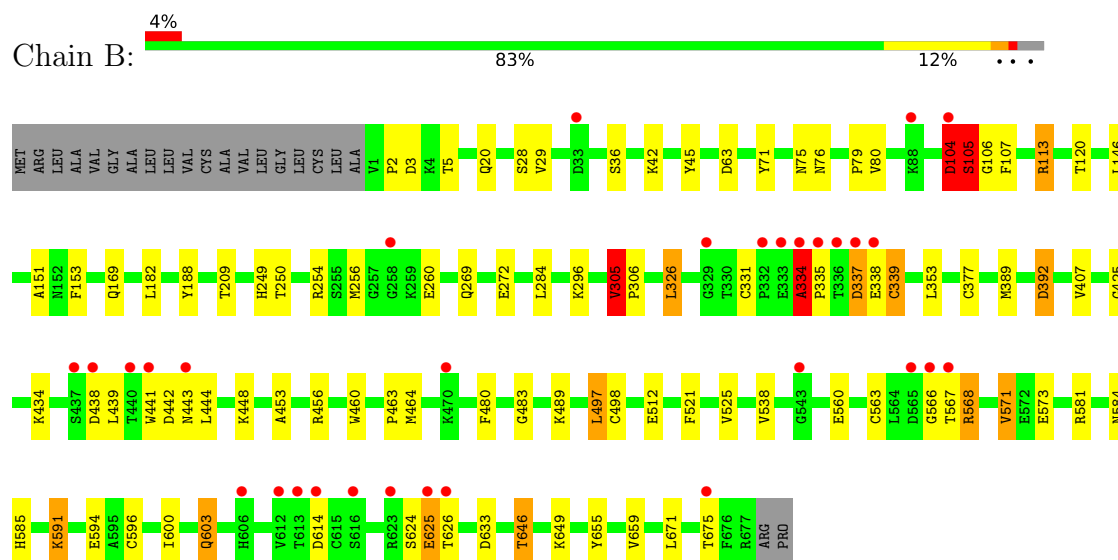
3 Residue-property plots

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

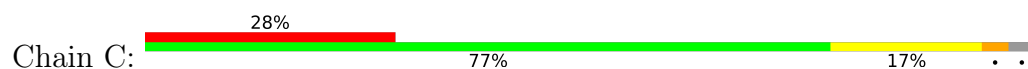
• Molecule 1: Serotransferrin

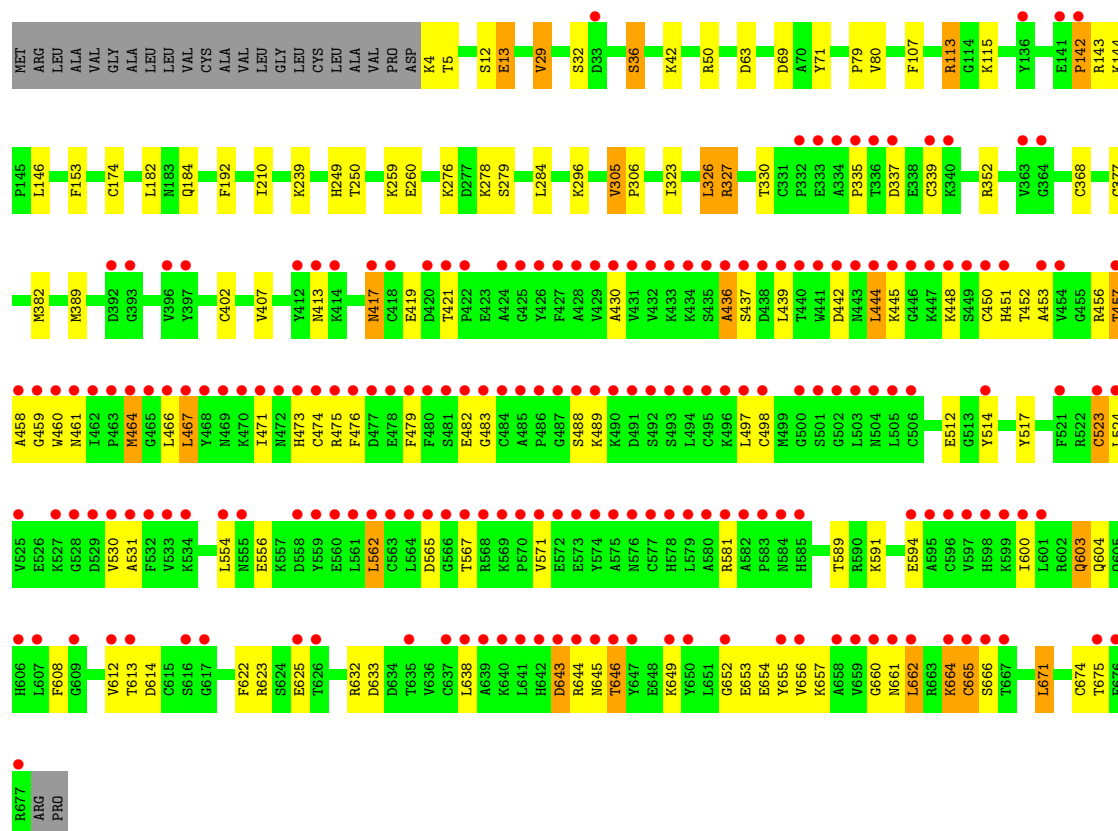


• Molecule 1: Serotransferrin

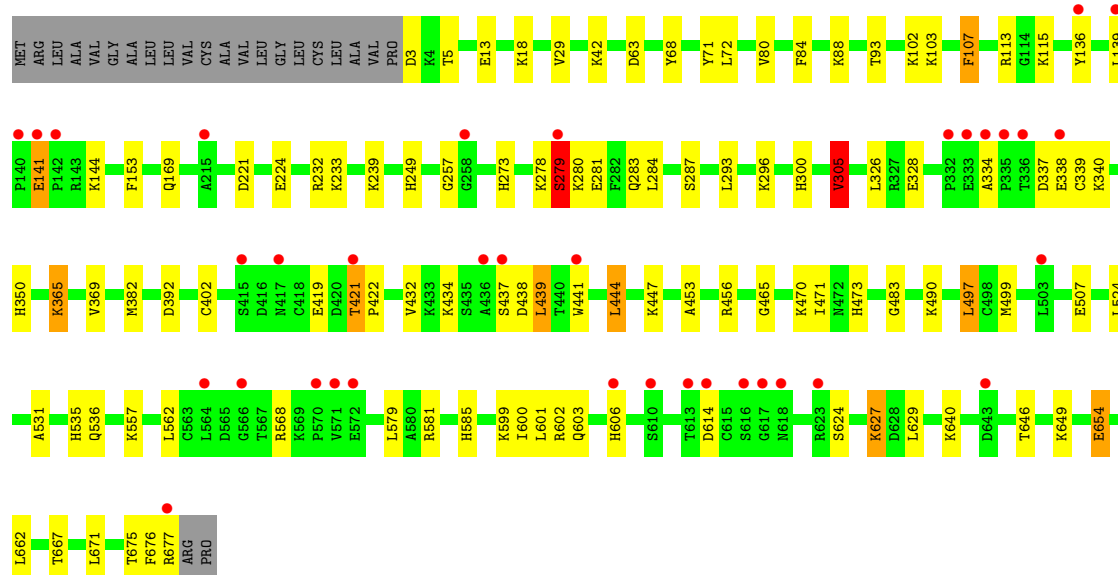
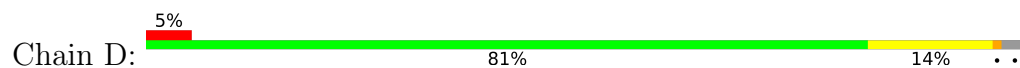


• Molecule 1: Serotransferrin

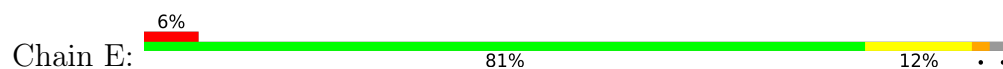


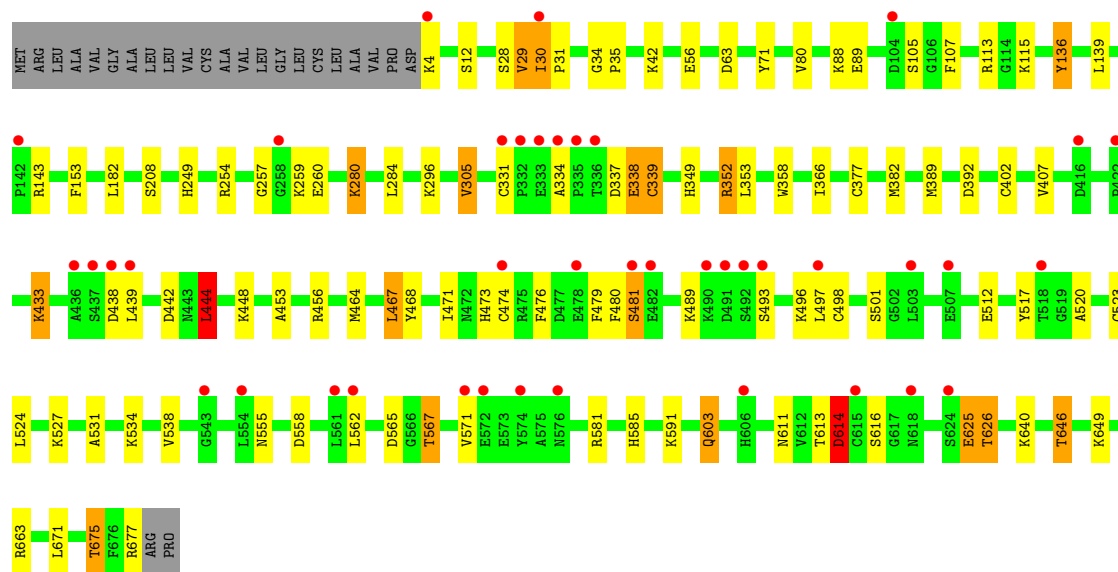


• Molecule 1: Serotransferrin

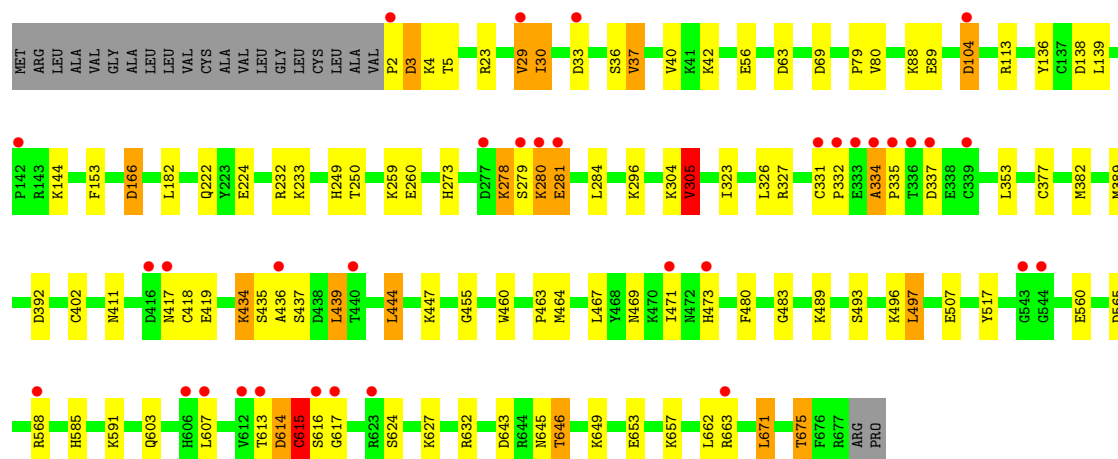
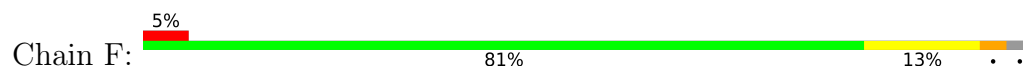


• Molecule 1: Serotransferrin





• Molecule 1: Serotransferrin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	254.53Å 173.00Å 150.15Å 90.00° 123.26° 90.00°	Depositor
Resolution (Å)	29.95 – 2.10 29.95 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.4 (29.95-2.10) 94.4 (29.95-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.180 , 0.230 0.182 , 0.224	Depositor DCC
R_{free} test set	15031 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33928	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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: SO4, BCT, FE, P6G

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/5278	0.82	2/7144 (0.0%)
1	B	0.52	0/5298	0.83	7/7169 (0.1%)
1	C	0.48	0/5240	0.83	4/7097 (0.1%)
1	D	0.52	0/5311	0.83	7/7184 (0.1%)
1	E	0.50	0/5320	0.83	7/7196 (0.1%)
1	F	0.51	0/5309	0.85	4/7183 (0.1%)
All	All	0.50	0/31756	0.83	31/42973 (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	2
1	E	0	2
All	All	0	4

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	13	GLU	N-CA-C	7.53	119.57	111.36
1	F	337	ASP	N-CA-C	-7.01	103.86	113.18
1	F	278	LYS	N-CA-C	-6.56	105.24	112.72
1	D	107	PHE	N-CA-C	6.25	118.37	110.24
1	B	305	VAL	N-CA-CB	5.86	116.50	110.23
1	E	331	CYS	CA-C-N	5.83	125.84	119.89
1	E	331	CYS	C-N-CA	5.83	125.84	119.89
1	C	13	GLU	N-CA-C	5.82	117.70	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	SER	N-CA-C	5.70	122.95	110.80
1	A	105	SER	N-CA-C	-5.68	106.69	113.97
1	D	279	SER	N-CA-C	5.58	122.68	110.80
1	E	614	ASP	N-CA-C	5.53	122.57	110.80
1	E	136	TYR	N-CA-C	5.43	117.20	111.28
1	E	34	GLY	CA-C-N	5.43	125.19	119.76
1	E	34	GLY	C-N-CA	5.43	125.19	119.76
1	F	281	GLU	N-CA-C	-5.38	105.94	112.88
1	C	662	LEU	N-CA-C	-5.37	104.51	111.71
1	E	444	LEU	N-CA-C	-5.33	106.73	113.18
1	B	334	ALA	CA-C-N	5.31	124.94	119.05
1	B	334	ALA	C-N-CA	5.31	124.94	119.05
1	C	368	CYS	N-CA-C	5.31	118.05	109.40
1	C	461	ASN	N-CA-C	5.19	116.63	111.07
1	F	305	VAL	N-CA-CB	5.19	115.79	110.23
1	D	438	ASP	N-CA-C	-5.16	106.74	112.57
1	D	305	VAL	CA-C-N	5.13	123.40	119.66
1	D	305	VAL	C-N-CA	5.13	123.40	119.66
1	B	209	THR	N-CA-C	5.11	116.53	111.07
1	D	305	VAL	N-CA-CB	5.10	115.68	110.23
1	A	664	LYS	N-CA-C	-5.01	102.86	110.28
1	B	331	CYS	CA-C-N	5.01	125.01	119.90
1	B	331	CYS	C-N-CA	5.01	125.01	119.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	278	LYS	Peptide
1	D	279	SER	Peptide
1	E	613	THR	Peptide
1	E	614	ASP	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5160	0	4928	57	0
1	B	5179	0	4949	56	0
1	C	5124	0	4868	86	0
1	D	5193	0	4970	57	0
1	E	5202	0	4992	52	0
1	F	5191	0	4969	64	0
2	A	8	0	1	0	0
2	B	8	0	0	0	0
2	C	8	0	1	3	0
2	D	8	0	1	0	0
2	E	8	0	1	0	0
2	F	8	0	1	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	25	0	0	1	0
4	B	45	0	0	1	0
4	C	35	0	0	0	0
4	D	45	0	0	1	0
4	E	45	0	0	0	0
4	F	25	0	0	0	0
5	A	57	0	78	4	0
5	B	38	0	52	6	0
5	C	57	0	78	4	0
5	D	38	0	52	6	0
5	E	38	0	52	4	0
5	F	38	0	52	6	0
6	A	352	0	0	7	0
6	B	454	0	0	8	0
6	C	305	0	0	11	0
6	D	398	0	0	11	0
6	E	431	0	0	8	0
6	F	393	0	0	5	0
All	All	33928	0	30045	367	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 6.

