Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:57 PM BST

PDB ID	:	5VTA
Title	:	Co-Crystal Structure of DPPIV with a Chemibody Inhibitor
Authors	:	Wang, Z.; Johnstone, S.; Cheng, A.
Deposited on	:	2017-05-16
Resolution	:	2.80 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 following versions of software and data (see references ⓘ) were used in the production of this report:

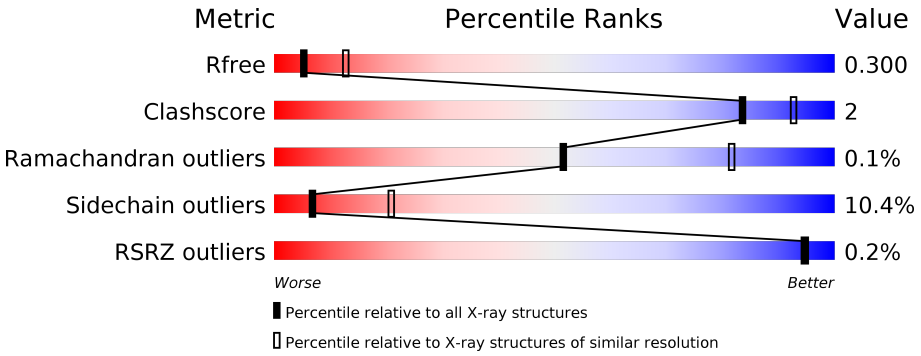
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	739	89% 9%
1	B	739	87% 10%
1	C	739	84% 13%
1	D	739	87% 11%
2	E	213	% 80% 15%
2	G	213	38% 9% 53%

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Mol	Chain	Length	Quality of chain
2	J	213	
2	L	213	
3	F	217	
3	H	217	
3	I	217	
3	K	217	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 33875 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5929	3798	981	1124	26			
1	B	718	Total	C	N	O	S	0	1	0
			5852	3752	967	1107	26			
1	C	728	Total	C	N	O	S	0	0	0
			5929	3798	981	1124	26			
1	D	727	Total	C	N	O	S	0	0	0
			5921	3792	980	1123	26			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	768	HIS	-	expression tag	UNP P14740
A	769	HIS	-	expression tag	UNP P14740
A	770	HIS	-	expression tag	UNP P14740
A	771	HIS	-	expression tag	UNP P14740
A	772	HIS	-	expression tag	UNP P14740
A	773	HIS	-	expression tag	UNP P14740
A	774	HIS	-	expression tag	UNP P14740
A	775	HIS	-	expression tag	UNP P14740
B	768	HIS	-	expression tag	UNP P14740
B	769	HIS	-	expression tag	UNP P14740
B	770	HIS	-	expression tag	UNP P14740
B	771	HIS	-	expression tag	UNP P14740
B	772	HIS	-	expression tag	UNP P14740
B	773	HIS	-	expression tag	UNP P14740
B	774	HIS	-	expression tag	UNP P14740
B	775	HIS	-	expression tag	UNP P14740
C	768	HIS	-	expression tag	UNP P14740
C	769	HIS	-	expression tag	UNP P14740
C	770	HIS	-	expression tag	UNP P14740
C	771	HIS	-	expression tag	UNP P14740
C	772	HIS	-	expression tag	UNP P14740

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Chain	Residue	Modelled	Actual	Comment	Reference
C	773	HIS	-	expression tag	UNP P14740
C	774	HIS	-	expression tag	UNP P14740
C	775	HIS	-	expression tag	UNP P14740
D	768	HIS	-	expression tag	UNP P14740
D	769	HIS	-	expression tag	UNP P14740
D	770	HIS	-	expression tag	UNP P14740
D	771	HIS	-	expression tag	UNP P14740
D	772	HIS	-	expression tag	UNP P14740
D	773	HIS	-	expression tag	UNP P14740
D	774	HIS	-	expression tag	UNP P14740
D	775	HIS	-	expression tag	UNP P14740

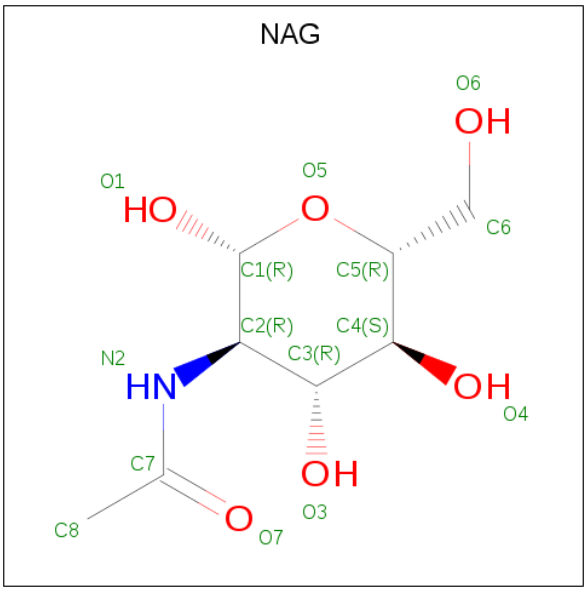
- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	208	Total	C	N	O	S	0	0	0
			1578	986	268	317	7			
2	E	204	Total	C	N	O	S	0	0	0
			1546	966	263	310	7			
2	G	100	Total	C	N	O	S	0	0	0
			747	467	131	144	5			
2	J	89	Total	C	N	O	S	0	0	0
			669	420	119	125	5			

- Molecule 3 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	217	Total	C	N	O	S	0	0	0
			1639	1040	267	327	5			
3	F	217	Total	C	N	O	S	0	0	0
			1639	1040	267	327	5			
3	I	115	Total	C	N	O	S	0	0	0
			899	573	146	177	3			
3	K	110	Total	C	N	O	S	0	0	0
			860	549	141	167	3			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0

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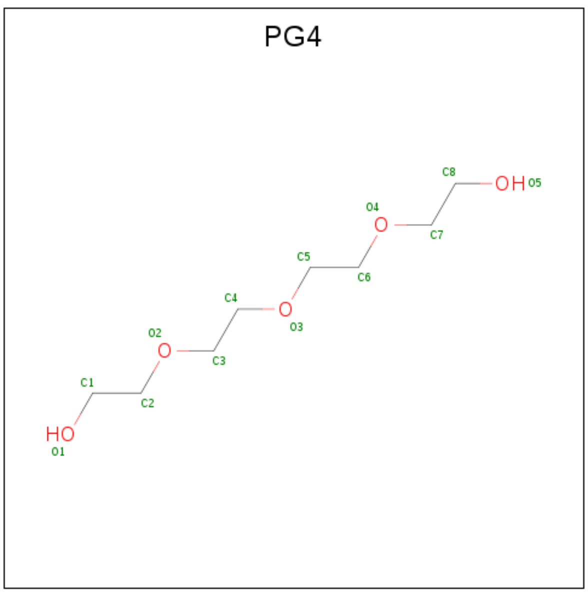
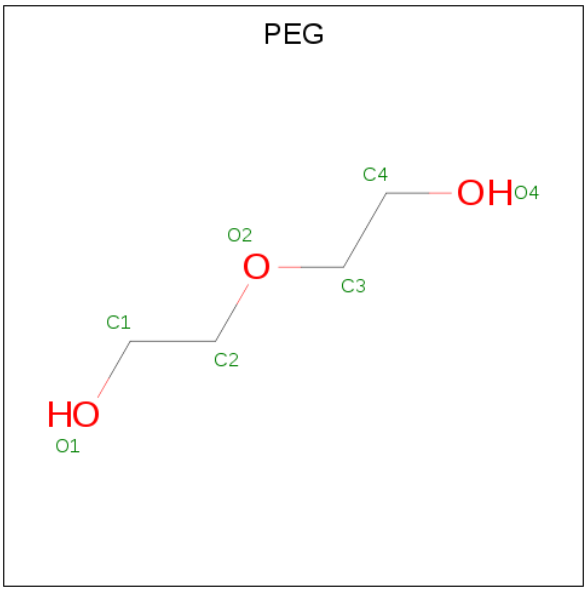
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