All (367) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:ALA:H	1:C:437:SER:HA	1.23	1.00
1:B:566:GLY:H	1:B:567:THR:HA	1.39	0.85
1:A:113:ARG:HD2	1:E:254:ARG:HD2	1.59	0.82
1:F:42:LYS:HZ2	5:F:711:P6G:H91	1.45	0.80
1:A:646:THR:HG22	1:A:649:LYS:H	1.48	0.79
1:E:646:THR:HG22	1:E:649:LYS:H	1.48	0.78
1:D:169:GLN:NE2	6:D:936:HOH:O	2.16	0.78
1:C:436:ALA:N	1:C:437:SER:HA	2.00	0.76
1:C:524:LEU:HB2	1:C:531:ALA:HB2	1.67	0.76
1:C:657:LYS:O	1:C:661:ASN:N	2.19	0.76
1:A:327:ARG:NH2	6:A:825:HOH:O	2.19	0.75
1:F:435:SER:H	1:F:436:ALA:HA	1.50	0.75
1:A:365:LYS:HZ2	5:A:712:P6G:H92	1.52	0.75
1:C:664:LYS:O	6:C:942:HOH:O	2.04	0.74
1:D:507:GLU:OE2	6:D:979:HOH:O	2.06	0.74
1:C:327:ARG:NH2	6:C:858:HOH:O	2.22	0.72
1:D:42:LYS:HZ3	5:D:714:P6G:H122	1.54	0.72
1:A:439:LEU:O	1:A:568:ARG:NH1	2.23	0.72
1:C:665:CYS:SG	6:C:1067:HOH:O	2.49	0.71
1:C:662:LEU:O	6:C:942:HOH:O	2.09	0.70
1:E:565:ASP:OD1	1:E:567:THR:OG1	2.10	0.70
1:F:483:GLY:HA2	1:F:497:LEU:HD22	1.74	0.69
1:E:208:SER:HB2	5:E:714:P6G:H112	1.74	0.69
1:B:20:GLN:NE2	6:B:1222:HOH:O	2.26	0.69
1:E:493:SER:HA	1:E:496:LYS:HD3	1.74	0.69
1:C:646:THR:HG22	1:C:649:LYS:H	1.57	0.68
1:C:603:GLN:OE1	1:C:604:GLN:NE2	2.24	0.68
1:C:69:ASP:OD1	1:C:327:ARG:NH1	2.26	0.67
1:D:239:LYS:NZ	6:D:1053:HOH:O	2.27	0.67
1:C:483:GLY:HA2	1:C:497:LEU:HD22	1.76	0.66
1:A:439:LEU:HD21	1:A:447:LYS:HG2	1.76	0.66
1:A:465:GLY:O	1:A:469:ASN:ND2	2.28	0.66
1:B:339:CYS:SG	6:B:1202:HOH:O	2.53	0.65
1:F:4:LYS:NZ	1:F:33:ASP:O	2.26	0.65
1:F:616:SER:HB2	1:F:617:GLY:HA2	1.77	0.65
1:F:671:LEU:O	1:F:675:THR:HB	1.95	0.65
1:B:254:ARG:HD2	1:F:113:ARG:HD2	1.78	0.65
1:D:350:HIS:ND1	6:D:991:HOH:O	2.29	0.65
1:F:493:SER:HA	1:F:496:LYS:HD2	1.79	0.64
1:B:646:THR:HG22	1:B:649:LYS:H	1.63	0.64
1:A:441:TRP:CD1	1:A:442:ASP:H	2.15	0.64
1:A:324:ARG:NH2	6:A:1126:HOH:O	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:646:THR:HG22	1:F:649:LYS:H	1.63	0.63
1:B:104:ASP:O	1:B:106:GLY:N	2.31	0.63
1:F:323:ILE:O	1:F:327:ARG:HG2	1.98	0.63
1:B:591:LYS:NZ	6:B:949:HOH:O	2.32	0.63
1:C:115:LYS:NZ	6:C:954:HOH:O	2.28	0.63
1:B:2:PRO:HD2	1:B:5:THR:OG1	1.99	0.63
1:F:434:LYS:HD2	1:F:560:GLU:HG3	1.79	0.63
1:E:56:GLU:OE1	5:E:715:P6G:O19	2.14	0.62
1:D:654:GLU:CD	1:D:654:GLU:H	2.07	0.62
1:A:254:ARG:HD2	1:C:113:ARG:HD2	1.82	0.62
1:C:452:THR:OG1	2:C:702:BCT:O3	2.08	0.61
1:C:5:THR:HG22	1:C:36:SER:HB2	1.83	0.61
1:C:79:PRO:HB3	1:C:250:THR:HG21	1.82	0.61
1:E:113:ARG:HD3	6:E:1031:HOH:O	1.99	0.61
1:F:42:LYS:NZ	5:F:711:P6G:H91	2.16	0.60
1:D:600:ILE:HD11	5:D:715:P6G:H122	1.83	0.60
1:F:5:THR:HG22	1:F:36:SER:HB2	1.82	0.60
1:C:63:ASP:HA	1:C:249:HIS:CD2	2.37	0.60
1:C:413:ASN:ND2	6:C:1006:HOH:O	2.34	0.60
1:A:323:ILE:O	1:A:327:ARG:HG2	2.02	0.60
1:C:664:LYS:O	1:C:666:SER:N	2.34	0.60
1:F:304:LYS:NZ	6:F:1103:HOH:O	2.34	0.60
1:D:249:HIS:CE1	1:D:296:LYS:HD2	2.37	0.59
1:F:643:ASP:O	1:F:645:ASN:ND2	2.36	0.59
1:E:105:SER:O	6:E:827:HOH:O	2.16	0.59
1:A:352:ARG:NH2	6:A:1076:HOH:O	2.34	0.59
1:B:566:GLY:N	1:B:567:THR:HA	2.06	0.58
1:C:646:THR:HB	1:C:649:LYS:HD2	1.84	0.58
1:A:524:LEU:HB2	1:A:531:ALA:HB2	1.85	0.58
1:F:40:VAL:HG13	5:F:711:P6G:H141	1.85	0.58
1:C:517:TYR:OH	1:C:632:ARG:NH1	2.36	0.58
1:F:278:LYS:O	1:F:280:LYS:HG2	2.03	0.58
1:F:507:GLU:OE2	6:F:865:HOH:O	2.17	0.57
1:A:483:GLY:HA2	1:A:497:LEU:HD22	1.85	0.57
1:E:42:LYS:HD2	5:E:715:P6G:H61	1.87	0.57
1:A:432:VAL:HG11	1:A:439:LEU:HD12	1.87	0.57
1:B:42:LYS:HZ3	5:B:715:P6G:C14	2.18	0.57
1:D:441:TRP:HZ2	1:D:579:LEU:HD21	1.70	0.57
1:D:80:VAL:C	1:D:305:VAL:HG13	2.29	0.57
1:B:596:CYS:HB2	6:B:1202:HOH:O	2.05	0.56
1:C:456:ARG:NE	2:C:702:BCT:O1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:514:TYR:CD2	1:C:523:CYS:HB2	2.40	0.56
1:F:417:ASN:O	1:F:419:GLU:N	2.37	0.56
1:A:441:TRP:HE3	1:A:562:LEU:HD13	1.69	0.56
1:D:654:GLU:HG2	6:D:849:HOH:O	2.05	0.56
1:C:671:LEU:O	1:C:675:THR:HG22	2.06	0.56
5:D:714:P6G:O19	6:D:897:HOH:O	2.18	0.55
5:A:712:P6G:O1	6:A:1097:HOH:O	2.16	0.54
1:F:79:PRO:HB3	1:F:250:THR:HG21	1.88	0.54
1:C:50:ARG:HD3	5:C:713:P6G:H182	1.90	0.54
1:F:392:ASP:HA	1:F:585:HIS:CD2	2.43	0.54
1:C:464:MET:HG3	1:C:476:PHE:CG	2.43	0.54
1:E:80:VAL:C	1:E:305:VAL:HG13	2.33	0.54
1:C:660:GLY:C	1:C:662:LEU:H	2.15	0.54
1:E:677:ARG:NH2	6:E:1197:HOH:O	2.40	0.54
1:B:453:ALA:HB3	1:B:456:ARG:HD3	1.91	0.53
1:C:107:PHE:CD1	1:C:115:LYS:HE2	2.43	0.53
1:B:483:GLY:HA2	1:B:497:LEU:HD22	1.90	0.53
1:C:323:ILE:O	1:C:327:ARG:HG2	2.09	0.53
1:D:453:ALA:HB3	1:D:456:ARG:HD3	1.90	0.53
1:F:436:ALA:HB3	1:F:437:SER:HA	1.90	0.53
1:A:41:LYS:O	5:A:710:P6G:H32	2.08	0.53
1:A:570:PRO:HG2	1:A:573:GLU:HG3	1.90	0.53
1:D:646:THR:HG23	1:D:649:LYS:H	1.73	0.53
1:F:23:ARG:HA	1:F:37:VAL:HG13	1.91	0.53
1:B:42:LYS:NZ	5:B:715:P6G:H172	2.23	0.52
1:B:80:VAL:C	1:B:305:VAL:HG13	2.33	0.52
1:D:93:THR:H	1:D:677:ARG:HH21	1.55	0.52
1:B:42:LYS:HZ3	5:B:715:P6G:H142	1.74	0.52
1:B:392:ASP:HA	1:B:585:HIS:CD2	2.44	0.52
1:C:565:ASP:HB3	1:F:273:HIS:CD2	2.44	0.52
1:A:41:LYS:NZ	6:A:1091:HOH:O	2.43	0.52
1:B:76:ASN:ND2	1:B:256:MET:HE2	2.25	0.52
1:F:138:ASP:OD1	6:F:897:HOH:O	2.19	0.52
1:C:467:LEU:HD11	1:C:479:PHE:CE1	2.44	0.52
1:A:136:TYR:HA	1:A:139:LEU:HG	1.91	0.51
1:C:142:PRO:O	1:C:143:ARG:HB2	2.10	0.51
1:C:451:HIS:ND1	1:C:459:GLY:O	2.33	0.51
1:D:42:LYS:HD2	5:D:714:P6G:H92	1.91	0.51
1:D:136:TYR:HA	1:D:139:LEU:HG	1.90	0.51
1:F:113:ARG:HG3	1:F:153:PHE:CD1	2.45	0.51
1:D:535:HIS:CD2	1:D:536:GLN:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:483:GLY:HA2	1:D:497:LEU:HD22	1.92	0.51
1:A:80:VAL:C	1:A:305:VAL:HG13	2.36	0.51
1:A:407:VAL:HG22	1:A:408:LEU:HG	1.91	0.51
1:C:608:PHE:HA	1:C:612:VAL:HG21	1.93	0.51
1:E:433:LYS:HG2	6:E:1039:HOH:O	2.11	0.51
1:F:613:THR:O	1:F:614:ASP:HB2	2.10	0.51
1:C:279:SER:HB2	1:F:565:ASP:HB3	1.92	0.50
1:C:623:ARG:NH2	1:C:633:ASP:O	2.43	0.50
1:F:42:LYS:HD2	5:F:711:P6G:H52	1.93	0.50
1:F:80:VAL:C	1:F:305:VAL:HG13	2.36	0.50
1:E:136:TYR:HA	1:E:139:LEU:HG	1.93	0.50
1:C:664:LYS:C	1:C:666:SER:H	2.20	0.50
1:E:464:MET:HE3	1:E:476:PHE:CG	2.46	0.50
1:F:63:ASP:HA	1:F:249:HIS:CD2	2.46	0.50
1:D:365:LYS:HZ3	5:D:715:P6G:H151	1.77	0.50
1:E:30:ILE:HD13	1:E:35:PRO:HD2	1.94	0.50
1:B:655:TYR:O	1:B:659:VAL:HG23	2.12	0.50
1:C:417:ASN:O	1:C:419:GLU:N	2.43	0.50
1:C:483:GLY:C	1:C:497:LEU:HB2	2.37	0.50
1:D:337:ASP:OD1	6:D:1068:HOH:O	2.19	0.50
1:C:42:LYS:HZ1	5:C:713:P6G:H21	1.77	0.50
1:C:565:ASP:HB2	1:F:29:VAL:HG22	1.93	0.50
1:E:453:ALA:HB3	1:E:456:ARG:HD3	1.94	0.49
1:F:517:TYR:HE2	1:F:632:ARG:HD2	1.77	0.49
1:E:442:ASP:OD1	1:E:442:ASP:N	2.44	0.49
1:C:498:CYS:HA	1:C:514:TYR:HD2	1.77	0.49
1:F:653:GLU:N	1:F:653:GLU:OE1	2.44	0.49
1:C:467:LEU:HD21	1:C:479:PHE:CG	2.47	0.49
1:C:436:ALA:H	1:C:437:SER:CA	2.10	0.49
1:A:93:THR:OG1	1:A:677:ARG:HG2	2.13	0.49
1:B:249:HIS:CE1	1:B:296:LYS:HD2	2.47	0.49
1:A:63:ASP:HA	1:A:249:HIS:CD2	2.48	0.49
1:D:103:LYS:HE2	1:D:221:ASP:O	2.13	0.49
1:D:113:ARG:HG3	1:D:153:PHE:CD1	2.48	0.49
1:A:69:ASP:OD1	1:A:327:ARG:NH1	2.46	0.48
1:A:364:GLY:N	6:A:887:HOH:O	2.44	0.48
1:C:80:VAL:C	1:C:305:VAL:HG13	2.38	0.48
1:B:377:CYS:HB3	1:B:389:MET:SD	2.53	0.48
1:C:29:VAL:HG21	1:F:565:ASP:O	2.13	0.48
1:A:362:SER:HB2	1:A:365:LYS:HB2	1.95	0.48
5:C:712:P6G:O19	5:C:712:P6G:O1	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:667:THR:HG22	6:D:1044:HOH:O	2.14	0.48
1:E:113:ARG:HG3	1:E:153:PHE:CD1	2.48	0.48
1:F:435:SER:N	1:F:436:ALA:HA	2.23	0.48
1:A:441:TRP:O	1:A:443:ASN:N	2.47	0.48
1:B:151:ALA:HB1	1:B:169:GLN:HB2	1.96	0.48
1:B:464:MET:HE1	1:B:480:PHE:HE2	1.79	0.48
1:B:594:GLU:OE2	6:B:1174:HOH:O	2.20	0.47
1:C:278:LYS:NZ	6:C:1088:HOH:O	2.46	0.47
1:D:432:VAL:HG11	1:D:439:LEU:HD12	1.96	0.47
1:D:382:MET:SD	1:D:402:CYS:HB3	2.54	0.47
1:D:562:LEU:HD23	1:D:568:ARG:HG2	1.96	0.47
1:D:627:LYS:HB3	1:D:629:LEU:HG	1.96	0.47
1:F:166:ASP:OD1	1:F:166:ASP:N	2.47	0.47
1:E:392:ASP:HA	1:E:585:HIS:CD2	2.49	0.47
1:C:474:CYS:HA	6:C:1067:HOH:O	2.14	0.47
1:C:652:GLY:O	1:C:656:VAL:HG23	2.13	0.47
1:F:411:ASN:ND2	1:F:418:CYS:O	2.48	0.47
1:A:76:ASN:ND2	1:A:256:MET:HE2	2.29	0.47
1:B:538:VAL:HG11	1:B:571:VAL:HG21	1.95	0.47
1:B:563:CYS:HB2	1:B:566:GLY:HA3	1.95	0.47
1:E:444:LEU:HD12	1:E:444:LEU:HA	1.78	0.47
1:E:517:TYR:CZ	1:E:534:LYS:HD3	2.49	0.47
1:A:672:GLU:HA	1:A:675:THR:HG22	1.97	0.47
1:A:436:ALA:N	1:A:437:SER:HA	2.30	0.47
1:A:27:LYS:NZ	6:A:942:HOH:O	2.47	0.47
1:B:42:LYS:NZ	5:B:715:P6G:H112	2.30	0.47
1:D:107:PHE:CD1	1:D:115:LYS:HE3	2.49	0.47
1:D:444:LEU:O	1:D:447:LYS:HB2	2.15	0.47
1:D:599:LYS:HE3	5:D:715:P6G:H181	1.97	0.47
1:B:334:ALA:HA	1:B:335:PRO:HD3	1.81	0.47
1:C:645:ASN:ND2	6:C:1052:HOH:O	2.44	0.46
1:D:18:LYS:HD3	1:D:293:LEU:HB2	1.97	0.46
1:D:646:THR:HG22	1:D:649:LYS:HD3	1.97	0.46
1:F:56:GLU:OE1	5:F:711:P6G:O19	2.22	0.46
1:F:435:SER:H	1:F:436:ALA:CA	2.23	0.46
1:C:613:THR:HA	1:C:614:ASP:HA	1.58	0.46
1:E:377:CYS:HB3	1:E:389:MET:SD	2.55	0.46
1:C:450:CYS:HB2	1:C:531:ALA:HA	1.97	0.46
1:C:603:GLN:NE2	6:C:1100:HOH:O	2.49	0.46
1:E:249:HIS:CE1	1:E:296:LYS:HD2	2.51	0.46
1:B:120:THR:HG22	1:B:188:TYR:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:ASP:HA	1:D:585:HIS:CD2	2.51	0.46
1:B:3:ASP:OD1	1:B:3:ASP:N	2.49	0.46
1:D:419:GLU:OE1	1:D:602:ARG:NH2	2.48	0.46
1:E:498:CYS:HB3	1:E:512:GLU:OE1	2.15	0.46
1:E:524:LEU:HB2	1:E:531:ALA:HB2	1.98	0.46
5:E:715:P6G:H91	5:E:715:P6G:H121	1.40	0.46
1:A:542:THR:HB	1:A:555:ASN:HA	1.98	0.46
1:C:377:CYS:HB3	1:C:389:MET:SD	2.55	0.46
1:D:524:LEU:HB2	1:D:531:ALA:HB2	1.96	0.46
1:A:644:ARG:HB3	1:A:650:TYR:HA	1.98	0.46
1:B:105:SER:HB2	1:B:107:PHE:CE1	2.50	0.46
1:D:63:ASP:HA	1:D:249:HIS:CD2	2.51	0.46
1:A:433:LYS:HE3	1:A:524:LEU:O	2.16	0.46
1:C:600:ILE:O	1:C:603:GLN:HG3	2.16	0.46
1:B:63:ASP:HA	1:B:249:HIS:CD2	2.51	0.45
1:F:382:MET:SD	1:F:402:CYS:HB3	2.55	0.45
1:B:448:LYS:HD2	1:B:497:LEU:HD21	1.98	0.45
1:B:460:TRP:C	1:B:463:PRO:HD2	2.41	0.45
1:F:2:PRO:O	1:F:3:ASP:HB2	2.16	0.45
1:F:224:GLU:OE2	1:F:232:ARG:HD3	2.17	0.45
1:A:420:ASP:OD1	1:A:640:LYS:NZ	2.45	0.45
1:B:42:LYS:HZ1	5:B:715:P6G:H172	1.82	0.45
1:A:308:ARG:HH11	1:A:376:ASP:HA	1.80	0.45
1:B:600:ILE:O	1:B:603:GLN:HG3	2.17	0.45
1:C:453:ALA:HB3	1:C:456:ARG:HD3	1.98	0.45
1:C:623:ARG:NH1	1:C:633:ASP:HB3	2.32	0.45
1:C:458:ALA:N	2:C:702:BCT:O2	2.50	0.45
1:F:249:HIS:CE1	1:F:296:LYS:HD2	2.52	0.45
1:C:335:PRO:C	1:C:337:ASP:H	2.25	0.45
1:D:671:LEU:O	1:D:675:THR:HG22	2.17	0.45
1:A:462:ILE:HB	1:A:463:PRO:HD3	1.99	0.45
1:F:280:LYS:HB3	1:F:281:GLU:H	1.56	0.45
1:F:460:TRP:C	1:F:463:PRO:HD2	2.42	0.45
1:B:438:ASP:O	1:B:443:ASN:ND2	2.48	0.45
1:F:136:TYR:HA	1:F:139:LEU:HG	1.99	0.45
1:A:437:SER:HB3	1:F:104:ASP:OD1	2.18	0.44
1:B:42:LYS:HZ3	5:B:715:P6G:H141	1.82	0.44
1:C:113:ARG:HG3	1:C:153:PHE:CD1	2.52	0.44
1:E:603:GLN:HE21	1:E:603:GLN:HB2	1.59	0.44
1:E:677:ARG:HD2	1:E:677:ARG:N	2.31	0.44
1:B:269:GLN:NE2	6:B:983:HOH:O	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:353:LEU:HA	1:F:353:LEU:HD23	1.74	0.44
1:E:107:PHE:CD1	1:E:115:LYS:HE2	2.52	0.44
1:F:69:ASP:OD1	1:F:327:ARG:NH1	2.47	0.44
1:D:84:PHE:HZ	1:D:88:LYS:HE3	1.82	0.44
1:D:224:GLU:HB2	1:D:233:LYS:O	2.18	0.44
1:A:640:LYS:HB3	4:A:705:SO4:O3	2.18	0.44
1:B:521:PHE:O	1:B:525:VAL:HG23	2.18	0.44
1:B:337:ASP:HA	1:B:338:GLU:HA	1.65	0.44
1:C:457:THR:HG23	1:C:655:TYR:CE1	2.52	0.44
1:F:334:ALA:HA	1:F:335:PRO:HD2	1.87	0.44
1:A:336:THR:HB	1:E:349:HIS:HB2	2.00	0.44
1:C:305:VAL:HA	1:C:306:PRO:HD3	1.90	0.44
1:A:4:LYS:HG3	1:A:5:THR:H	1.83	0.43
1:C:382:MET:SD	1:C:402:CYS:HB3	2.58	0.43
1:E:468:TYR:HB2	1:E:476:PHE:HZ	1.83	0.43
1:C:644:ARG:HA	1:C:649:LYS:HB3	2.00	0.43
1:F:233:LYS:NZ	6:F:957:HOH:O	2.34	0.43
1:F:455:GLY:H	1:F:460:TRP:CG	2.36	0.43
1:A:441:TRP:H	1:A:562:LEU:HD11	1.83	0.43
1:B:434:LYS:HG3	1:B:560:GLU:HG3	2.00	0.43
1:E:334:ALA:HB3	1:E:337:ASP:OD1	2.18	0.43
1:E:353:LEU:HD23	1:E:353:LEU:HA	1.81	0.43
1:D:471:ILE:HD12	1:D:473:HIS:CE1	2.53	0.43
1:E:143:ARG:HB3	6:E:1200:HOH:O	2.17	0.43
1:C:460:TRP:O	1:C:464:MET:HB2	2.19	0.43
1:E:448:LYS:HD2	1:E:497:LEU:HD21	2.00	0.43
1:E:280:LYS:H	1:E:280:LYS:CD	2.31	0.43
1:A:464:MET:HE1	1:A:480:PHE:HE2	1.84	0.43
1:C:249:HIS:CE1	1:C:296:LYS:HD2	2.54	0.43
1:E:464:MET:HE1	1:E:480:PHE:HE2	1.84	0.43
1:E:527:LYS:HE2	6:E:1170:HOH:O	2.19	0.43
1:A:444:LEU:O	1:A:447:LYS:HB2	2.19	0.42
1:C:498:CYS:HA	1:C:514:TYR:CD2	2.54	0.42
1:F:278:LYS:O	1:F:280:LYS:N	2.52	0.42
1:F:444:LEU:HD12	1:F:444:LEU:HA	1.86	0.42
1:A:439:LEU:HD22	1:A:439:LEU:HA	1.82	0.42
1:B:105:SER:HB2	1:B:107:PHE:HE1	1.84	0.42
1:C:430:ALA:HB3	1:C:562:LEU:HB2	2.00	0.42
1:C:442:ASP:C	1:C:444:LEU:H	2.27	0.42
1:D:601:LEU:HD23	1:D:601:LEU:HA	1.90	0.42
1:C:471:ILE:HD12	1:C:473:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:467:LEU:HD21	1:E:479:PHE:CE1	2.55	0.42
1:A:249:HIS:CE1	1:A:296:LYS:HD2	2.55	0.42
1:D:419:GLU:OE2	1:D:606:HIS:NE2	2.53	0.42
1:F:464:MET:HE1	1:F:480:PHE:HE2	1.84	0.42
1:A:554:LEU:HD22	1:A:559:TYR:OH	2.19	0.42
1:D:224:GLU:OE2	1:D:232:ARG:HD3	2.20	0.42
1:D:434:LYS:HD3	1:D:557:LYS:O	2.20	0.42
1:A:441:TRP:CG	1:A:442:ASP:H	2.38	0.42
1:A:565:ASP:OD1	1:A:567:THR:OG1	2.36	0.42
1:E:382:MET:SD	1:E:402:CYS:HB3	2.60	0.42
1:A:625:GLU:HB2	1:A:626:THR:H	1.65	0.42
1:C:643:ASP:O	1:C:649:LYS:HD3	2.20	0.42
1:D:340:LYS:NZ	6:D:1143:HOH:O	2.52	0.42
1:E:63:ASP:HA	1:E:249:HIS:CD2	2.54	0.42
1:E:538:VAL:HB	1:E:571:VAL:HG11	2.02	0.42
1:A:457:THR:HG23	1:A:655:TYR:CE1	2.54	0.42
1:B:567:THR:C	1:B:568:ARG:HG2	2.44	0.42
1:C:498:CYS:HB3	1:C:512:GLU:CD	2.44	0.42
1:E:349:HIS:HA	1:E:352:ARG:HB3	2.02	0.42
1:F:377:CYS:HB3	1:F:389:MET:SD	2.59	0.42
1:B:75:ASN:ND2	6:B:1047:HOH:O	2.43	0.41
1:B:460:TRP:O	1:B:463:PRO:HD2	2.20	0.41
1:D:279:SER:CB	1:D:283:GLN:HG3	2.50	0.41
1:B:625:GLU:HA	1:B:626:THR:HA	1.67	0.41
1:D:141:GLU:HA	6:D:1079:HOH:O	2.19	0.41
1:E:625:GLU:HA	1:E:626:THR:HA	1.70	0.41
1:D:18:LYS:HD2	1:D:287:SER:HB2	2.01	0.41
1:D:279:SER:CB	1:D:280:LYS:HA	2.50	0.41
1:D:421:THR:HA	1:D:422:PRO:HD2	1.89	0.41
1:D:465:GLY:HA2	1:D:662:LEU:HD13	2.02	0.41
1:E:471:ILE:HD12	1:E:473:HIS:CE1	2.55	0.41
1:E:520:ALA:O	1:E:523:CYS:HB3	2.21	0.41
1:C:662:LEU:HG	6:C:942:HOH:O	2.20	0.41
1:B:260:GLU:HB2	4:B:707:SO4:O3	2.21	0.41
1:D:300:HIS:ND1	4:D:710:SO4:O2	2.42	0.41
1:E:517:TYR:CE2	1:E:534:LYS:HD3	2.56	0.41
1:B:305:VAL:HA	1:B:306:PRO:HD3	1.92	0.41
1:C:622:PHE:HZ	1:C:638:LEU:HG	1.84	0.41
1:E:29:VAL:HG12	1:E:30:ILE:HG23	2.03	0.41
1:E:358:TRP:CE2	1:E:366:ILE:HG13	2.55	0.41
1:F:331:CYS:HA	1:F:332:PRO:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:614:ASP:HB3	1:F:615:CYS:H	1.67	0.41
1:B:425:GLY:HA2	1:B:584:ASN:OD1	2.21	0.41
1:E:555:ASN:HB2	1:E:558:ASP:OD2	2.21	0.41
1:F:113:ARG:HG2	1:F:153:PHE:O	2.21	0.41
1:F:439:LEU:HD21	1:F:447:LYS:HG2	2.03	0.41
1:A:483:GLY:C	1:A:497:LEU:HB2	2.46	0.41
1:B:79:PRO:HB3	1:B:250:THR:HG21	2.02	0.41
1:D:273:HIS:HD2	6:D:1160:HOH:O	2.04	0.41
1:A:30:ILE:HD13	1:A:35:PRO:HD2	2.02	0.41
1:B:45:TYR:OH	6:B:910:HOH:O	2.22	0.41
1:C:4:LYS:HA	1:C:4:LYS:HD2	1.85	0.41
1:C:402:CYS:HA	1:C:674:CYS:HB3	2.03	0.41
1:C:654:GLU:OE1	1:F:88:LYS:NZ	2.54	0.41
1:E:675:THR:HG21	6:E:1132:HOH:O	2.21	0.41
1:F:444:LEU:O	1:F:447:LYS:HB2	2.21	0.41
1:A:239:LYS:HE2	1:A:239:LYS:HB2	1.92	0.41
1:B:113:ARG:HG3	1:B:153:PHE:CE1	2.56	0.41
1:B:624:SER:OG	1:B:633:ASP:OD1	2.33	0.41
1:C:42:LYS:NZ	5:C:713:P6G:H91	2.35	0.41
1:C:192:PHE:CE1	1:C:210:ILE:HG13	2.55	0.41
1:C:326:LEU:HD23	1:C:326:LEU:HA	1.88	0.41
1:E:12:SER:HA	6:E:938:HOH:O	2.21	0.41
1:B:146:LEU:HD22	1:B:326:LEU:HD22	2.02	0.40
1:D:471:ILE:HD12	1:D:473:HIS:NE2	2.36	0.40
1:E:30:ILE:HD12	1:E:31:PRO:O	2.20	0.40
1:A:365:LYS:HZ2	5:A:712:P6G:C9	2.29	0.40
1:A:441:TRP:N	1:A:562:LEU:HD21	2.37	0.40
1:D:676:PHE:O	1:D:677:ARG:HB2	2.21	0.40
1:C:174:CYS:O	1:C:174:CYS:SG	2.79	0.40
1:C:448:LYS:O	1:C:530:VAL:HG12	2.21	0.40
1:D:68:TYR:CE2	1:D:72:LEU:HD11	2.56	0.40
1:B:498:CYS:HB3	1:B:512:GLU:OE1	2.21	0.40
1:C:146:LEU:HD22	1:C:326:LEU:HD22	2.03	0.40
1:C:466:LEU:HD23	1:C:466:LEU:HA	1.90	0.40
1:D:470:LYS:HE2	1:D:470:LYS:HB3	1.88	0.40
5:F:711:P6G:H81	6:F:890:HOH:O	2.22	0.40
1:C:589:THR:HG21	1:C:594:GLU:HA	2.03	0.40
1:F:29:VAL:HG12	1:F:30:ILE:HG22	2.03	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	672/698 (96%)	621 (92%)	42 (6%)	9 (1%)	9	6
1	B	675/698 (97%)	630 (93%)	39 (6%)	6 (1%)	14	10
1	C	672/698 (96%)	617 (92%)	46 (7%)	9 (1%)	9	6
1	D	673/698 (96%)	630 (94%)	37 (6%)	6 (1%)	14	10
1	E	672/698 (96%)	632 (94%)	35 (5%)	5 (1%)	18	15
1	F	674/698 (97%)	623 (92%)	43 (6%)	8 (1%)	10	7
All	All	4038/4188 (96%)	3753 (93%)	242 (6%)	43 (1%)	11	8