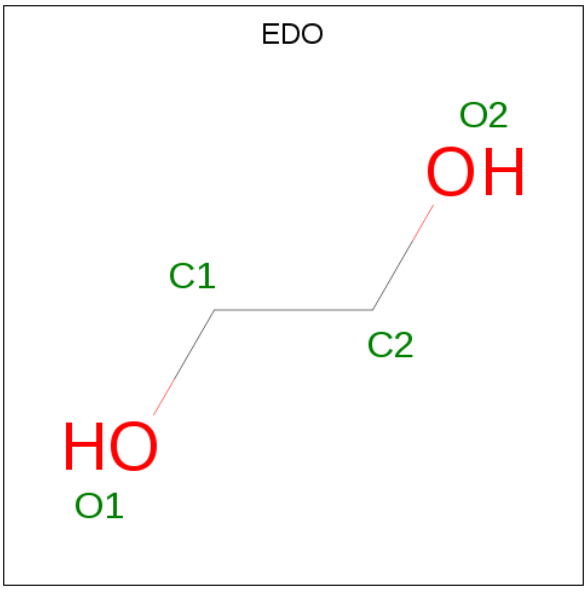
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 8 5	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		

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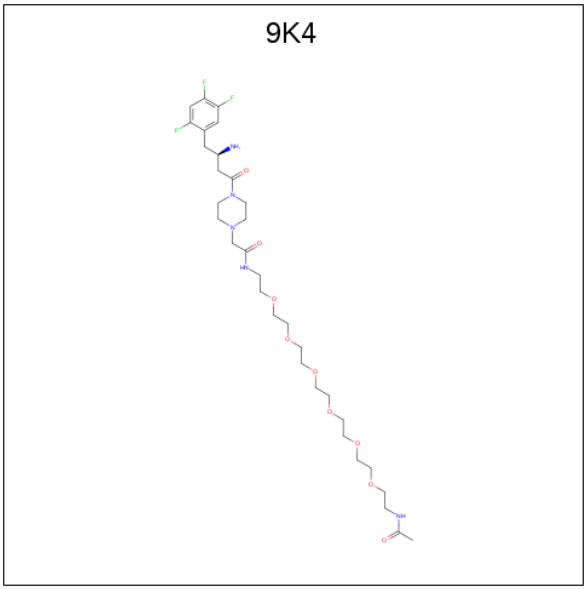
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is 2-{4-[(3R)-3-amino-4-(2,4,5-trifluorophenyl)butanoyl]piperazin-1-yl}-N-(22-oxo-3,6,9,12,15,18-hexaoxa-21-azatricosan-1-yl)acetamide (three-letter code: 9K4) (formula: $C_{32}H_{52}F_3N_5O_9$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	F	N	O	0	0
			43	28	3	4	8		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	F	N	O	0	0
			49	32	3	5	9		
8	C	1	Total	C	F	N	O	0	0
			40	26	3	4	7		
8	D	1	Total	C	F	N	O	0	0
			49	32	3	5	9		

- Molecule 9 is water.

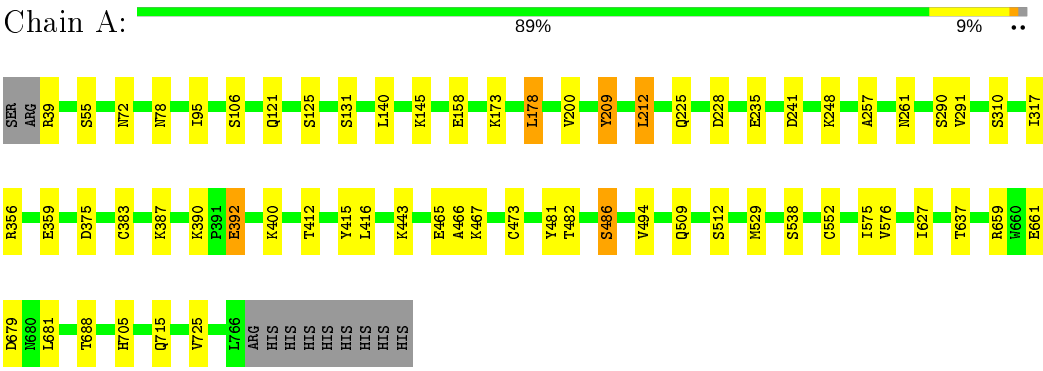
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	36	Total	O	0	0
			36	36		
9	B	28	Total	O	0	0
			28	28		
9	C	24	Total	O	0	0
			24	24		
9	D	16	Total	O	0	0
			16	16		
9	L	2	Total	O	0	0
			2	2		
9	E	2	Total	O	0	0
			2	2		
9	H	5	Total	O	0	0
			5	5		
9	F	2	Total	O	0	0
			2	2		
9	G	1	Total	O	0	0
			1	1		
9	J	1	Total	O	0	0
			1	1		
9	K	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

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

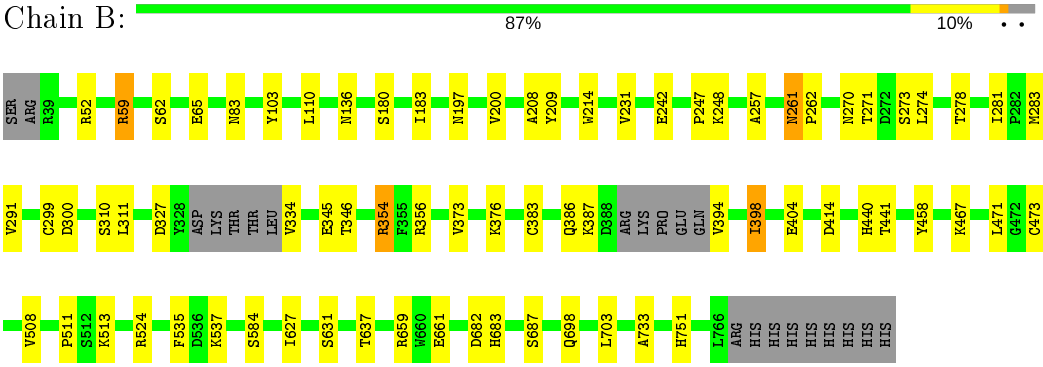
- Molecule 1: Dipeptidyl peptidase 4

Chain A:



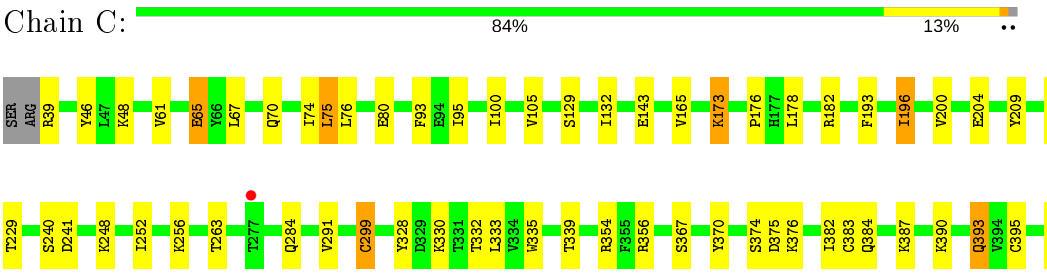
- Molecule 1: Dipeptidyl peptidase 4

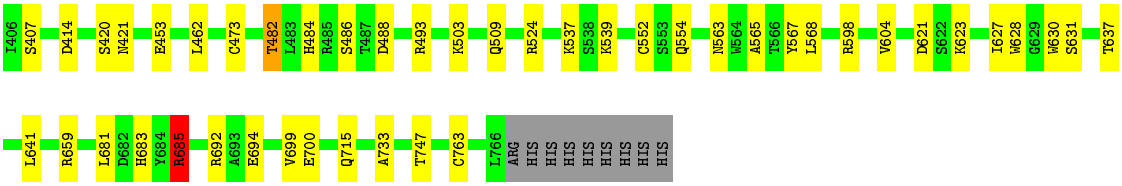
Chain B:



- Molecule 1: Dipeptidyl peptidase 4

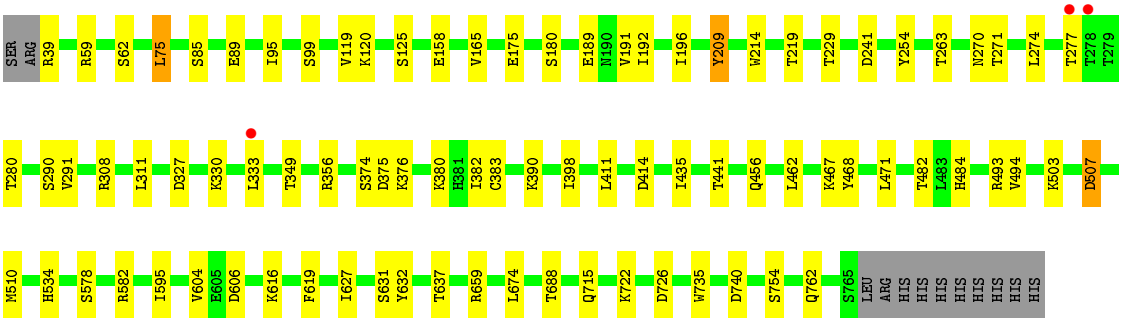
Chain C:





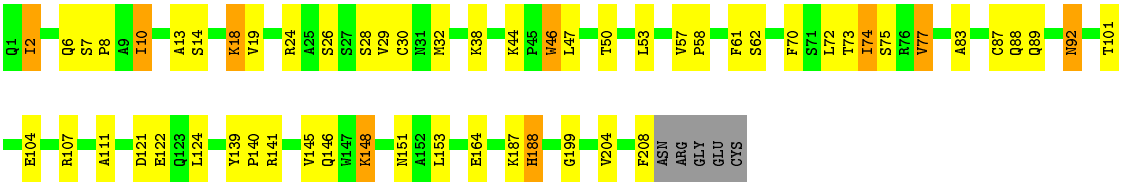
• Molecule 1: Dipeptidyl peptidase 4

Chain D:



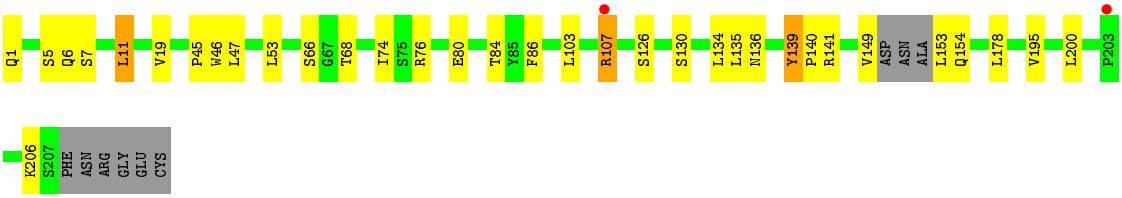
• Molecule 2: Fab light chain

Chain L:



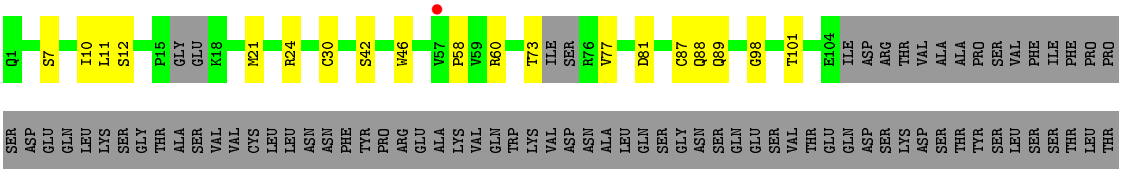
• Molecule 2: Fab light chain

Chain E:



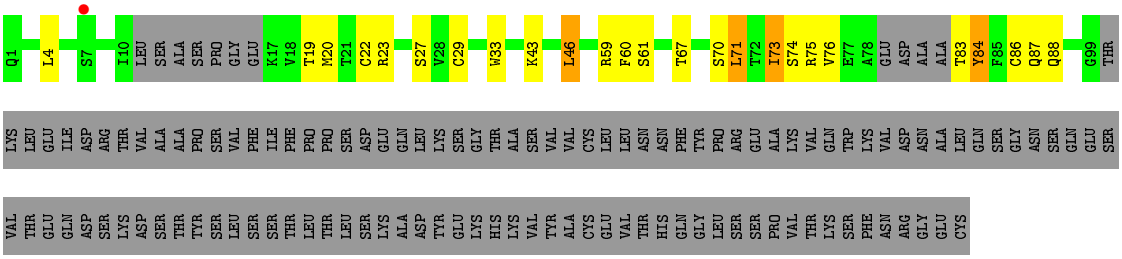
• Molecule 2: Fab light chain

Chain G:



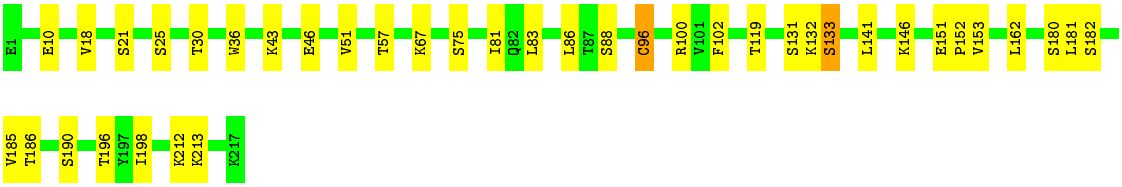
• Molecule 2: Fab light chain

Chain J:



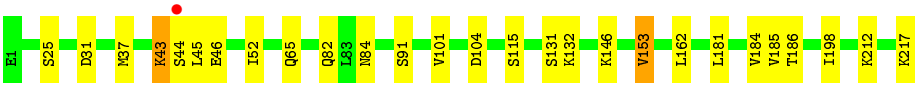
• Molecule 3: Fab heavy chain

Chain H:



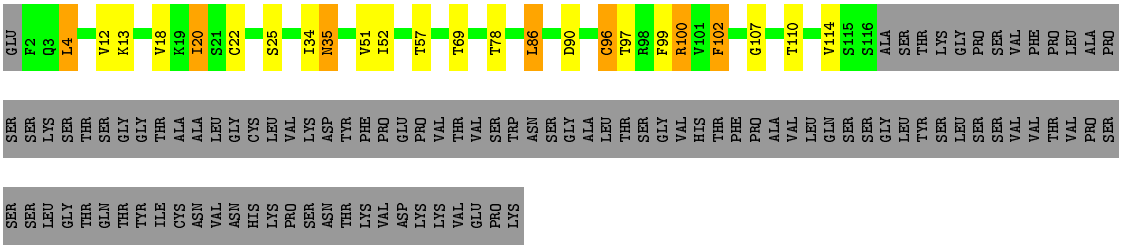
• Molecule 3: Fab heavy chain

Chain F:



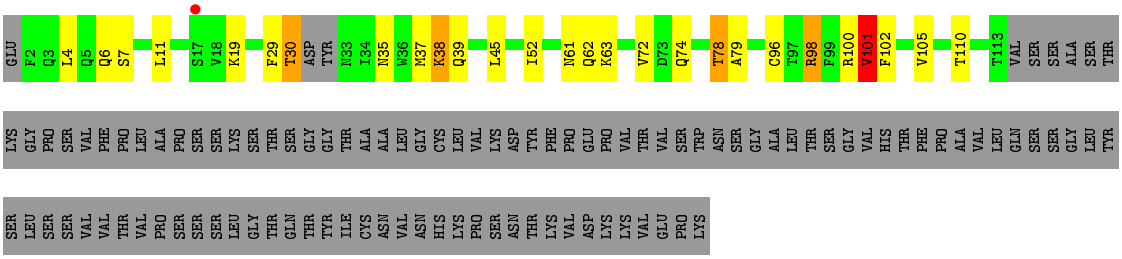
• Molecule 3: Fab heavy chain

Chain I:



• Molecule 3: Fab heavy chain

Chain K:


GLU F2 Q3 L4 Q5 Q6 S7 L11 S17 V18 K19 F29 T30 ASP TYR N33 I34 N35 W36 M37 K38 Q39 L45 I52 N61 Q62 K63 V72 D73 Q74 T78 A79 C96 T97 R98 F99 R100 V101 F102 V105 T110 T113 VAL SER SER ALA SER THR
LYS GLY PRO SER VAL PHE PRO LEU ALA PRO SER SER LYS SER THR SER GLY GLY THR ALA ALA LEU GLY CYS LEU VAL LYS ASP TYR PHE PRO GLU PRO VAL THR VAL SER TRP ASN SER GLY ALA LEU THR SER GLY VAL HIS THR PHE PRO ALA VAL LEU GLN SER SER GLY LEU TYR
SER LEU SER SER VAL VAL THR VAL PRO SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS LYS VAL GLU PRO LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	120.33Å 123.23Å 129.02Å 62.34° 77.21° 75.91°	Depositor
Resolution (Å)	30.00 – 2.80 29.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.5 (30.00-2.80) 88.6 (29.96-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.250 , 0.300 0.253 , 0.300	Depositor DCC
R_{free} test set	6869 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 13.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	33875	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PG4, 9K4, NAG, EDO