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	416	ASP
1	A	442	ASP
1	A	614	ASP
1	B	104	ASP
1	B	105	SER
1	E	614	ASP
1	F	279	SER
1	F	614	ASP
1	B	442	ASP
1	C	439	LEU
1	C	445	LYS
1	C	625	GLU
1	D	339	CYS
1	D	437	SER
1	E	338	GLU
1	E	481	SER
1	F	3	ASP
1	A	334	ALA
1	A	415	SER
1	A	665	CYS

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Mol	Chain	Res	Type
1	C	457	THR
1	C	665	CYS
1	F	439	LEU
1	F	615	CYS
1	F	624	SER
1	A	624	SER
1	B	334	ALA
1	C	436	ALA
1	D	334	ALA
1	D	624	SER
1	F	280	LYS
1	A	257	GLY
1	A	339	CYS
1	B	625	GLU
1	C	417	ASN
1	D	614	ASP
1	E	339	CYS
1	B	614	ASP
1	C	664	LYS
1	D	257	GLY
1	F	334	ALA
1	E	257	GLY
1	C	142	PRO

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	547/585 (94%)	513 (94%)	34 (6%)	16	14
1	B	547/585 (94%)	517 (94%)	30 (6%)	19	18
1	C	539/585 (92%)	496 (92%)	43 (8%)	11	8
1	D	555/585 (95%)	529 (95%)	26 (5%)	23	24
1	E	560/585 (96%)	520 (93%)	40 (7%)	13	11
1	F	553/585 (94%)	519 (94%)	34 (6%)	17	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3301/3510 (94%)	3094 (94%)	207 (6%)	16	14

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	20	GLN
1	A	29	VAL
1	A	30	ILE
1	A	71	TYR
1	A	104	ASP
1	A	113	ARG
1	A	165	THR
1	A	184	GLN
1	A	224	GLU
1	A	239	LYS
1	A	260	GLU
1	A	279	SER
1	A	281	GLU
1	A	283	GLN
1	A	284	LEU
1	A	305	VAL
1	A	326	LEU
1	A	330	THR
1	A	339	CYS
1	A	377	CYS
1	A	407	VAL
1	A	413	ASN
1	A	439	LEU
1	A	444	LEU
1	A	467	LEU
1	A	489	LYS
1	A	562	LEU
1	A	581	ARG
1	A	603	GLN
1	A	611	ASN
1	A	646	THR
1	A	671	LEU
1	A	675	THR
1	B	28	SER
1	B	29	VAL
1	B	36	SER

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Mol	Chain	Res	Type
1	B	71	TYR
1	B	104	ASP
1	B	113	ARG
1	B	182	LEU
1	B	272	GLU
1	B	284	LEU
1	B	305	VAL
1	B	326	LEU
1	B	337	ASP
1	B	339	CYS
1	B	353	LEU
1	B	392	ASP
1	B	407	VAL
1	B	439	LEU
1	B	441	TRP
1	B	444	LEU
1	B	489	LYS
1	B	497	LEU
1	B	568	ARG
1	B	571	VAL
1	B	573	GLU
1	B	581	ARG
1	B	591	LYS
1	B	603	GLN
1	B	646	THR
1	B	671	LEU
1	B	675	THR
1	C	12	SER
1	C	13	GLU
1	C	29	VAL
1	C	32	SER
1	C	36	SER
1	C	71	TYR
1	C	113	ARG
1	C	144	LYS
1	C	182	LEU
1	C	184	GLN
1	C	239	LYS
1	C	259	LYS
1	C	260	GLU
1	C	276	LYS
1	C	284	LEU

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Mol	Chain	Res	Type
1	C	305	VAL
1	C	326	LEU
1	C	327	ARG
1	C	330	THR
1	C	339	CYS
1	C	352	ARG
1	C	407	VAL
1	C	421	THR
1	C	444	LEU
1	C	464	MET
1	C	467	LEU
1	C	475	ARG
1	C	482	GLU
1	C	488	SER
1	C	489	LYS
1	C	523	CYS
1	C	554	LEU
1	C	556	GLU
1	C	562	LEU
1	C	567	THR
1	C	571	VAL
1	C	581	ARG
1	C	591	LYS
1	C	603	GLN
1	C	643	ASP
1	C	646	THR
1	C	653	GLU
1	C	671	LEU
1	D	3	ASP
1	D	5	THR
1	D	29	VAL
1	D	71	TYR
1	D	102	LYS
1	D	141	GLU
1	D	144	LYS
1	D	281	GLU
1	D	284	LEU
1	D	305	VAL
1	D	326	LEU
1	D	328	GLU
1	D	338	GLU
1	D	365	LYS

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Mol	Chain	Res	Type
1	D	369	VAL
1	D	421	THR
1	D	439	LEU
1	D	444	LEU
1	D	490	LYS
1	D	497	LEU
1	D	499	MET
1	D	581	ARG
1	D	603	GLN
1	D	627	LYS
1	D	640	LYS
1	D	654	GLU
1	E	4	LYS
1	E	28	SER
1	E	29	VAL
1	E	30	ILE
1	E	71	TYR
1	E	88	LYS
1	E	89	GLU
1	E	182	LEU
1	E	259	LYS
1	E	260	GLU
1	E	280	LYS
1	E	284	LEU
1	E	305	VAL
1	E	338	GLU
1	E	339	CYS
1	E	352	ARG
1	E	407	VAL
1	E	433	LYS
1	E	438	ASP
1	E	439	LEU
1	E	444	LEU
1	E	467	LEU
1	E	474	CYS
1	E	481	SER
1	E	489	LYS
1	E	501	SER
1	E	562	LEU
1	E	567	THR
1	E	581	ARG
1	E	591	LYS

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Mol	Chain	Res	Type
1	E	603	GLN
1	E	611	ASN
1	E	616	SER
1	E	625	GLU
1	E	626	THR
1	E	640	LYS
1	E	646	THR
1	E	663	ARG
1	E	671	LEU
1	E	675	THR
1	F	29	VAL
1	F	30	ILE
1	F	37	VAL
1	F	89	GLU
1	F	104	ASP
1	F	144	LYS
1	F	166	ASP
1	F	182	LEU
1	F	222	GLN
1	F	259	LYS
1	F	260	GLU
1	F	284	LEU
1	F	305	VAL
1	F	326	LEU
1	F	434	LYS
1	F	444	LEU
1	F	467	LEU
1	F	469	ASN
1	F	471	ILE
1	F	473	HIS
1	F	489	LYS
1	F	497	LEU
1	F	568	ARG
1	F	591	LYS
1	F	603	GLN
1	F	607	LEU
1	F	615	CYS
1	F	627	LYS
1	F	646	THR
1	F	657	LYS
1	F	662	LEU
1	F	663	ARG

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Mol	Chain	Res	Type
1	F	671	LEU
1	F	675	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	75	ASN
1	A	76	ASN
1	A	169	GLN
1	A	289	HIS
1	A	555	ASN
1	A	603	GLN
1	B	55	ASN
1	B	76	ASN
1	B	230	ASN
1	B	289	HIS
1	B	540	GLN
1	B	606	HIS
1	B	642	HIS
1	C	55	ASN
1	C	169	GLN
1	C	230	ASN
1	C	269	GLN
1	C	289	HIS
1	C	598	HIS
1	D	55	ASN
1	D	230	ASN
1	D	289	HIS
1	D	510	ASN
1	E	169	GLN
1	E	230	ASN
1	E	325	ASN
1	E	349	HIS
1	E	553	ASN
1	E	642	HIS
1	F	55	ASN
1	F	172	GLN
1	F	606	HIS
1	F	645	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 82 ligands modelled in this entry, 12 are monoatomic - leaving 70 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	SO4	D	712	-	4,4,4	0.22	0	6,6,6	0.13	0
5	P6G	C	712	-	18,18,18	0.73	0	17,17,17	1.45	0
2	BCT	A	702	3	3,3,3	0.67	0	2,3,3	0.41	0
4	SO4	D	710	-	4,4,4	0.22	0	6,6,6	0.20	0
2	BCT	D	702	3	3,3,3	0.60	0	2,3,3	0.44	0
5	P6G	B	714	-	18,18,18	0.75	0	17,17,17	1.32	2 (11%)
2	BCT	E	701	3	3,3,3	0.68	0	2,3,3	0.62	0
4	SO4	A	707	-	4,4,4	0.21	0	6,6,6	0.15	0
2	BCT	A	701	3	3,3,3	0.44	0	2,3,3	0.68	0
4	SO4	D	705	-	4,4,4	0.24	0	6,6,6	0.11	0
5	P6G	F	710	-	18,18,18	0.72	0	17,17,17	1.54	1 (5%)
4	SO4	B	707	-	4,4,4	0.26	0	6,6,6	0.13	0
5	P6G	B	715	-	18,18,18	0.72	0	17,17,17	1.51	1 (5%)
2	BCT	E	702	3	3,3,3	0.42	0	2,3,3	0.90	0
4	SO4	C	708	-	4,4,4	0.23	0	6,6,6	0.15	0
4	SO4	B	712	-	4,4,4	0.26	0	6,6,6	0.07	0
4	SO4	A	706	-	4,4,4	0.27	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	C	710	-	4,4,4	0.26	0	6,6,6	0.09	0
4	SO4	E	705	-	4,4,4	0.25	0	6,6,6	0.07	0
4	SO4	F	708	-	4,4,4	0.26	0	6,6,6	0.11	0
5	P6G	C	713	-	18,18,18	0.68	0	17,17,17	1.56	1 (5%)
2	BCT	D	701	3	3,3,3	0.44	0	2,3,3	0.43	0
4	SO4	C	707	-	4,4,4	0.24	0	6,6,6	0.23	0
4	SO4	F	707	-	4,4,4	0.24	0	6,6,6	0.15	0
4	SO4	C	706	-	4,4,4	0.26	0	6,6,6	0.12	0
2	BCT	C	701	3	3,3,3	0.43	0	2,3,3	0.35	0
5	P6G	A	710	-	18,18,18	0.71	0	17,17,17	1.51	0
4	SO4	E	712	-	4,4,4	0.25	0	6,6,6	0.14	0
4	SO4	F	705	-	4,4,4	0.24	0	6,6,6	0.12	0
2	BCT	B	702	3	3,3,3	0.48	0	2,3,3	0.92	0
5	P6G	A	711	-	18,18,18	0.66	0	17,17,17	1.56	2 (11%)
4	SO4	A	705	-	4,4,4	0.27	0	6,6,6	0.16	0
4	SO4	E	706	-	4,4,4	0.72	0	6,6,6	0.89	0
4	SO4	D	707	-	4,4,4	0.23	0	6,6,6	0.13	0
4	SO4	A	709	-	4,4,4	0.25	0	6,6,6	0.11	0
4	SO4	E	708	-	4,4,4	0.25	0	6,6,6	0.06	0
5	P6G	C	714	-	18,18,18	0.67	0	17,17,17	1.56	0
4	SO4	E	710	-	4,4,4	0.24	0	6,6,6	0.12	0
4	SO4	D	713	-	4,4,4	0.26	0	6,6,6	0.05	0
4	SO4	D	708	-	4,4,4	0.21	0	6,6,6	0.15	0
4	SO4	D	709	-	4,4,4	0.28	0	6,6,6	0.17	0
5	P6G	A	712	-	18,18,18	0.71	0	17,17,17	1.49	0
2	BCT	F	702	3	3,3,3	0.78	0	2,3,3	0.63	0
5	P6G	D	715	-	18,18,18	0.62	0	17,17,17	1.77	3 (17%)
5	P6G	E	715	-	18,18,18	0.74	0	17,17,17	1.42	0
4	SO4	C	709	-	4,4,4	0.27	0	6,6,6	0.16	0
4	SO4	E	707	-	4,4,4	0.25	0	6,6,6	0.17	0
2	BCT	C	702	3	3,3,3	0.74	0	2,3,3	0.60	0
2	BCT	F	701	3	3,3,3	0.38	0	2,3,3	0.19	0
4	SO4	B	709	-	4,4,4	0.24	0	6,6,6	0.19	0
4	SO4	C	711	-	4,4,4	0.24	0	6,6,6	0.09	0
4	SO4	F	706	-	4,4,4	0.29	0	6,6,6	0.12	0
4	SO4	D	706	-	4,4,4	0.25	0	6,6,6	0.13	0
5	P6G	F	711	-	18,18,18	0.71	0	17,17,17	1.66	2 (11%)
4	SO4	B	708	-	4,4,4	0.25	0	6,6,6	0.24	0
4	SO4	B	710	-	4,4,4	0.26	0	6,6,6	0.21	0
2	BCT	B	701	3	3,3,3	0.33	0	2,3,3	0.86	0
4	SO4	B	713	-	4,4,4	0.25	0	6,6,6	0.15	0
5	P6G	E	714	-	18,18,18	0.69	0	17,17,17	1.58	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	706	-	4,4,4	0.28	0	6,6,6	0.16	0
4	SO4	E	711	-	4,4,4	0.23	0	6,6,6	0.13	0
4	SO4	A	708	-	4,4,4	0.28	0	6,6,6	0.09	0
4	SO4	B	705	-	4,4,4	0.24	0	6,6,6	0.22	0
4	SO4	C	705	-	4,4,4	0.23	0	6,6,6	0.11	0
4	SO4	D	711	-	4,4,4	0.25	0	6,6,6	0.13	0
4	SO4	F	709	-	4,4,4	0.25	0	6,6,6	0.12	0
5	P6G	D	714	-	18,18,18	0.70	0	17,17,17	1.58	0
4	SO4	E	713	-	4,4,4	0.24	0	6,6,6	0.05	0
4	SO4	E	709	-	4,4,4	0.24	0	6,6,6	0.18	0
4	SO4	B	711	-	4,4,4	0.27	0	6,6,6	0.13	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
5	P6G	C	712	-	-	11/16/16/16	-
5	P6G	A	710	-	-	10/16/16/16	-
5	P6G	E	714	-	-	9/16/16/16	-
5	P6G	B	714	-	-	4/16/16/16	-
5	P6G	D	715	-	-	9/16/16/16	-
5	P6G	E	715	-	-	12/16/16/16	-
5	P6G	F	710	-	-	8/16/16/16	-
5	P6G	D	714	-	-	14/16/16/16	-
5	P6G	A	711	-	-	10/16/16/16	-
5	P6G	B	715	-	-	10/16/16/16	-
5	P6G	C	713	-	-	7/16/16/16	-
5	P6G	F	711	-	-	13/16/16/16	-
5	P6G	C	714	-	-	11/16/16/16	-
5	P6G	A	712	-	-	11/16/16/16	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	714	P6G	C14-O13-C12	2.46	124.04	113.26
5	F	711	P6G	O4-C5-C6	2.34	121.00	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	711	P6G	C8-O7-C6	2.23	123.00	113.26
5	D	715	P6G	O7-C6-C5	2.22	120.46	110.35
5	C	713	P6G	O10-C9-C8	2.19	120.33	110.35
5	D	715	P6G	O13-C12-C11	2.15	120.13	110.35
5	B	714	P6G	O13-C14-C15	2.12	120.01	110.35
5	A	711	P6G	O16-C17-C18	2.06	119.17	110.11
5	D	715	P6G	O4-C5-C6	2.05	119.69	110.35
5	B	715	P6G	O16-C17-C18	2.04	119.11	110.11
5	F	710	P6G	O16-C17-C18	2.04	119.11	110.11
5	E	714	P6G	C17-O16-C15	2.03	122.16	113.26
5	B	714	P6G	O4-C3-C2	2.01	118.96	110.11
5	A	711	P6G	O13-C12-C11	2.00	119.48	110.35

There are no chirality outliers.

All (139) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	714	P6G	C12-C11-O10-C9
5	E	715	P6G	C12-C11-O10-C9
5	C	712	P6G	C14-C15-O16-C17
5	E	714	P6G	C2-C3-O4-C5
5	F	710	P6G	C6-C5-O4-C3
5	B	715	P6G	C11-C12-O13-C14
5	B	715	P6G	C8-C9-O10-C11
5	E	714	P6G	O10-C11-C12-O13
5	F	711	P6G	O13-C14-C15-O16
5	C	714	P6G	C11-C12-O13-C14
5	A	711	P6G	O4-C5-C6-O7
5	F	711	P6G	O4-C5-C6-O7
5	D	715	P6G	O13-C14-C15-O16
5	F	711	P6G	C12-C11-O10-C9
5	E	715	P6G	O4-C5-C6-O7
5	C	714	P6G	O4-C5-C6-O7
5	A	710	P6G	C14-C15-O16-C17
5	E	715	P6G	O10-C11-C12-O13
5	F	710	P6G	O4-C5-C6-O7
5	A	710	P6G	O1-C2-C3-O4
5	C	712	P6G	O16-C17-C18-O19
5	D	714	P6G	O1-C2-C3-O4
5	E	714	P6G	O1-C2-C3-O4
5	A	712	P6G	C5-C6-O7-C8
5	C	712	P6G	C9-C8-O7-C6

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Mol	Chain	Res	Type	Atoms
5	A	711	P6G	O13-C14-C15-O16
5	D	714	P6G	O13-C14-C15-O16
5	F	711	P6G	O10-C11-C12-O13
5	C	712	P6G	O13-C14-C15-O16
5	A	710	P6G	O16-C17-C18-O19
5	A	712	P6G	O16-C17-C18-O19
5	C	714	P6G	O1-C2-C3-O4
5	C	712	P6G	O7-C8-C9-O10
5	B	715	P6G	O10-C11-C12-O13
5	C	714	P6G	O13-C14-C15-O16
5	C	713	P6G	O1-C2-C3-O4
5	E	715	P6G	O16-C17-C18-O19
5	F	711	P6G	O1-C2-C3-O4
5	F	711	P6G	O16-C17-C18-O19
5	F	711	P6G	O7-C8-C9-O10
5	A	710	P6G	O13-C14-C15-O16
5	D	714	P6G	O7-C8-C9-O10
5	D	715	P6G	O4-C5-C6-O7
5	C	712	P6G	O4-C5-C6-O7
5	C	713	P6G	O16-C17-C18-O19
5	D	715	P6G	O1-C2-C3-O4
5	F	710	P6G	O16-C17-C18-O19
5	A	711	P6G	O7-C8-C9-O10
5	A	712	P6G	C12-C11-O10-C9
5	B	715	P6G	O4-C5-C6-O7
5	C	714	P6G	O7-C8-C9-O10
5	A	712	P6G	O1-C2-C3-O4
5	F	710	P6G	O1-C2-C3-O4
5	A	710	P6G	C11-C12-O13-C14
5	B	715	P6G	C14-C15-O16-C17
5	E	715	P6G	O13-C14-C15-O16
5	E	714	P6G	O13-C14-C15-O16
5	E	714	P6G	C8-C9-O10-C11
5	A	710	P6G	O4-C5-C6-O7
5	B	715	P6G	O7-C8-C9-O10
5	A	711	P6G	C14-C15-O16-C17
5	C	714	P6G	C6-C5-O4-C3
5	D	715	P6G	O7-C8-C9-O10
5	A	710	P6G	O7-C8-C9-O10
5	F	710	P6G	O10-C11-C12-O13
5	F	710	P6G	O7-C8-C9-O10
5	E	714	P6G	O7-C8-C9-O10

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Mol	Chain	Res	Type	Atoms
5	D	714	P6G	O10-C11-C12-O13
5	F	711	P6G	C15-C14-O13-C12
5	D	715	P6G	O10-C11-C12-O13
5	D	714	P6G	C9-C8-O7-C6
5	F	710	P6G	O13-C14-C15-O16
5	C	712	P6G	O1-C2-C3-O4
5	C	712	P6G	C8-C9-O10-C11
5	A	712	P6G	C15-C14-O13-C12
5	B	715	P6G	O1-C2-C3-O4
5	D	714	P6G	C18-C17-O16-C15
5	A	712	P6G	C2-C3-O4-C5
5	B	715	P6G	C5-C6-O7-C8
5	E	715	P6G	C11-C12-O13-C14
5	E	715	P6G	C18-C17-O16-C15
5	F	711	P6G	C2-C3-O4-C5
5	C	714	P6G	C15-C14-O13-C12
5	C	713	P6G	C9-C8-O7-C6
5	D	715	P6G	C6-C5-O4-C3
5	E	714	P6G	C6-C5-O4-C3
5	D	715	P6G	C11-C12-O13-C14
5	E	714	P6G	C5-C6-O7-C8
5	C	714	P6G	C12-C11-O10-C9
5	A	711	P6G	C8-C9-O10-C11
5	B	714	P6G	C5-C6-O7-C8
5	B	714	P6G	C9-C8-O7-C6
5	C	712	P6G	C5-C6-O7-C8
5	B	714	P6G	C6-C5-O4-C3
5	B	714	P6G	O4-C5-C6-O7
5	D	714	P6G	O16-C17-C18-O19
5	D	715	P6G	O16-C17-C18-O19
5	C	713	P6G	O13-C14-C15-O16
5	E	715	P6G	O7-C8-C9-O10
5	E	715	P6G	C8-C9-O10-C11
5	C	712	P6G	C11-C12-O13-C14
5	C	714	P6G	O16-C17-C18-O19
5	A	711	P6G	C5-C6-O7-C8
5	E	715	P6G	O1-C2-C3-O4
5	A	711	P6G	C15-C14-O13-C12
5	F	711	P6G	C5-C6-O7-C8
5	C	714	P6G	C14-C15-O16-C17
5	C	713	P6G	C12-C11-O10-C9
5	A	711	P6G	O1-C2-C3-O4

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Mol	Chain	Res	Type	Atoms
5	A	712	P6G	C9-C8-O7-C6
5	A	710	P6G	C15-C14-O13-C12
5	D	714	P6G	C15-C14-O13-C12
5	A	712	P6G	O10-C11-C12-O13
5	B	715	P6G	C6-C5-O4-C3
5	F	710	P6G	C9-C8-O7-C6
5	B	715	P6G	C9-C8-O7-C6
5	A	712	P6G	C6-C5-O4-C3
5	A	710	P6G	C2-C3-O4-C5
5	A	711	P6G	C11-C12-O13-C14
5	A	712	P6G	O13-C14-C15-O16
5	D	715	P6G	C18-C17-O16-C15
5	F	711	P6G	C14-C15-O16-C17
5	C	714	P6G	O10-C11-C12-O13
5	E	715	P6G	C5-C6-O7-C8
5	F	711	P6G	C9-C8-O7-C6
5	E	714	P6G	C15-C14-O13-C12
5	F	711	P6G	C18-C17-O16-C15
5	D	714	P6G	C14-C15-O16-C17
5	D	714	P6G	C2-C3-O4-C5
5	A	711	P6G	C6-C5-O4-C3
5	D	714	P6G	C11-C12-O13-C14
5	A	710	P6G	C18-C17-O16-C15
5	A	712	P6G	C11-C12-O13-C14
5	C	712	P6G	O10-C11-C12-O13
5	E	715	P6G	C2-C3-O4-C5
5	C	713	P6G	C5-C6-O7-C8
5	D	714	P6G	C5-C6-O7-C8
5	D	714	P6G	O4-C5-C6-O7
5	C	713	P6G	O7-C8-C9-O10

There are no ring outliers.

14 monomers are involved in 36 short contacts:

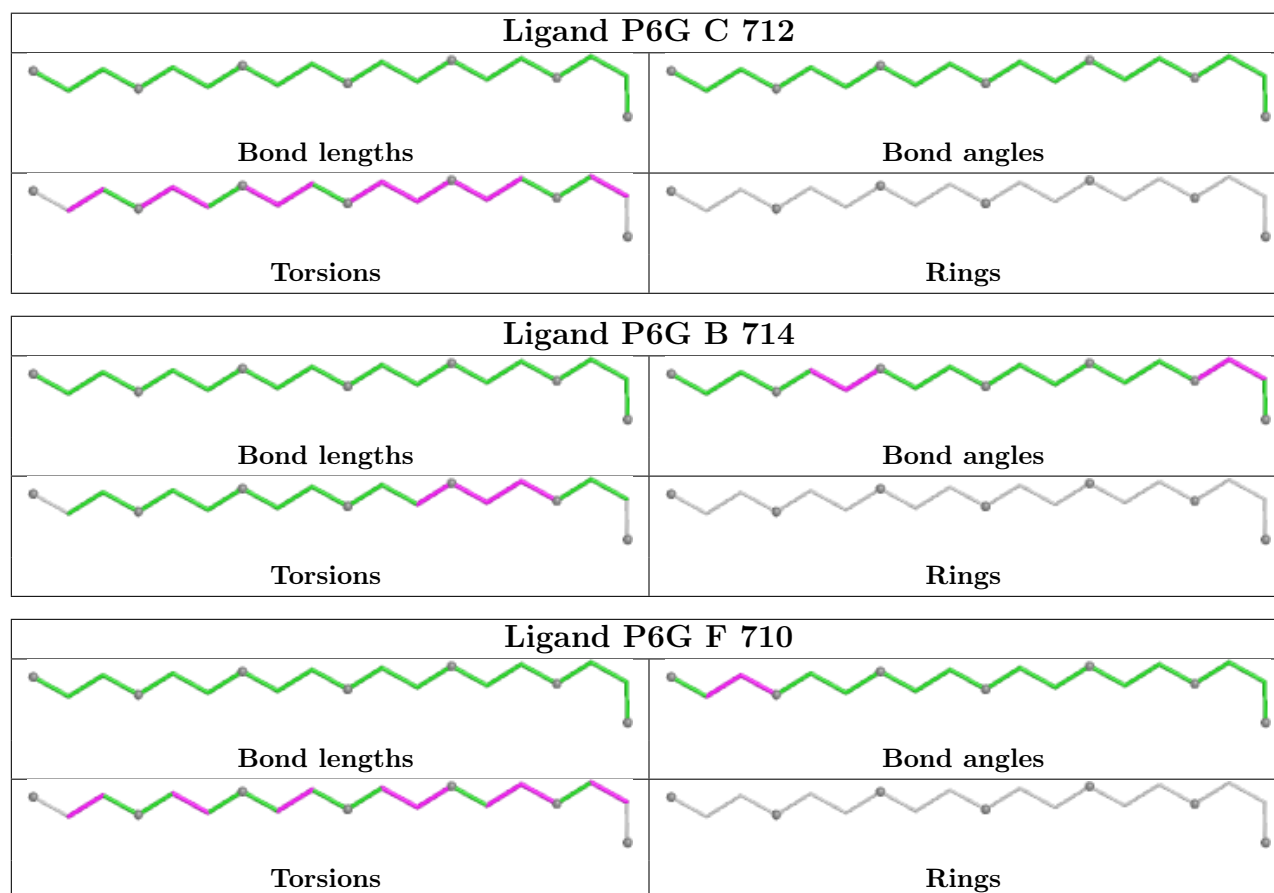
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	712	P6G	1	0
4	D	710	SO4	1	0
4	B	707	SO4	1	0
5	B	715	P6G	6	0
5	C	713	P6G	3	0
5	A	710	P6G	1	0
4	A	705	SO4	1	0

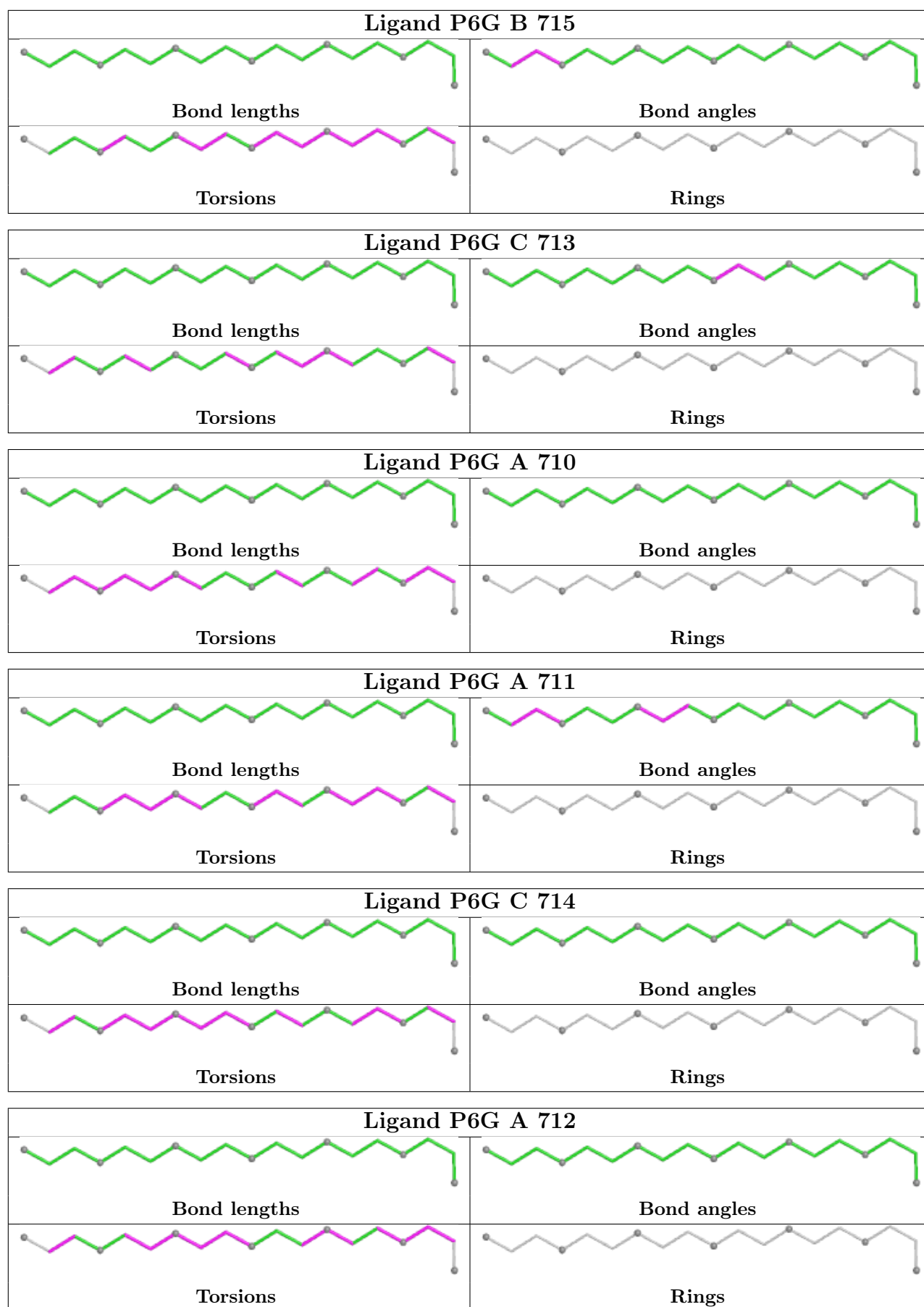
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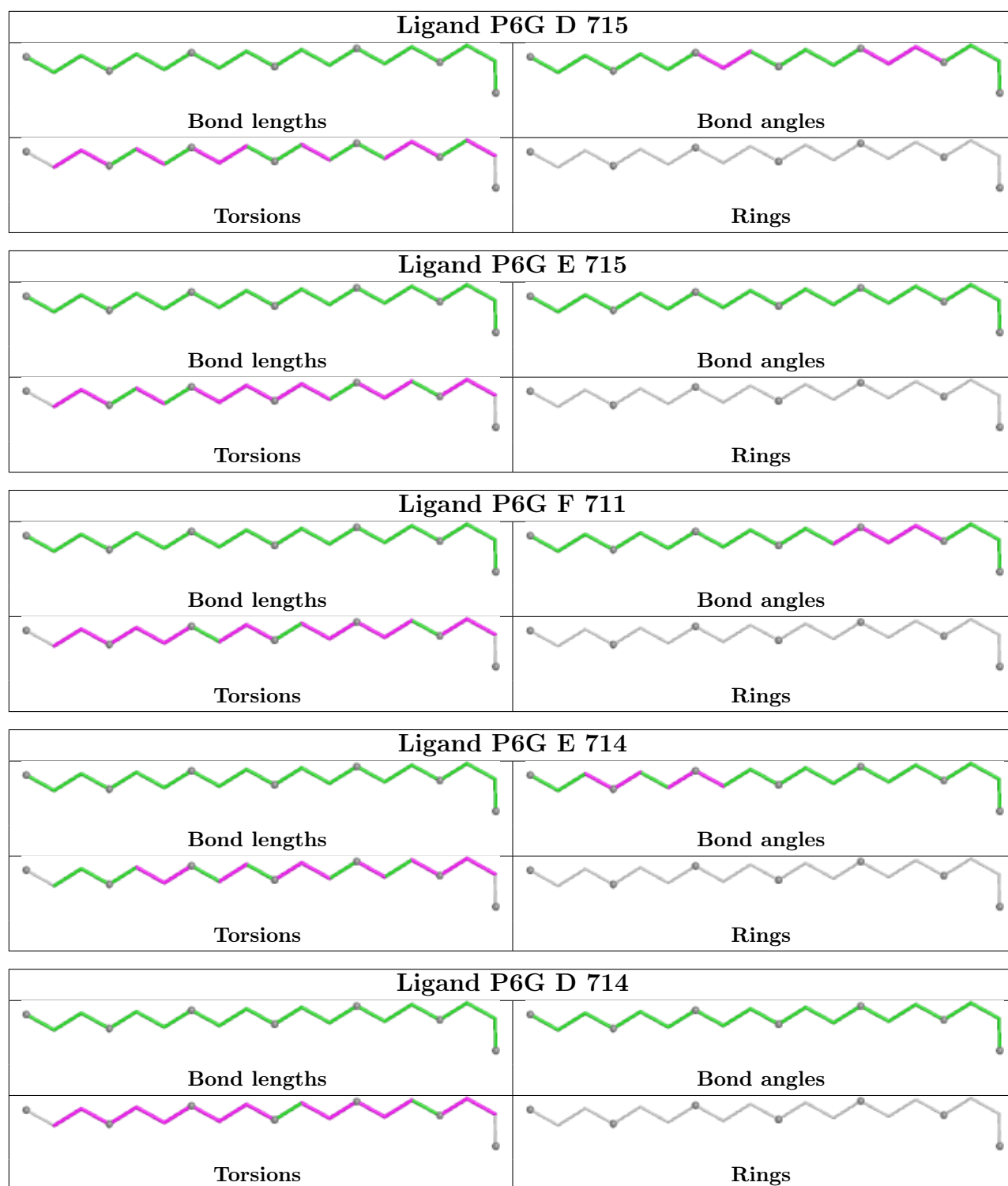
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	712	P6G	3	0
5	D	715	P6G	3	0
5	E	715	P6G	3	0
2	C	702	BCT	3	0
5	F	711	P6G	6	0
5	E	714	P6G	1	0
5	D	714	P6G	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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	674/698 (96%)	0.05	31 (4%) 37 39	15, 39, 77, 97	0
1	B	677/698 (96%)	-0.03	31 (4%) 37 39	13, 33, 72, 97	0
1	C	674/698 (96%)	1.02	194 (28%) 1 1	13, 46, 117, 151	0
1	D	675/698 (96%)	-0.05	36 (5%) 32 34	16, 34, 66, 94	0
1	E	674/698 (96%)	0.12	41 (6%) 27 29	13, 35, 73, 93	0
1	F	676/698 (96%)	0.02	34 (5%) 34 36	13, 36, 70, 98	0
All	All	4050/4188 (96%)	0.19	367 (9%) 15 15	13, 36, 83, 151	0