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	0.56	0/6098	0.73	0/8291
1	B	0.59	0/6022	0.76	0/8186
1	C	0.56	0/6098	0.73	1/8291 (0.0%)
1	D	0.55	0/6090	0.73	0/8280
2	E	0.54	0/1583	0.72	0/2152
2	G	0.57	0/767	0.73	0/1041
2	J	0.55	0/688	0.68	0/933
2	L	0.61	0/1617	0.75	0/2200
3	F	0.55	0/1679	0.70	0/2287
3	H	0.54	0/1679	0.73	1/2287 (0.0%)
3	I	0.57	0/920	0.75	1/1249 (0.1%)
3	K	0.61	0/879	0.82	2/1191 (0.2%)
All	All	0.56	0/34120	0.74	5/46388 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	685	ARG	NE-CZ-NH2	9.34	124.97	120.30
3	H	151	GLU	C-N-CD	-5.76	107.93	120.60
3	K	98	ARG	NE-CZ-NH1	5.52	123.06	120.30
3	K	98	ARG	NE-CZ-NH2	-5.39	117.61	120.30
3	I	100	ARG	NE-CZ-NH1	5.14	122.87	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5929	0	5664	23	0
1	B	5852	0	5581	18	0
1	C	5929	0	5663	34	0
1	D	5921	0	5652	26	0
2	E	1546	0	1499	9	0
2	G	747	0	716	3	0
2	J	669	0	642	5	0
2	L	1578	0	1524	23	0
3	F	1639	0	1613	8	0
3	H	1639	0	1613	7	0
3	I	899	0	870	8	0
3	K	860	0	837	7	0
4	A	70	0	65	1	0
4	B	56	0	52	1	0
4	C	84	0	78	1	0
4	D	84	0	78	1	0
5	A	13	0	18	0	0
6	A	14	0	20	0	0
6	D	7	0	10	1	0
7	A	16	0	24	1	0
7	B	4	0	6	1	0
7	C	20	0	30	0	0
8	A	43	0	0	0	0
8	B	49	0	0	1	0
8	C	40	0	0	2	0
8	D	49	0	0	0	0
9	A	36	0	0	0	0
9	B	28	0	0	0	0
9	C	24	0	0	0	0
9	D	16	0	0	0	0
9	E	2	0	0	0	0
9	F	2	0	0	0	0
9	G	1	0	0	0	0
9	H	5	0	0	0	0
9	J	1	0	0	0	0
9	K	1	0	0	0	0
9	L	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	33875	0	32255	161	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 2.