All (367) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	564	LEU	9.8
1	C	479	PHE	8.1
1	C	573	GLU	7.0
1	C	567	THR	6.9
1	C	566	GLY	6.9
1	C	468	TYR	6.6
1	C	561	LEU	6.4
1	F	334	ALA	6.1
1	C	480	PHE	6.0
1	C	441	TRP	6.0
1	C	417	ASN	6.0
1	C	444	LEU	5.9
1	C	425	GLY	5.9
1	C	474	CYS	5.8
1	C	466	LEU	5.8
1	C	578	HIS	5.8
1	C	639	ALA	5.8
1	C	483	GLY	5.7
1	C	476	PHE	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	467	LEU	5.5
1	C	470	LYS	5.4
1	C	471	ILE	5.4
1	C	462	ILE	5.4
1	C	562	LEU	5.3
1	C	448	LYS	5.3
1	C	569	LYS	5.3
1	A	436	ALA	5.3
1	C	431	VAL	5.2
1	C	446	GLY	5.2
1	C	336	THR	5.2
1	F	335	PRO	5.1
1	C	440	THR	5.1
1	C	612	VAL	5.1
1	C	665	CYS	5.0
1	C	449	SER	4.9
1	B	334	ALA	4.8
1	C	531	ALA	4.8
1	C	575	ALA	4.8
1	C	579	LEU	4.8
1	F	337	ASP	4.8
1	C	582	ALA	4.8
1	C	662	LEU	4.7
1	C	495	CYS	4.7
1	C	493	SER	4.7
1	B	332	PRO	4.7
1	C	447	LYS	4.7
1	C	494	LEU	4.7
1	C	485	ALA	4.6
1	C	478	GLU	4.5
1	C	571	VAL	4.5
1	C	577	CYS	4.5
1	C	661	ASN	4.5
1	B	336	THR	4.5
1	C	481	SER	4.5
1	C	430	ALA	4.5
1	B	441	TRP	4.4
1	C	565	ASP	4.4
1	C	576	ASN	4.4
1	C	570	PRO	4.4
1	C	659	VAL	4.4
1	C	563	CYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	333	GLU	4.4
1	C	532	PHE	4.4
1	A	336	THR	4.3
1	C	424	ALA	4.3
1	C	443	ASN	4.3
1	C	496	LYS	4.3
1	C	432	VAL	4.3
1	C	580	ALA	4.2
1	C	497	LEU	4.2
1	C	463	PRO	4.2
1	C	574	TYR	4.2
1	B	335	PRO	4.1
1	C	426	TYR	4.1
1	C	428	ALA	4.1
1	C	439	LEU	4.1
1	C	429	VAL	4.1
1	E	543	GLY	4.1
1	C	421	THR	4.1
1	C	473	HIS	4.1
1	A	435	SER	4.1
1	A	333	GLU	4.1
1	C	436	ALA	4.0
1	C	560	GLU	4.0
1	C	484	CYS	4.0
1	C	655	TYR	4.0
1	E	258	GLY	3.9
1	D	441	TRP	3.9
1	C	469	ASN	3.9
1	F	104	ASP	3.9
1	C	335	PRO	3.9
1	E	334	ALA	3.9
1	B	438	ASP	3.8
1	C	333	GLU	3.8
1	C	445	LYS	3.8
1	D	617	GLY	3.8
1	A	618	ASN	3.7
1	C	607	LEU	3.7
1	A	335	PRO	3.7
1	C	427	PHE	3.7
1	C	492	SER	3.7
1	A	334	ALA	3.7
1	C	465	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	625	GLU	3.7
1	C	460	TRP	3.7
1	C	528	GLY	3.7
1	A	443	ASN	3.7
1	C	658	ALA	3.7
1	E	436	ALA	3.7
1	A	439	LEU	3.6
1	C	450	CYS	3.6
1	B	566	GLY	3.6
1	B	567	THR	3.6
1	F	279	SER	3.6
1	D	335	PRO	3.6
1	C	650	TYR	3.6
1	C	396	VAL	3.5
1	D	421	THR	3.5
1	C	647	TYR	3.5
1	C	572	GLU	3.5
1	C	435	SER	3.5
1	C	559	TYR	3.4
1	C	505	LEU	3.4
1	E	438	ASP	3.4
1	C	334	ALA	3.4
1	E	503	LEU	3.4
1	C	568	ARG	3.3
1	F	471	ILE	3.3
1	C	491	ASP	3.3
1	D	613	THR	3.3
1	C	613	THR	3.3
1	D	258	GLY	3.3
1	C	656	VAL	3.3
1	B	437	SER	3.2
1	D	140	PRO	3.2
1	C	638	LEU	3.2
1	C	660	GLY	3.2
1	C	363	VAL	3.2
1	F	436	ALA	3.2
1	C	397	TYR	3.2
1	B	33	ASP	3.2
1	C	422	PRO	3.2
1	D	417	ASN	3.2
1	C	477	ASP	3.2
1	B	613	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	457	THR	3.2
1	F	440	THR	3.2
1	C	472	ASN	3.2
1	C	525	VAL	3.1
1	C	581	ARG	3.1
1	C	642	HIS	3.1
1	C	502	GLY	3.1
1	D	215	ALA	3.1
1	D	334	ALA	3.1
1	D	142	PRO	3.1
1	F	332	PRO	3.1
1	F	417	ASN	3.1
1	B	623	ARG	3.1
1	C	524	LEU	3.1
1	A	441	TRP	3.1
1	F	2	PRO	3.0
1	C	420	ASP	3.0
1	C	606	HIS	3.0
1	C	418	CYS	3.0
1	C	458	ALA	3.0
1	C	464	MET	3.0
1	C	437	SER	3.0
1	D	437	SER	3.0
1	E	478	GLU	3.0
1	B	612	VAL	3.0
1	C	554	LEU	3.0
1	E	624	SER	3.0
1	E	482	GLU	3.0
1	B	626	THR	3.0
1	A	104	ASP	3.0
1	C	433	LYS	3.0
1	A	613	THR	3.0
1	C	585	HIS	3.0
1	B	333	GLU	2.9
1	E	333	GLU	2.9
1	C	461	ASN	2.9
1	C	503	LEU	2.9
1	E	554	LEU	2.9
1	E	104	ASP	2.9
1	F	416	ASP	2.9
1	F	142	PRO	2.9
1	E	615	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	337	ASP	2.9
1	C	337	ASP	2.9
1	C	600	ILE	2.9
1	F	336	THR	2.9
1	E	437	SER	2.9
1	C	640	LYS	2.9
1	C	652	GLY	2.9
1	C	529	ASP	2.9
1	C	555	ASN	2.9
1	F	606	HIS	2.9
1	C	454	VAL	2.8
1	D	333	GLU	2.8
1	F	29	VAL	2.8
1	A	332	PRO	2.8
1	C	332	PRO	2.8
1	C	490	LYS	2.8
1	D	606	HIS	2.8
1	C	666	SER	2.8
1	D	623	ARG	2.8
1	C	451	HIS	2.8
1	C	625	GLU	2.8
1	D	436	ALA	2.8
1	B	440	THR	2.7
1	A	337	ASP	2.7
1	C	438	ASP	2.7
1	C	530	VAL	2.7
1	C	339	CYS	2.7
1	D	279	SER	2.7
1	C	33	ASP	2.7
1	C	442	ASP	2.7
1	C	644	ARG	2.7
1	C	141	GLU	2.7
1	B	614	ASP	2.7
1	C	596	CYS	2.7
1	C	414	LYS	2.7
1	C	475	ARG	2.7
1	C	486	PRO	2.6
1	C	584	ASN	2.6
1	E	332	PRO	2.6
1	E	606	HIS	2.6
1	A	437	SER	2.6
1	E	481	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	277	ASP	2.6
1	B	258	GLY	2.6
1	C	142	PRO	2.6
1	A	624	SER	2.6
1	C	599	LYS	2.6
1	C	506	CYS	2.6
1	C	594	GLU	2.6
1	A	327	ARG	2.6
1	D	141	GLU	2.6
1	C	487	GLY	2.6
1	C	617	GLY	2.5
1	F	617	GLY	2.5
1	F	280	LYS	2.5
1	C	646	THR	2.5
1	D	643	ASP	2.5
1	F	607	LEU	2.5
1	A	625	GLU	2.5
1	F	612	VAL	2.5
1	D	614	ASP	2.5
1	C	626	THR	2.5
1	E	518	THR	2.5
1	E	572	GLU	2.5
1	C	412	TYR	2.5
1	D	136	TYR	2.5
1	E	474	CYS	2.5
1	F	331	CYS	2.5
1	A	415	SER	2.5
1	B	616	SER	2.5
1	C	583	PRO	2.5
1	C	598	HIS	2.5
1	F	473	HIS	2.5
1	E	618	ASN	2.5
1	C	482	GLU	2.4
1	D	570	PRO	2.4
1	F	663	ARG	2.4
1	C	364	GLY	2.4
1	A	4	LYS	2.4
1	C	489	LYS	2.4
1	D	503	LEU	2.4
1	D	618	ASN	2.4
1	F	281	GLU	2.4
1	C	616	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	527	LYS	2.4
1	C	675	THR	2.4
1	C	677	ARG	2.4
1	D	332	PRO	2.4
1	E	439	LEU	2.4
1	B	329	GLY	2.4
1	A	416	ASP	2.4
1	C	645	ASN	2.3
1	F	616	SER	2.3
1	B	104	ASP	2.3
1	E	416	ASP	2.3
1	C	340	LYS	2.3
1	C	649	LYS	2.3
1	A	616	SER	2.3
1	E	492	SER	2.3
1	A	417	ASN	2.3
1	A	438	ASP	2.3
1	A	614	ASP	2.3
1	C	601	LEU	2.3
1	C	641	LEU	2.3
1	E	497	LEU	2.3
1	C	664	LYS	2.3
1	C	501	SER	2.3
1	D	338	GLU	2.3
1	B	675	THR	2.3
1	C	498	CYS	2.3
1	C	136	TYR	2.3
1	E	574	TYR	2.3
1	B	606	HIS	2.2
1	E	493	SER	2.2
1	C	521	PHE	2.2
1	C	676	PHE	2.2
1	A	471	ILE	2.2
1	C	667	THR	2.2
1	C	504	ASN	2.2
1	A	338	GLU	2.2
1	B	88	LYS	2.2
1	B	443	ASN	2.2
1	C	434	LYS	2.2
1	C	597	VAL	2.2
1	D	571	VAL	2.2
1	E	142	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	490	LYS	2.2
1	A	549	PRO	2.2
1	D	336	THR	2.2
1	F	613	THR	2.2
1	B	565	ASP	2.2
1	C	533	VAL	2.2
1	C	643	ASP	2.2
1	B	338	GLU	2.1
1	D	572	GLU	2.1
1	E	507	GLU	2.1
1	B	543	GLY	2.1
1	C	459	GLY	2.1
1	F	543	GLY	2.1
1	D	415	SER	2.1
1	F	33	ASP	2.1
1	C	393	GLY	2.1
1	C	500	GLY	2.1
1	C	534	LYS	2.1
1	E	561	LEU	2.1
1	C	392	ASP	2.1
1	C	635	THR	2.1
1	C	609	GLY	2.1
1	D	677	ARG	2.1
1	A	28	SER	2.1
1	C	488	SER	2.1
1	E	562	LEU	2.1
1	C	523	CYS	2.1
1	C	413	ASN	2.1
1	E	576	ASN	2.1
1	F	544	GLY	2.1
1	E	4	LYS	2.1
1	E	30	ILE	2.1
1	A	612	VAL	2.1
1	C	453	ALA	2.1
1	D	610	SER	2.1
1	D	616	SER	2.1
1	D	564	LEU	2.0
1	C	558	ASP	2.0
1	E	331	CYS	2.0
1	F	568	ARG	2.0
1	F	623	ARG	2.0
1	E	335	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	336	THR	2.0
1	B	470	LYS	2.0
1	C	514	TYR	2.0
1	D	566	GLY	2.0
1	E	571	VAL	2.0
1	C	595	ALA	2.0
1	D	139	LEU	2.0
1	E	491	ASP	2.0
1	C	637	CYS	2.0
1	F	339	CYS	2.0
1	E	422	PRO	2.0
1	A	617	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
4	SO4	A	705	5/5	0.70	0.18	93,94,95,97	0
4	SO4	F	705	5/5	0.71	0.15	97,97,98,100	0
4	SO4	B	713	5/5	0.74	0.17	105,107,108,109	0
4	SO4	E	713	5/5	0.75	0.12	93,95,95,96	0
4	SO4	B	708	5/5	0.77	0.16	86,88,92,96	0
4	SO4	C	711	5/5	0.78	0.14	106,109,109,110	0
4	SO4	D	706	5/5	0.80	0.11	101,103,106,109	0
4	SO4	F	706	5/5	0.80	0.14	89,92,95,98	0
4	SO4	E	705	5/5	0.81	0.13	107,108,109,110	0
4	SO4	C	706	5/5	0.81	0.10	94,95,97,98	0
4	SO4	F	709	5/5	0.81	0.08	89,89,92,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	709	5/5	0.82	0.11	97,97,99,99	0
4	SO4	B	707	5/5	0.82	0.17	85,87,90,92	0
5	P6G	C	714	19/19	0.82	0.16	56,79,99,100	0
5	P6G	D	715	19/19	0.82	0.19	56,74,84,86	0
5	P6G	A	711	19/19	0.83	0.16	46,66,84,85	0
4	SO4	B	706	5/5	0.83	0.13	72,79,81,82	0
4	SO4	A	707	5/5	0.83	0.14	77,87,88,92	0
5	P6G	F	711	19/19	0.84	0.19	28,48,98,100	0
4	SO4	E	708	5/5	0.85	0.11	94,95,96,96	0
4	SO4	C	709	5/5	0.85	0.10	76,77,80,80	0
5	P6G	A	712	19/19	0.85	0.15	74,81,91,92	0
5	P6G	C	713	19/19	0.85	0.15	43,57,83,83	0
4	SO4	A	708	5/5	0.85	0.15	95,98,99,100	0
4	SO4	E	706	5/5	0.85	0.54	111,112,113,113	5
4	SO4	F	708	5/5	0.85	0.11	80,85,87,90	0
4	SO4	E	710	5/5	0.86	0.10	73,73,75,79	0
4	SO4	D	712	5/5	0.86	0.12	95,95,99,100	0
5	P6G	D	714	19/19	0.87	0.15	41,54,79,79	0
4	SO4	B	712	5/5	0.87	0.08	77,80,83,84	0
5	P6G	E	715	19/19	0.87	0.15	44,56,71,71	0
4	SO4	E	709	5/5	0.87	0.10	76,77,79,81	0
4	SO4	A	706	5/5	0.88	0.10	51,66,69,77	0
4	SO4	F	707	5/5	0.88	0.13	85,87,87,90	0
4	SO4	D	713	5/5	0.88	0.11	72,73,74,78	0
4	SO4	C	710	5/5	0.88	0.11	73,77,79,83	0
5	P6G	E	714	19/19	0.89	0.14	28,45,83,84	0
5	P6G	B	715	19/19	0.90	0.13	32,46,94,95	0
5	P6G	A	710	19/19	0.90	0.12	37,48,77,77	0
4	SO4	C	708	5/5	0.90	0.09	70,75,76,79	0
4	SO4	B	709	5/5	0.90	0.09	66,67,68,73	0
4	SO4	E	711	5/5	0.91	0.10	73,77,84,87	0
4	SO4	D	709	5/5	0.91	0.07	70,72,75,76	0
4	SO4	C	705	5/5	0.91	0.12	77,78,83,83	0
5	P6G	C	712	19/19	0.92	0.12	28,48,79,81	0
5	P6G	F	710	19/19	0.92	0.12	37,48,68,71	0
4	SO4	D	707	5/5	0.92	0.10	57,58,59,65	0
4	SO4	B	710	5/5	0.93	0.17	44,61,65,72	0
4	SO4	D	710	5/5	0.93	0.16	55,55,65,66	0
4	SO4	D	711	5/5	0.93	0.07	62,67,73,74	0
4	SO4	B	711	5/5	0.93	0.09	63,68,74,77	0
5	P6G	B	714	19/19	0.93	0.12	22,32,87,87	0
2	BCT	E	702	4/4	0.94	0.09	26,28,29,30	0

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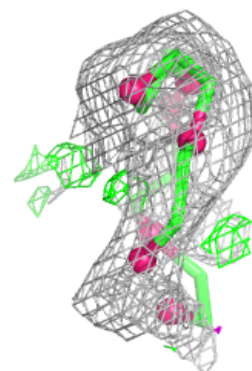
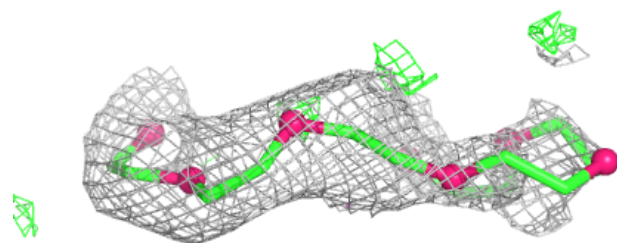
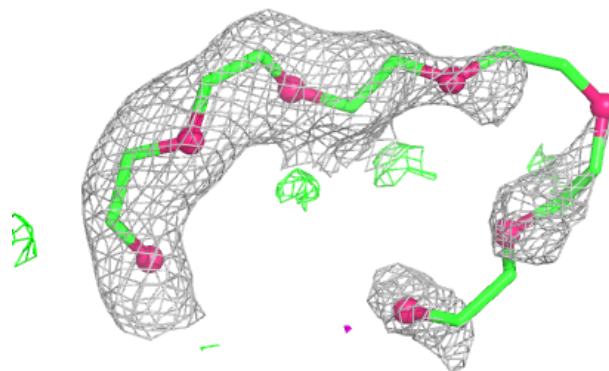
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BCT	C	702	4/4	0.94	0.11	32,36,38,44	0
4	SO4	D	705	5/5	0.94	0.09	68,71,72,78	0
2	BCT	B	702	4/4	0.95	0.07	27,27,28,31	0
4	SO4	C	707	5/5	0.95	0.13	38,55,63,63	0
4	SO4	E	707	5/5	0.95	0.12	41,55,61,63	0
4	SO4	D	708	5/5	0.96	0.13	46,49,58,58	0
2	BCT	D	702	4/4	0.96	0.09	23,26,29,32	0
4	SO4	B	705	5/5	0.96	0.08	44,45,49,50	0
4	SO4	E	712	5/5	0.96	0.11	44,48,49,50	0
2	BCT	A	702	4/4	0.96	0.06	28,31,34,38	0
2	BCT	B	701	4/4	0.96	0.06	13,14,15,16	0
2	BCT	C	701	4/4	0.97	0.05	14,15,15,17	0
2	BCT	A	701	4/4	0.97	0.05	14,14,16,19	0
2	BCT	D	701	4/4	0.97	0.06	15,17,21,24	0
3	FE	C	703	1/1	0.98	0.03	38,38,38,38	0
3	FE	E	704	1/1	0.98	0.05	32,32,32,32	0
2	BCT	E	701	4/4	0.98	0.04	14,17,17,18	0
2	BCT	F	701	4/4	0.98	0.04	8,9,10,11	0
2	BCT	F	702	4/4	0.98	0.05	19,20,21,24	0
3	FE	A	704	1/1	0.99	0.04	34,34,34,34	0
3	FE	F	704	1/1	0.99	0.05	31,31,31,31	0
3	FE	D	703	1/1	0.99	0.05	26,26,26,26	0
3	FE	D	704	1/1	0.99	0.04	20,20,20,20	0
3	FE	F	703	1/1	1.00	0.04	16,16,16,16	0
3	FE	C	704	1/1	1.00	0.02	16,16,16,16	0
3	FE	B	703	1/1	1.00	0.02	29,29,29,29	0
3	FE	B	704	1/1	1.00	0.04	15,15,15,15	0
3	FE	E	703	1/1	1.00	0.04	19,19,19,19	0
3	FE	A	703	1/1	1.00	0.04	19,19,19,19	0

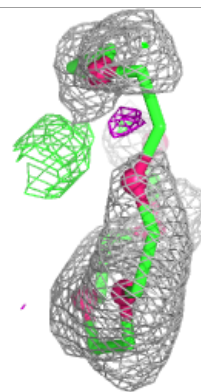
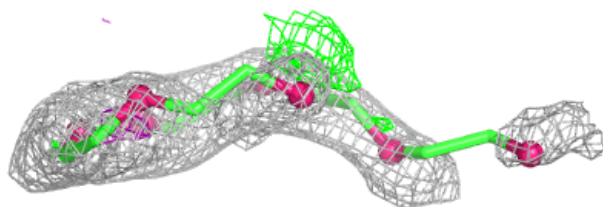
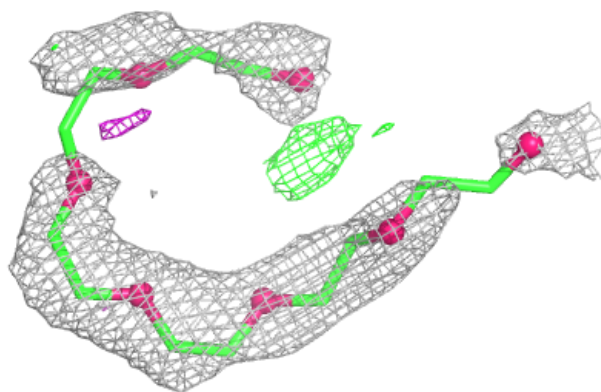
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around P6G C 714:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

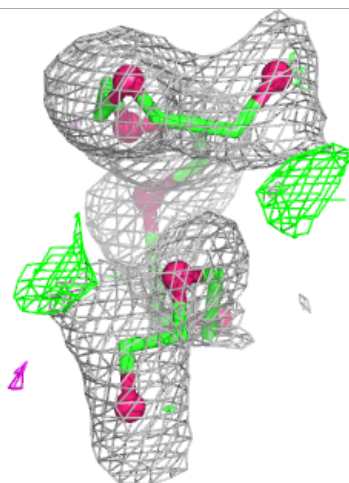
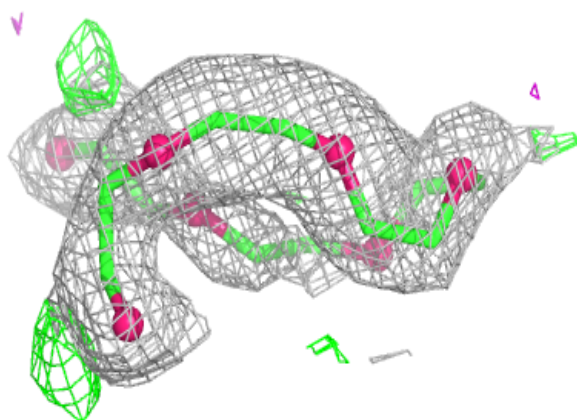
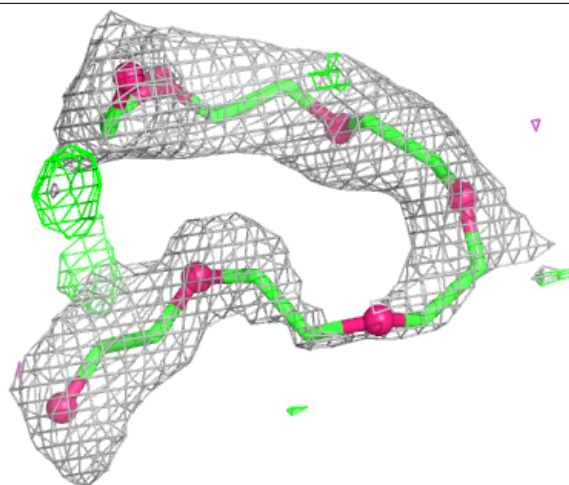
**Electron density around P6G D 715:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



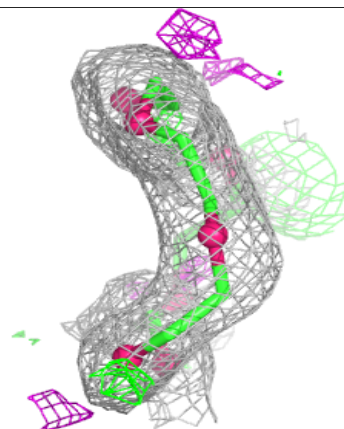
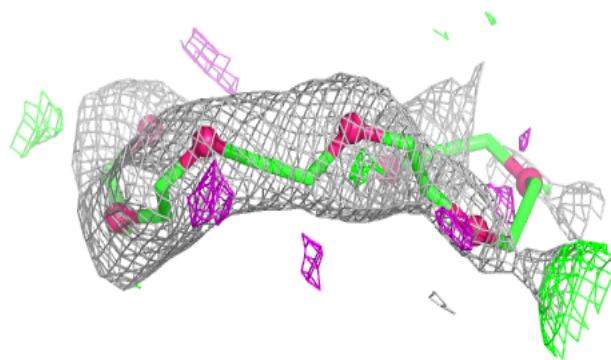
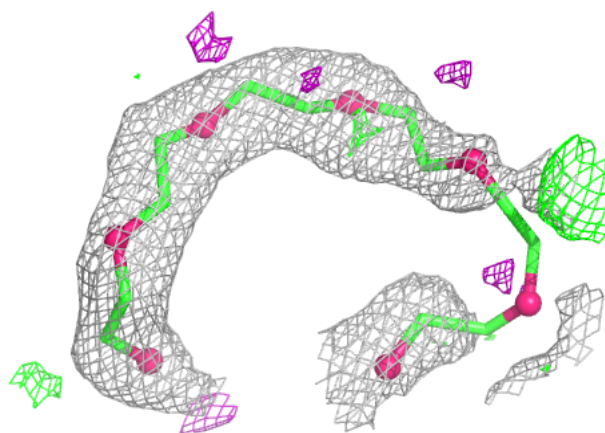
Electron density around P6G A 711:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



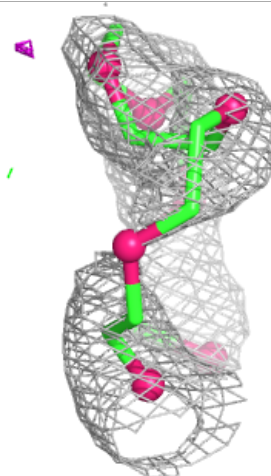
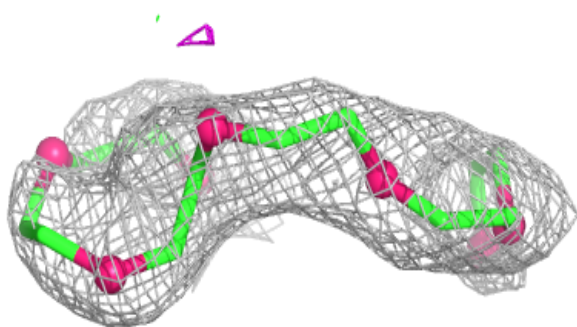
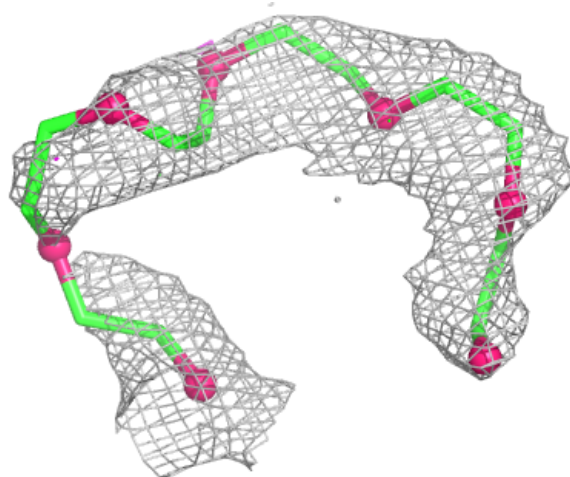
Electron density around P6G F 711:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



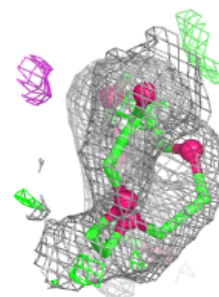
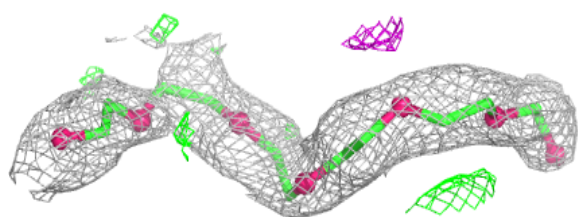
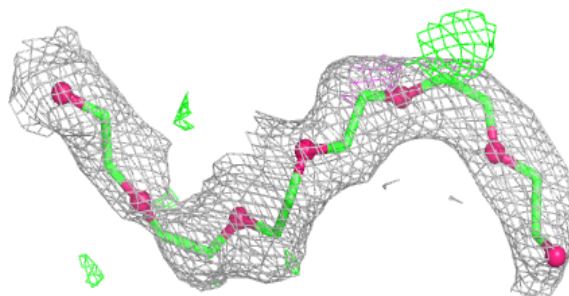
Electron density around P6G A 712:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

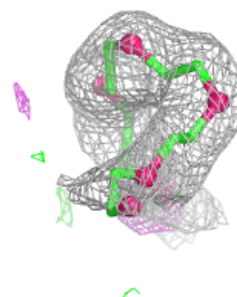
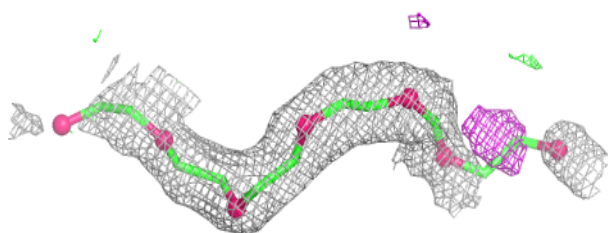
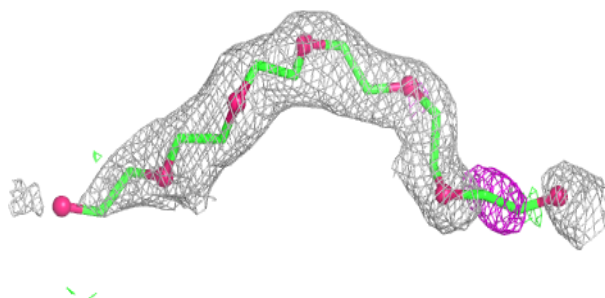