All (161) 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)
2:E:134:LEU:HD22	3:F:184:VAL:HG11	1.61	0.80
1:D:219:THR:HG22	1:D:270:ASN:HD21	1.57	0.69
2:J:60:PHE:CE1	2:J:73:ILE:HD13	2.31	0.66
2:L:47:LEU:HD11	2:L:72:LEU:HD13	1.77	0.65
3:K:39:GLN:HB2	3:K:45:LEU:HD23	1.79	0.64
8:B:806:9K4:N41	2:G:30:CYS:SG	2.72	0.63
1:C:382:ILE:HG13	1:C:405:VAL:HG11	1.80	0.63
1:D:75:LEU:HB3	1:D:85:SER:O	1.99	0.63
1:A:121:GLN:HE21	1:A:125:SER:HB2	1.69	0.58
1:A:681:LEU:HG	1:A:681:LEU:O	2.04	0.57
1:B:261:ASN:HD22	1:B:262:PRO:HD2	1.67	0.57
2:E:107:ARG:HG2	2:E:140:PRO:HB3	1.86	0.57
1:B:83:ASN:ND2	4:B:801:NAG:H83	2.19	0.56
1:C:240:SER:O	1:D:722:LYS:NZ	2.37	0.56
1:A:55:SER:HA	1:A:481:TYR:CE1	2.40	0.56
2:L:148:LYS:HE3	2:L:151:ASN:HA	1.87	0.56
3:F:162:LEU:HD21	3:F:185:VAL:HG21	1.89	0.55
2:E:47:LEU:HG	2:E:53:LEU:HD23	1.88	0.55
1:A:466:ALA:O	1:A:486:SER:OG	2.16	0.55
1:A:241:ASP:OD1	2:J:67:THR:OG1	2.20	0.55
1:C:659:ARG:HH22	1:C:685:ARG:HD3	1.72	0.54
2:J:33:TRP:HB2	2:J:46:LEU:HB2	1.90	0.54
2:L:61:PHE:CD2	2:L:74:ILE:HG22	2.43	0.54
3:H:83:LEU:HB3	3:H:86:LEU:HD21	1.89	0.54
1:A:392:GLU:OE2	1:A:392:GLU:N	2.41	0.54
1:C:354:ARG:HD3	1:C:552:CYS:SG	2.48	0.54
2:L:153:LEU:HD23	2:L:153:LEU:O	2.08	0.53
1:A:173:LYS:NZ	1:A:178:LEU:O	2.41	0.53
3:K:101:VAL:HG12	3:K:102:PHE:HD1	1.73	0.53
1:B:354:ARG:NH1	1:B:404:GLU:OE1	2.41	0.53
1:C:565:ALA:HA	1:C:568:LEU:HD12	1.90	0.53
1:C:733:ALA:HB1	1:D:735:TRP:CZ3	2.44	0.52
2:E:139:TYR:N	2:E:139:TYR:HD1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:ARG:HH21	1:C:685:ARG:HG2	1.75	0.51
1:C:132:ILE:HG21	1:C:176:PRO:HB3	1.93	0.51
1:C:393:GLN:N	1:C:393:GLN:HE21	2.09	0.51
2:L:13:ALA:HB2	2:L:19:VAL:HG11	1.91	0.51
1:C:95:ILE:HD11	3:F:52:ILE:HG13	1.93	0.51
1:B:458:TYR:CD1	1:B:471:LEU:HD22	2.47	0.50
1:B:398:ILE:HD12	1:B:440:HIS:CE1	2.46	0.50
1:C:328:TYR:HB2	1:C:335:TRP:CH2	2.47	0.50
1:D:219:THR:HG22	1:D:270:ASN:ND2	2.25	0.50
2:L:122:GLU:OE1	3:H:212:LYS:NZ	2.45	0.50
3:H:153:VAL:CG2	3:H:181:LEU:HD21	2.42	0.49
1:C:212:LEU:HD12	1:C:212:LEU:O	2.12	0.49
1:C:65:GLU:HB2	1:C:76:LEU:HD21	1.94	0.49
2:L:74:ILE:HD11	2:L:77:VAL:HG12	1.94	0.49
2:E:139:TYR:N	2:E:139:TYR:CD1	2.80	0.49
2:L:111:ALA:HB2	2:L:199:GLY:HA3	1.95	0.49
1:A:355:PHE:O	1:A:670:ARG:NH1	2.46	0.49
1:C:61:VAL:HG11	1:C:67:LEU:HD13	1.94	0.49
1:D:471:LEU:HD12	1:D:484:HIS:NE2	2.27	0.48
3:F:37:MET:HB3	3:F:45:LEU:HD12	1.96	0.48
1:A:95:ILE:HD12	1:A:140:LEU:HD21	1.95	0.48
1:C:46:TYR:CE1	1:C:563:ASN:HA	2.49	0.48
1:D:467:LYS:HG2	1:D:468:TYR:CE1	2.49	0.48
1:C:621:ASP:OD1	1:C:623:LYS:N	2.46	0.47
1:C:65:GLU:CB	1:C:76:LEU:HD21	2.45	0.47
4:C:805:NAG:H83	4:C:805:NAG:H3	1.97	0.47
3:H:162:LEU:HD21	3:H:185:VAL:HG21	1.97	0.47
2:L:121:ASP:N	2:L:121:ASP:OD1	2.48	0.46
3:K:100:ARG:O	3:K:100:ARG:HG2	2.15	0.46
1:D:125:SER:HB3	1:D:209:TYR:CG	2.50	0.46
1:D:631:SER:OG	1:D:632:TYR:N	2.47	0.46
1:D:99:SER:HB2	2:L:92:ASN:HA	1.96	0.46
1:D:192:ILE:HG12	4:D:806:NAG:H82	1.97	0.46
2:J:71:LEU:O	2:J:71:LEU:HD23	2.15	0.46
1:C:173:LYS:NZ	1:C:178:LEU:O	2.49	0.46
3:I:20:ILE:HD12	3:I:110:THR:HB	1.98	0.46
1:D:582:ARG:N	1:D:606:ASP:OD2	2.48	0.46
2:L:47:LEU:CD2	2:L:53:LEU:HD23	2.45	0.46
2:L:8:PRO:O	2:L:101:THR:HG23	2.16	0.46
1:D:214:TRP:CZ3	1:D:271:THR:HG21	2.51	0.46
3:F:153:VAL:HG12	3:F:181:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:57:VAL:HG22	2:L:58:PRO:HD2	1.98	0.46
2:L:32:MET:CE	2:L:87:CYS:HB2	2.46	0.45
1:A:725:VAL:HG22	1:B:751:HIS:CG	2.51	0.45
1:C:370:TYR:CZ	1:C:384:GLN:HG3	2.51	0.45
2:L:32:MET:HG3	2:L:70:PHE:CG	2.51	0.45
1:B:627:ILE:HG23	1:B:637:THR:HG23	1.98	0.45
1:C:165:VAL:HG11	1:C:196:ILE:HG12	1.99	0.45
1:C:299:CYS:O	1:C:356:ARG:NH1	2.50	0.45
2:J:84:TYR:N	2:J:84:TYR:CD1	2.85	0.45
2:L:38:LYS:HG3	2:L:83:ALA:HB2	1.99	0.45
1:C:70:GLN:HB3	1:C:75:LEU:HD21	1.99	0.45
3:H:153:VAL:HG23	3:H:181:LEU:HD21	1.98	0.44
3:I:52:ILE:HD12	3:I:57:THR:HB	2.00	0.44
2:L:47:LEU:HD23	2:L:53:LEU:HD23	1.99	0.44
1:C:598:ARG:HA	1:C:683:HIS:CD2	2.53	0.44
1:C:256:LYS:NZ	1:C:715:GLN:OE1	2.48	0.44
1:D:627:ILE:HG23	1:D:637:THR:HG23	1.99	0.44
1:D:722:LYS:HG3	6:D:807:PEG:H41	1.98	0.44
1:A:212:LEU:HD12	1:A:212:LEU:O	2.18	0.44
1:A:257:ALA:HB3	1:A:661:GLU:HA	1.98	0.44
3:F:82:GLN:NE2	3:F:84:ASN:OD1	2.51	0.44
3:I:12:VAL:HG21	3:I:86:LEU:HD23	2.00	0.44
1:B:584:SER:HB3	7:B:805:EDO:H12	1.99	0.44
1:C:681:LEU:O	1:C:681:LEU:HG	2.17	0.44
1:A:529:MET:HE2	1:A:575:ILE:HG21	2.00	0.44
2:E:45:PRO:HG2	3:F:104:ASP:O	2.18	0.44
2:G:87:CYS:O	2:G:98:GLY:N	2.50	0.44
1:B:386:GLN:OE1	1:B:386:GLN:N	2.50	0.43
1:D:274:LEU:HD23	1:D:280:THR:HG21	2.00	0.43
3:I:35:ASN:HD21	3:I:99:PHE:HB2	1.83	0.43
3:I:4:LEU:HB3	3:I:22:CYS:SG	2.58	0.43
1:A:627:ILE:HG23	1:A:637:THR:HG23	2.00	0.43
1:B:257:ALA:HB3	1:B:661:GLU:HA	2.00	0.43
1:C:93:PHE:HD1	1:C:100:ILE:HD12	1.83	0.43
1:D:120:LYS:NZ	1:D:740:ASP:OD2	2.49	0.43
1:A:659:ARG:HG3	1:A:688:THR:HG22	2.00	0.43
3:I:18:VAL:HG12	3:I:86:LEU:HD21	2.00	0.43
3:K:38:LYS:O	3:K:38:LYS:HG3	2.18	0.43
1:D:191:VAL:HG12	1:D:192:ILE:HD12	2.01	0.43
1:D:308:ARG:NE	1:D:327:ASP:OD2	2.52	0.43
3:H:36:TRP:CH2	3:H:96:CYS:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:LEU:O	1:B:733:ALA:HA	2.18	0.43
1:D:165:VAL:HG11	1:D:196:ILE:HG23	2.01	0.42
2:L:2:ILE:HG23	2:L:92:ASN:HD21	1.85	0.42
1:A:576:VAL:HG12	7:A:811:EDO:H12	2.01	0.42
1:B:59:ARG:NH1	1:B:103:TYR:O	2.53	0.42
1:C:747:THR:HG21	1:D:726:ASP:HA	2.01	0.42
1:A:317:ILE:HA	1:A:317:ILE:HD13	1.90	0.42
1:A:467:LYS:C	1:A:486:SER:OG	2.58	0.42
1:C:627:ILE:HG23	1:C:637:THR:HG23	2.01	0.42
3:K:61:ASN:OD1	3:K:62:GLN:N	2.53	0.42
1:A:678:GLU:CD	1:A:678:GLU:H	2.22	0.42
1:C:204:GLU:OE2	8:C:812:9K4:N11	2.53	0.42
1:B:683:HIS:O	1:B:687:SER:OG	2.29	0.41
3:I:102:PHE:H	3:I:102:PHE:HD1	1.68	0.41
3:F:43:LYS:N	3:F:43:LYS:HD3	2.35	0.41
1:A:482:THR:HG22	1:A:494:VAL:HG22	2.01	0.41
1:A:78:ASN:HB2	4:A:801:NAG:H82	2.03	0.41
1:D:471:LEU:HA	1:D:471:LEU:HD23	1.97	0.41
2:L:188:HIS:N	2:L:188:HIS:ND1	2.69	0.41
1:A:715:GLN:NE2	1:B:247:PRO:HD3	2.35	0.41
1:D:125:SER:HB3	1:D:209:TYR:CD1	2.56	0.41
2:E:6:GLN:HE22	2:E:86:PHE:HA	1.86	0.41
1:C:631:SER:HB3	8:C:812:9K4:C05	2.51	0.41
2:L:46:TRP:CZ2	2:L:57:VAL:HG23	2.56	0.41
1:A:125:SER:HB3	1:A:209:TYR:CD1	2.55	0.41
1:B:197:ASN:ND2	1:B:208:ALA:O	2.51	0.41
1:C:482:THR:OG1	1:C:484:HIS:NE2	2.53	0.41
1:D:595:ILE:C	1:D:595:ILE:HD12	2.41	0.41
3:K:78:THR:OG1	3:K:79:ALA:N	2.54	0.41
1:B:183:ILE:CD1	1:B:274:LEU:HD21	2.51	0.41
1:D:507:ASP:OD1	1:D:507:ASP:N	2.54	0.41
1:C:328:TYR:HB2	1:C:335:TRP:CZ3	2.56	0.40
2:L:10:ILE:HD11	2:L:104:GLU:HB3	2.04	0.40
1:C:74:ILE:N	1:C:74:ILE:HD12	2.36	0.40
3:I:96:CYS:O	3:I:107:GLY:N	2.54	0.40
1:D:659:ARG:HB2	1:D:688:THR:HG22	2.02	0.40
2:E:11:LEU:HD11	2:E:19:VAL:CG1	2.51	0.40
2:G:11:LEU:C	2:G:11:LEU:HD12	2.42	0.40
3:H:133:SER:O	3:H:133:SER:OG	2.38	0.40
3:K:29:PHE:O	3:K:30:THR:HB	2.22	0.40
1:B:214:TRP:CZ3	1:B:271:THR:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:LEU:HA	1:B:508:VAL:HG12	2.04	0.40
2:E:135:LEU:HD21	2:E:195:VAL:HG13	2.03	0.40
2:L:18:LYS:HB3	2:L:75:SER:O	2.22	0.40
1:C:641:LEU:HB3	1:C:699:VAL:HG21	2.02	0.40
2:L:139:TYR:HB2	2:L:140:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/739 (98%)	690 (95%)	36 (5%)	0	100	100
1	B	713/739 (96%)	682 (96%)	31 (4%)	0	100	100
1	C	726/739 (98%)	686 (94%)	40 (6%)	0	100	100
1	D	725/739 (98%)	676 (93%)	49 (7%)	0	100	100
2	E	200/213 (94%)	190 (95%)	10 (5%)	0	100	100
2	G	94/213 (44%)	89 (95%)	4 (4%)	1 (1%)	14	41
2	J	83/213 (39%)	80 (96%)	2 (2%)	1 (1%)	13	39
2	L	206/213 (97%)	196 (95%)	10 (5%)	0	100	100
3	F	215/217 (99%)	204 (95%)	10 (5%)	1 (0%)	29	61
3	H	215/217 (99%)	207 (96%)	7 (3%)	1 (0%)	29	61
3	I	113/217 (52%)	105 (93%)	8 (7%)	0	100	100
3	K	106/217 (49%)	100 (94%)	5 (5%)	1 (1%)	17	46
All	All	4122/4676 (88%)	3905 (95%)	212 (5%)	5 (0%)	51	81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	152	PRO
3	F	101	VAL
3	K	101	VAL
2	J	76	VAL
2	G	58	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	649/660 (98%)	608 (94%)	41 (6%)	18 46
1	B	640/660 (97%)	589 (92%)	51 (8%)	12 34
1	C	649/660 (98%)	584 (90%)	65 (10%)	7 22
1	D	648/660 (98%)	595 (92%)	53 (8%)	11 33
2	E	178/185 (96%)	154 (86%)	24 (14%)	4 11
2	G	84/185 (45%)	70 (83%)	14 (17%)	2 6
2	J	76/185 (41%)	55 (72%)	21 (28%)	0 1
2	L	181/185 (98%)	149 (82%)	32 (18%)	2 5
3	F	189/189 (100%)	173 (92%)	16 (8%)	10 31
3	H	189/189 (100%)	160 (85%)	29 (15%)	2 8
3	I	101/189 (53%)	85 (84%)	16 (16%)	2 8
3	K	96/189 (51%)	77 (80%)	19 (20%)	1 4
All	All	3680/4136 (89%)	3299 (90%)	381 (10%)	7 21

All (381) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	72	ASN
1	A	106	SER
1	A	131	SER
1	A	145	LYS
1	A	158	GLU

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Mol	Chain	Res	Type
1	A	178	LEU
1	A	200	VAL
1	A	209	TYR
1	A	212	LEU
1	A	225	GLN
1	A	228	ASP
1	A	235	GLU
1	A	248	LYS
1	A	261	ASN
1	A	290	SER
1	A	291	VAL
1	A	310	SER
1	A	330	LYS
1	A	356	ARG
1	A	359	GLU
1	A	375	ASP
1	A	383	CYS
1	A	387	LYS
1	A	390	LYS
1	A	392	GLU
1	A	400	LYS
1	A	412	THR
1	A	415	TYR
1	A	416	LEU
1	A	443	LYS
1	A	465	GLU
1	A	473	CYS
1	A	486	SER
1	A	509	GLN
1	A	512	SER
1	A	538	SER
1	A	552	CYS
1	A	678	GLU
1	A	679	ASP
1	A	705	HIS
1	B	52	ARG
1	B	59	ARG
1	B	62	SER
1	B	65	GLU
1	B	110	LEU
1	B	136	ASN
1	B	180	SER

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Mol	Chain	Res	Type
1	B	200	VAL
1	B	209	TYR
1	B	231	VAL
1	B	242	GLU
1	B	248	LYS
1	B	261	ASN
1	B	270	ASN
1	B	273	SER
1	B	278	THR
1	B	281	ILE
1	B	283	MET
1	B	285	ILE
1	B	290	SER
1	B	291	VAL
1	B	299	CYS
1	B	300	ASP
1	B	310	SER
1	B	311	LEU
1	B	327	ASP
1	B	334	VAL
1	B	345	GLU
1	B	346	THR
1	B	354	ARG
1	B	356	ARG
1	B	373	VAL
1	B	376	LYS
1	B	383	CYS
1	B	387	LYS
1	B	394	VAL
1	B	398	ILE
1	B	414	ASP
1	B	441	THR
1	B	467	LYS
1	B	473	CYS
1	B	489	GLN
1	B	511	PRO
1	B	513	LYS
1	B	524	ARG
1	B	535	PHE
1	B	537	LYS
1	B	631	SER
1	B	659	ARG

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Mol	Chain	Res	Type
1	B	682	ASP
1	B	698	GLN
1	C	39	ARG
1	C	48	LYS
1	C	65	GLU
1	C	75	LEU
1	C	80	GLU
1	C	105	VAL
1	C	129	SER
1	C	143	GLU
1	C	173	LYS
1	C	182	ARG
1	C	193	PHE
1	C	196	ILE
1	C	200	VAL
1	C	209	TYR
1	C	217	ASN
1	C	229	THR
1	C	241	ASP
1	C	248	LYS
1	C	252	ILE
1	C	263	THR
1	C	284	GLN
1	C	291	VAL
1	C	299	CYS
1	C	330	LYS
1	C	332	THR
1	C	333	LEU
1	C	339	THR
1	C	367	SER
1	C	374	SER
1	C	375	ASP
1	C	376	LYS
1	C	383	CYS
1	C	387	LYS
1	C	390	LYS
1	C	393	GLN
1	C	395	CYS
1	C	398	ILE
1	C	399	THR
1	C	405	VAL
1	C	407	SER

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Mol	Chain	Res	Type
1	C	414	ASP
1	C	420	SER
1	C	421	ASN
1	C	453	GLU
1	C	462	LEU
1	C	473	CYS
1	C	482	THR
1	C	486	SER
1	C	488	ASP
1	C	493	ARG
1	C	503	LYS
1	C	509	GLN
1	C	524	ARG
1	C	537	LYS
1	C	539	LYS
1	C	554	GLN
1	C	567	TYR
1	C	604	VAL
1	C	628	TRP
1	C	630	TRP
1	C	685	ARG
1	C	692	ARG
1	C	694	GLU
1	C	700	GLU
1	C	763	CYS
1	D	39	ARG
1	D	59	ARG
1	D	62	SER
1	D	75	LEU
1	D	89	GLU
1	D	95	ILE
1	D	119	VAL
1	D	158	GLU
1	D	175	GLU
1	D	180	SER
1	D	189	GLU
1	D	209	TYR
1	D	229	THR
1	D	241	ASP
1	D	254	TYR
1	D	263	THR
1	D	277	THR

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Mol	Chain	Res	Type
1	D	290	SER
1	D	291	VAL
1	D	311	LEU
1	D	330	LYS
1	D	333	LEU
1	D	349	THR
1	D	356	ARG
1	D	374	SER
1	D	375	ASP
1	D	376	LYS
1	D	380	LYS
1	D	382	ILE
1	D	383	CYS
1	D	390	LYS
1	D	398	ILE
1	D	411	LEU
1	D	414	ASP
1	D	435	ILE
1	D	441	THR
1	D	456	GLN
1	D	462	LEU
1	D	482	THR
1	D	493	ARG
1	D	494	VAL
1	D	503	LYS
1	D	507	ASP
1	D	510	MET
1	D	534	HIS
1	D	578	SER
1	D	604	VAL
1	D	616	LYS
1	D	619	PHE
1	D	674	LEU
1	D	715	GLN
1	D	754	SER
1	D	762	GLN
2	L	2	ILE
2	L	6	GLN
2	L	7	SER
2	L	10	ILE
2	L	14	SER
2	L	18	LYS