Electron density around P6G C 713:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

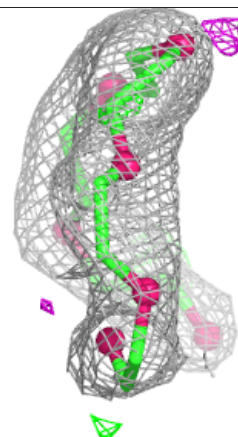
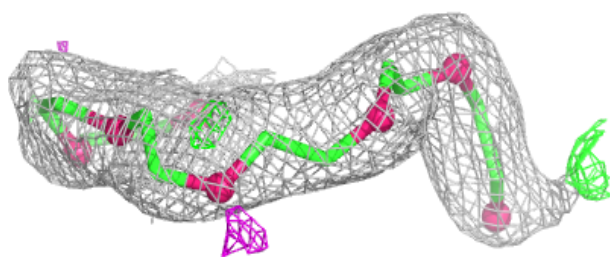
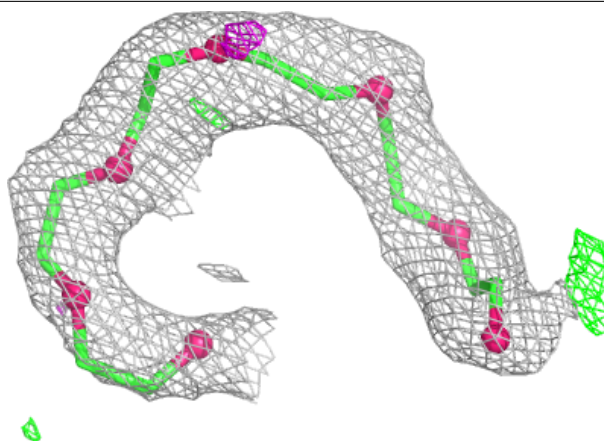
**Electron density around P6G D 714:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



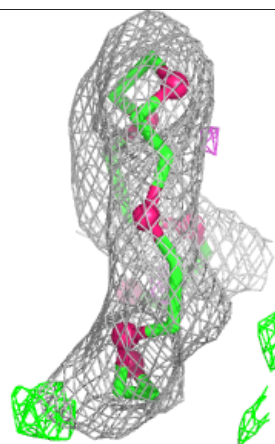
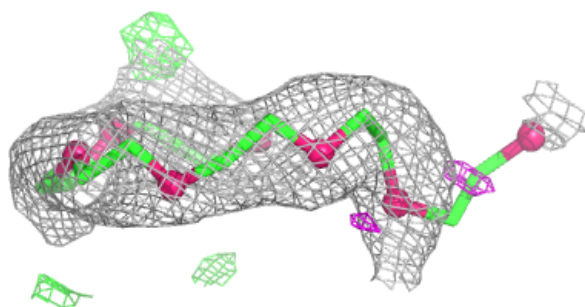
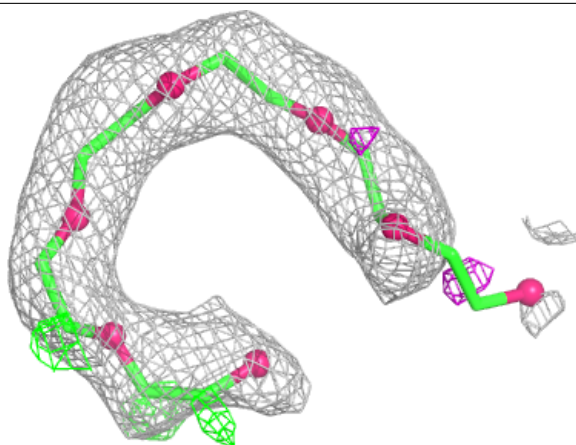
Electron density around P6G E 715:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

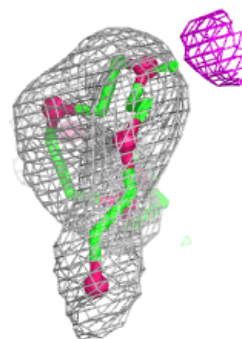
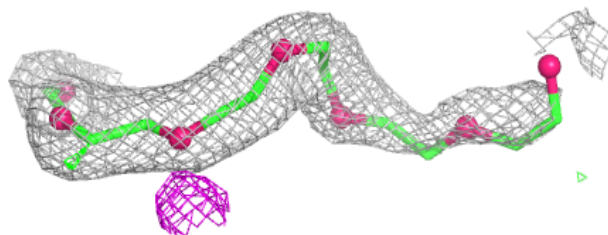
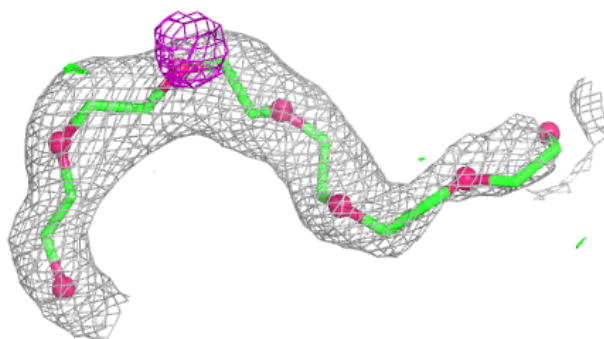


Electron density around P6G E 714:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

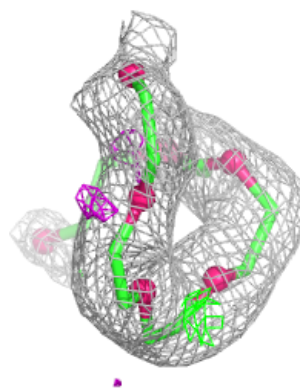
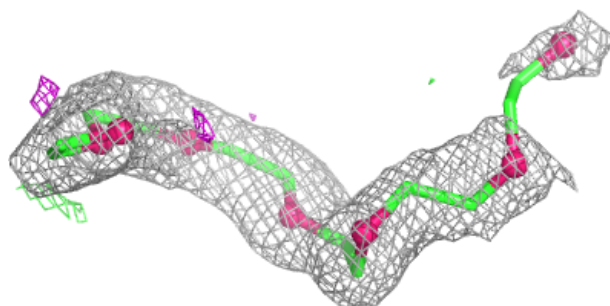
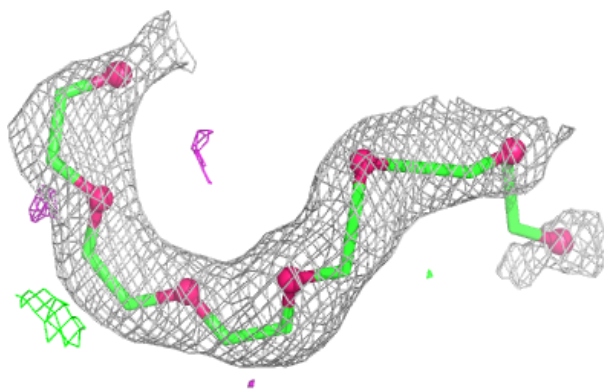
**Electron density around P6G B 715:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



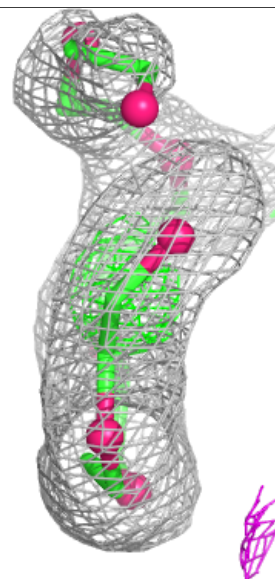
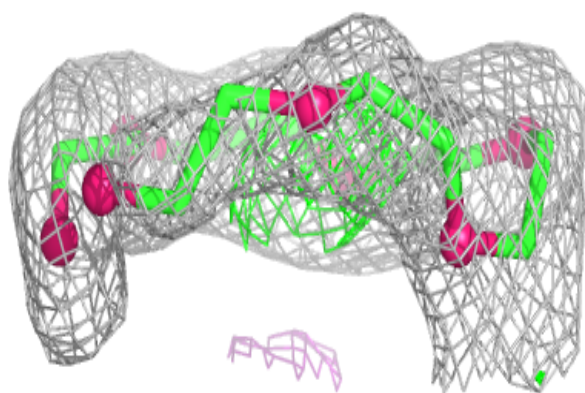
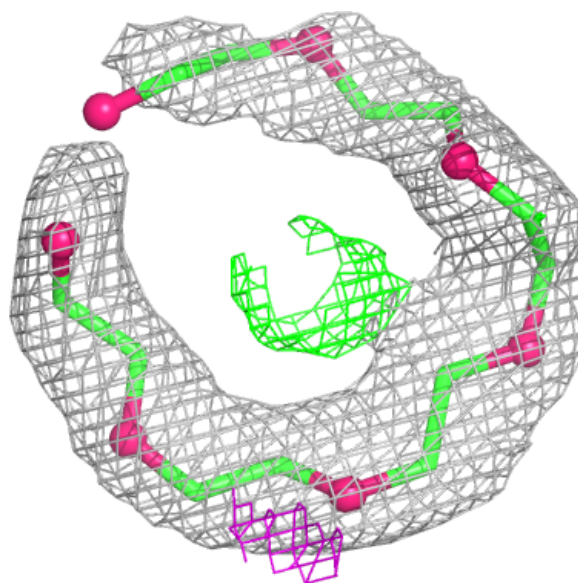
Electron density around P6G A 710:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



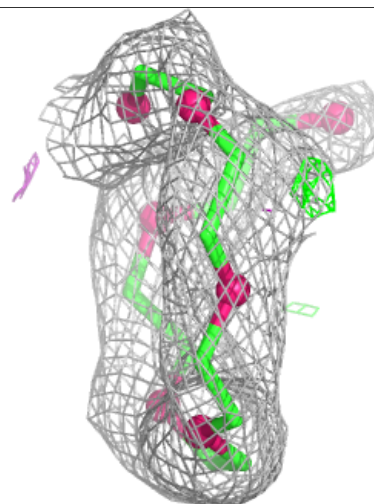
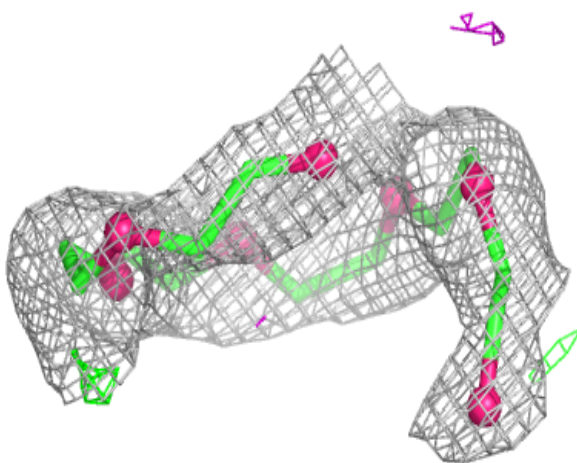
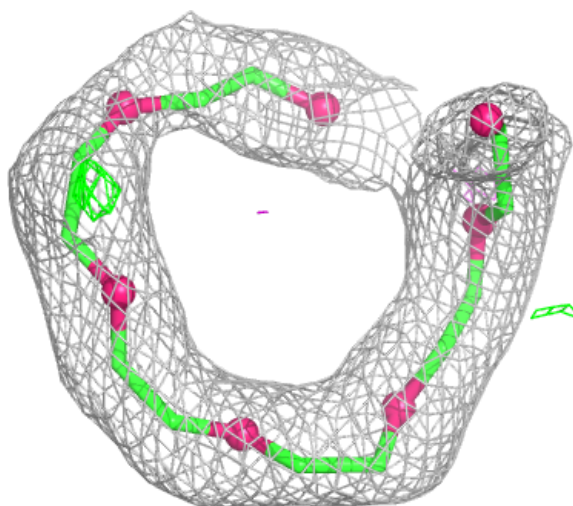
Electron density around P6G C 712:

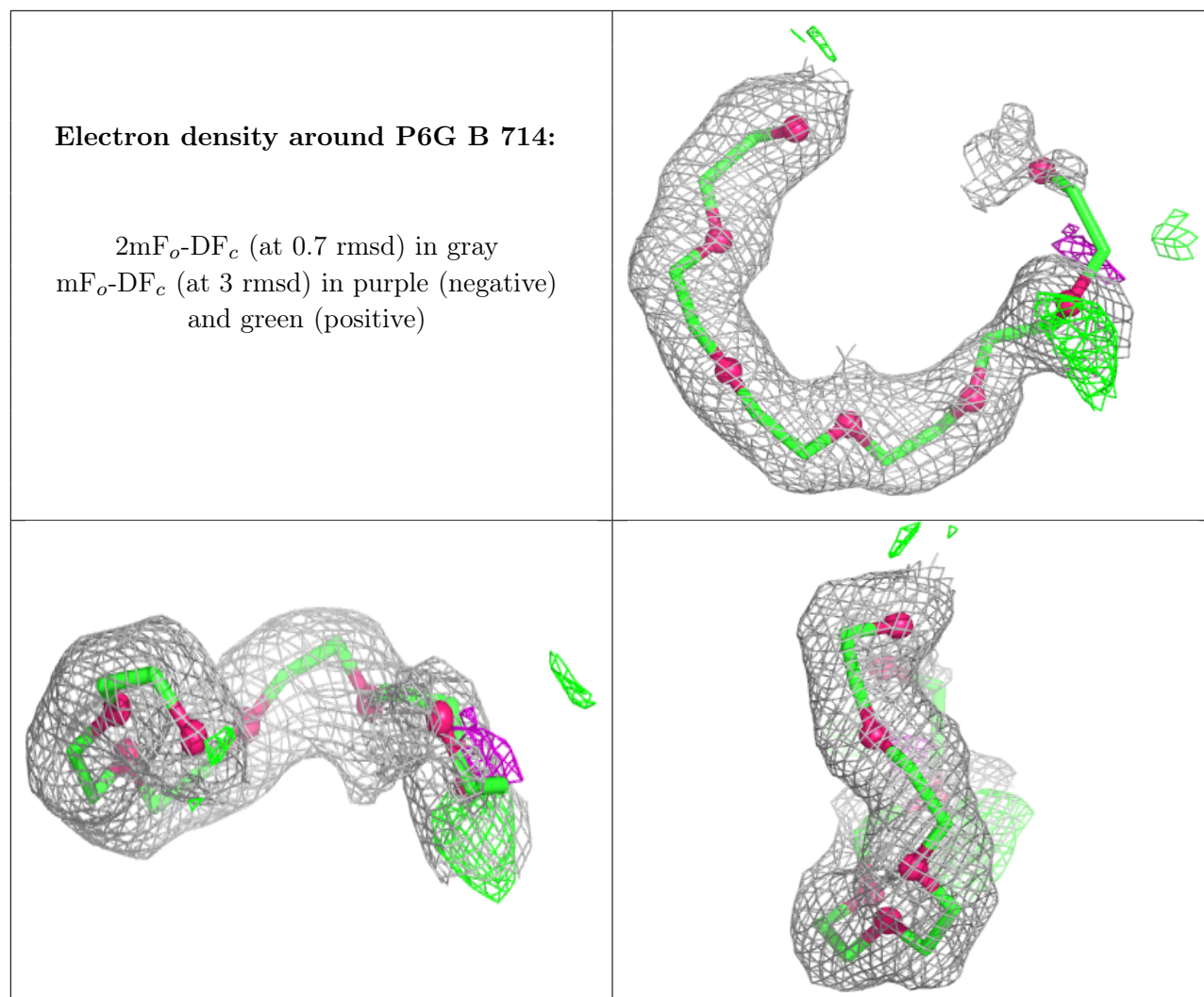
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around P6G F 710:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.