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Mol	Chain	Res	Type
2	L	24	ARG
2	L	26	SER
2	L	28	SER
2	L	29	VAL
2	L	30	CYS
2	L	44	LYS
2	L	46	TRP
2	L	50	THR
2	L	62	SER
2	L	73	THR
2	L	74	ILE
2	L	77	VAL
2	L	88	GLN
2	L	89	GLN
2	L	92	ASN
2	L	107	ARG
2	L	124	LEU
2	L	141	ARG
2	L	145	VAL
2	L	146	GLN
2	L	148	LYS
2	L	164	GLU
2	L	187	LYS
2	L	188	HIS
2	L	204	VAL
2	L	208	PHE
2	E	1	GLN
2	E	5	SER
2	E	7	SER
2	E	11	LEU
2	E	46	TRP
2	E	66	SER
2	E	68	THR
2	E	74	ILE
2	E	76	ARG
2	E	80	GLU
2	E	84	THR
2	E	103	LEU
2	E	107	ARG
2	E	126	SER
2	E	130	SER
2	E	136	ASN

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Mol	Chain	Res	Type
2	E	139	TYR
2	E	141	ARG
2	E	149	VAL
2	E	153	LEU
2	E	154	GLN
2	E	178	LEU
2	E	200	LEU
2	E	206	LYS
3	H	10	GLU
3	H	18	VAL
3	H	21	SER
3	H	25	SER
3	H	30	THR
3	H	43	LYS
3	H	46	GLU
3	H	51	VAL
3	H	57	THR
3	H	67	LYS
3	H	75	SER
3	H	81	ILE
3	H	88	SER
3	H	96	CYS
3	H	100	ARG
3	H	102	PHE
3	H	119	THR
3	H	131	SER
3	H	132	LYS
3	H	133	SER
3	H	141	LEU
3	H	146	LYS
3	H	180	SER
3	H	182	SER
3	H	186	THR
3	H	190	SER
3	H	196	THR
3	H	198	ILE
3	H	213	LYS
3	F	25	SER
3	F	31	ASP
3	F	43	LYS
3	F	44	SER
3	F	46	GLU

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Mol	Chain	Res	Type
3	F	65	GLN
3	F	91	SER
3	F	115	SER
3	F	131	SER
3	F	132	LYS
3	F	146	LYS
3	F	153	VAL
3	F	186	THR
3	F	198	ILE
3	F	212	LYS
3	F	217	LYS
2	G	7	SER
2	G	10	ILE
2	G	12	SER
2	G	21	MET
2	G	24	ARG
2	G	42	SER
2	G	46	TRP
2	G	60	ARG
2	G	73	THR
2	G	77	VAL
2	G	81	ASP
2	G	88	GLN
2	G	89	GLN
2	G	101	THR
3	I	4	LEU
3	I	13	LYS
3	I	20	ILE
3	I	25	SER
3	I	34	ILE
3	I	35	ASN
3	I	51	VAL
3	I	69	THR
3	I	78	THR
3	I	86	LEU
3	I	90	ASP
3	I	96	CYS
3	I	97	THR
3	I	100	ARG
3	I	102	PHE
3	I	114	VAL
2	J	4	LEU

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Mol	Chain	Res	Type
2	J	19	THR
2	J	20	MET
2	J	22	CYS
2	J	23	ARG
2	J	27	SER
2	J	29	CYS
2	J	43	LYS
2	J	46	LEU
2	J	59	ARG
2	J	61	SER
2	J	70	SER
2	J	71	LEU
2	J	73	ILE
2	J	74	SER
2	J	75	ARG
2	J	83	THR
2	J	84	TYR
2	J	86	CYS
2	J	87	GLN
2	J	88	GLN
3	K	4	LEU
3	K	6	GLN
3	K	7	SER
3	K	11	LEU
3	K	19	LYS
3	K	30	THR
3	K	35	ASN
3	K	37	MET
3	K	38	LYS
3	K	52	ILE
3	K	63	LYS
3	K	72	VAL
3	K	74	GLN
3	K	78	THR
3	K	96	CYS
3	K	98	ARG
3	K	101	VAL
3	K	105	VAL
3	K	110	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	261	ASN
1	A	686	ASN
1	B	261	ASN
1	B	270	ASN
1	B	440	HIS
1	B	506	GLN
1	B	528	GLN
1	C	136	ASN
1	C	393	GLN
1	C	686	ASN
1	C	762	GLN
1	D	49	ASN
1	D	121	GLN
1	D	261	ASN
1	D	270	ASN
1	D	284	GLN
1	D	384	GLN
1	D	506	GLN
1	D	750	GLN
2	L	88	GLN
2	L	89	GLN
2	E	136	ASN
3	H	39	GLN
3	H	65	GLN
3	F	82	GLN
3	F	84	ASN
2	G	52	ASN
2	G	88	GLN
3	I	62	GLN
3	I	84	ASN
2	J	30	ASN
2	J	51	ASN
2	J	87	GLN
3	K	84	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

39 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PEG	D	807	-	6,6,6	0.70	0	5,5,5	0.59	0
4	NAG	A	802	1	14,14,15	0.49	0	17,19,21	1.33	3 (17%)
4	NAG	A	805	1	14,14,15	0.63	0	17,19,21	1.39	2 (11%)
4	NAG	D	806	1	14,14,15	0.34	0	17,19,21	1.31	1 (5%)
4	NAG	D	801	1	14,14,15	0.45	0	17,19,21	1.45	1 (5%)
4	NAG	B	801	1	14,14,15	0.64	0	17,19,21	2.06	5 (29%)
8	9K4	C	812	-	41,41,50	2.53	7 (17%)	45,51,61	1.17	5 (11%)
4	NAG	D	805	1	14,14,15	0.35	0	17,19,21	1.69	3 (17%)
8	9K4	B	806	-	50,50,50	2.51	11 (22%)	55,61,61	1.35	5 (9%)
6	PEG	A	808	-	6,6,6	0.56	0	5,5,5	0.42	0
4	NAG	D	804	1	14,14,15	0.57	0	17,19,21	1.40	2 (11%)
8	9K4	A	813	-	44,44,50	2.44	7 (15%)	48,54,61	1.31	5 (10%)
4	NAG	A	801	1	14,14,15	0.76	1 (7%)	17,19,21	1.84	5 (29%)
4	NAG	C	805	1	14,14,15	0.51	0	17,19,21	2.19	5 (29%)
7	EDO	C	809	-	3,3,3	0.57	0	2,2,2	0.09	0
4	NAG	D	802	1	14,14,15	0.47	0	17,19,21	1.63	2 (11%)
4	NAG	A	803	1	14,14,15	0.53	0	17,19,21	1.91	5 (29%)
7	EDO	B	805	-	3,3,3	0.60	0	2,2,2	0.35	0
7	EDO	C	808	-	3,3,3	0.48	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	EDO	A	809	-	3,3,3	0.75	0	2,2,2	0.51	0
7	EDO	C	807	-	3,3,3	0.45	0	2,2,2	0.26	0
4	NAG	B	803	1	14,14,15	0.43	0	17,19,21	1.77	1 (5%)
4	NAG	C	801	1	14,14,15	0.56	0	17,19,21	1.94	2 (11%)
4	NAG	B	802	1	14,14,15	0.73	0	17,19,21	1.67	4 (23%)
6	PEG	A	807	-	6,6,6	0.45	0	5,5,5	0.35	0
7	EDO	A	810	-	3,3,3	0.46	0	2,2,2	0.31	0
5	PG4	A	806	-	12,12,12	0.58	0	11,11,11	0.41	0
4	NAG	C	804	1	14,14,15	0.33	0	17,19,21	1.53	3 (17%)
4	NAG	A	804	1	14,14,15	0.36	0	17,19,21	1.36	2 (11%)
4	NAG	B	804	1	14,14,15	0.63	1 (7%)	17,19,21	1.50	1 (5%)
7	EDO	A	811	-	3,3,3	0.44	0	2,2,2	0.07	0
7	EDO	C	811	-	3,3,3	0.47	0	2,2,2	0.23	0
7	EDO	C	810	-	3,3,3	0.58	0	2,2,2	0.07	0
4	NAG	C	806	1	14,14,15	0.43	0	17,19,21	1.57	3 (17%)
4	NAG	C	802	1	14,14,15	0.43	0	17,19,21	1.43	2 (11%)
8	9K4	D	808	-	50,50,50	2.59	12 (24%)	55,61,61	1.40	8 (14%)
4	NAG	C	803	1	14,14,15	0.45	0	17,19,21	2.11	1 (5%)
7	EDO	A	812	-	3,3,3	0.63	0	2,2,2	0.35	0
4	NAG	D	803	1	14,14,15	0.54	0	17,19,21	1.35	4 (23%)

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
6	PEG	D	807	-	-	1/4/4/4	-
4	NAG	A	802	1	-	0/6/23/26	0/1/1/1
4	NAG	A	805	1	-	2/6/23/26	0/1/1/1
4	NAG	D	806	1	-	2/6/23/26	0/1/1/1
4	NAG	D	801	1	-	2/6/23/26	0/1/1/1
4	NAG	B	801	1	-	3/6/23/26	0/1/1/1
8	9K4	C	812	-	-	10/32/42/51	0/2/2/2
4	NAG	D	805	1	-	2/6/23/26	0/1/1/1
8	9K4	B	806	-	-	11/41/51/51	0/2/2/2
6	PEG	A	808	-	-	4/4/4/4	-
4	NAG	D	804	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	9K4	A	813	-	-	13/35/45/51	0/2/2/2
4	NAG	A	801	1	-	3/6/23/26	0/1/1/1
4	NAG	C	805	1	-	5/6/23/26	0/1/1/1
7	EDO	C	809	-	-	1/1/1/1	-
4	NAG	D	802	1	-	2/6/23/26	0/1/1/1
4	NAG	A	803	1	-	2/6/23/26	0/1/1/1
7	EDO	B	805	-	-	1/1/1/1	-
7	EDO	C	808	-	-	0/1/1/1	-
7	EDO	A	809	-	-	1/1/1/1	-
7	EDO	C	807	-	-	1/1/1/1	-
4	NAG	B	803	1	-	2/6/23/26	0/1/1/1
4	NAG	C	801	1	-	2/6/23/26	0/1/1/1
4	NAG	B	802	1	-	0/6/23/26	0/1/1/1
6	PEG	A	807	-	-	3/4/4/4	-
7	EDO	A	810	-	-	1/1/1/1	-
5	PG4	A	806	-	-	8/10/10/10	-
4	NAG	C	804	1	-	2/6/23/26	0/1/1/1
4	NAG	A	804	1	-	0/6/23/26	0/1/1/1
4	NAG	B	804	1	-	2/6/23/26	0/1/1/1
7	EDO	A	811	-	-	0/1/1/1	-
7	EDO	C	811	-	-	1/1/1/1	-
7	EDO	C	810	-	-	0/1/1/1	-
4	NAG	C	806	1	-	2/6/23/26	0/1/1/1
4	NAG	C	802	1	-	2/6/23/26	0/1/1/1
8	9K4	D	808	-	-	18/41/51/51	0/2/2/2
4	NAG	C	803	1	-	2/6/23/26	0/1/1/1
7	EDO	A	812	-	-	1/1/1/1	-
4	NAG	D	803	1	-	3/6/23/26	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	808	9K4	C18-N17	-10.00	1.25	1.47
8	C	812	9K4	C18-N17	-9.47	1.26	1.47
8	A	813	9K4	C18-N17	-9.23	1.27	1.47
8	B	806	9K4	C18-N17	-9.11	1.27	1.47
8	A	813	9K4	C13-N14	7.38	1.50	1.35
8	B	806	9K4	C13-N14	7.37	1.50	1.35
8	D	808	9K4	C19-N20	7.08	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	812	9K4	C13-N14	6.93	1.49	1.35
8	B	806	9K4	C19-N20	6.83	1.48	1.33
8	D	808	9K4	C13-N14	6.74	1.48	1.35
8	A	813	9K4	C19-N20	6.72	1.48	1.33
8	C	812	9K4	C19-N20	6.67	1.48	1.33
8	D	808	9K4	C09-C08	5.85	1.59	1.51
8	B	806	9K4	C42-N41	5.27	1.49	1.34
8	D	808	9K4	C42-N41	4.99	1.48	1.34
8	B	806	9K4	C09-C08	4.73	1.57	1.51
8	C	812	9K4	C09-C08	4.33	1.57	1.51
8	A	813	9K4	C09-C08	4.15	1.57	1.51
8	D	808	9K4	C05-C06	3.02	1.42	1.37
8	D	808	9K4	C15-N14	-2.75	1.42	1.47
8	A	813	9K4	C15-N14	-2.63	1.42	1.47
8	C	812	9K4	C15-N14	-2.53	1.42	1.47
8	D	808	9K4	C48-N14	-2.48	1.42	1.47
8	B	806	9K4	C08-C06	2.46	1.42	1.38
8	D	808	9K4	C08-C06	2.37	1.42	1.38
8	B	806	9K4	C21-C22	2.37	1.58	1.50
8	A	813	9K4	C08-C06	2.33	1.42	1.38
8	C	812	9K4	C08-C06	2.32	1.42	1.38
8	D	808	9K4	O45-C42	-2.31	1.18	1.23
8	A	813	9K4	C21-C22	2.30	1.58	1.50
8	C	812	9K4	C21-C22	2.29	1.58	1.50
8	D	808	9K4	C21-C22	2.17	1.58	1.50
8	B	806	9K4	C15-N14	-2.17	1.43	1.47
8	D	808	9K4	C47-N17	-2.14	1.41	1.46
4	A	801	NAG	C1-C2	2.13	1.55	1.52
8	B	806	9K4	C12-C10	2.10	1.56	1.53
4	B	804	NAG	C1-C2	2.04	1.55	1.52
8	B	806	9K4	O45-C42	-2.03	1.18	1.23
8	B	806	9K4	C47-N17	-2.01	1.41	1.46

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	803	NAG	C1-O5-C5	8.37	123.53	112.19
4	B	803	NAG	C1-O5-C5	6.34	120.79	112.19
4	C	801	NAG	C1-O5-C5	6.14	120.51	112.19
4	C	805	NAG	C8-C7-N2	5.62	125.62	116.10
4	D	805	NAG	O5-C1-C2	-5.31	102.91	111.29
4	B	804	NAG	C1-O5-C5	5.30	119.38	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	808	9K4	C47-N17-C16	5.03	120.16	108.83
4	D	801	NAG	C1-O5-C5	4.91	118.85	112.19
4	A	803	NAG	C1-O5-C5	4.76	118.64	112.19
4	B	801	NAG	O5-C1-C2	-4.56	104.08	111.29
4	C	805	NAG	C2-N2-C7	4.42	129.20	122.90
4	D	802	NAG	O5-C1-C2	-4.39	104.36	111.29
8	A	813	9K4	C50-C08-C06	4.14	121.40	116.58
8	B	806	9K4	C50-C08-C06	4.08	121.33	116.58
8	B	806	9K4	C05-C06-C08	-4.02	118.71	123.98
4	B	801	NAG	C8-C7-N2	3.93	122.75	116.10
8	A	813	9K4	C05-C06-C08	-3.87	118.91	123.98
4	C	802	NAG	C1-O5-C5	3.74	117.26	112.19
4	A	801	NAG	C1-O5-C5	3.66	117.16	112.19
8	D	808	9K4	C43-C42-N41	3.62	122.50	116.09
4	A	804	NAG	C1-O5-C5	3.57	117.03	112.19
4	C	804	NAG	C1-O5-C5	3.54	116.99	112.19
4	C	806	NAG	C4-C3-C2	-3.54	105.83	111.02
4	D	804	NAG	O5-C1-C2	-3.51	105.74	111.29
4	A	803	NAG	O5-C1-C2	-3.41	105.91	111.29
4	D	802	NAG	C3-C4-C5	3.30	116.12	110.24
8	C	812	9K4	C50-C08-C06	3.28	120.39	116.58
4	D	805	NAG	C1-O5-C5	3.12	116.42	112.19
4	B	802	NAG	C1-C2-N2	-3.11	105.17	110.49
8	C	812	9K4	C05-C06-C08	-3.04	119.99	123.98
4	A	801	NAG	C3-C4-C5	-3.00	104.89	110.24
4	A	805	NAG	C1-O5-C5	2.99	116.24	112.19
4	C	805	NAG	O7-C7-N2	-2.94	116.54	121.95
4	A	803	NAG	O3-C3-C2	-2.94	103.39	109.47
4	B	801	NAG	C2-N2-C7	2.93	127.08	122.90
4	B	801	NAG	O7-C7-C8	-2.92	116.64	122.06
4	C	806	NAG	O5-C1-C2	-2.88	106.75	111.29
4	D	804	NAG	O5-C5-C6	2.87	111.71	107.20
8	A	813	9K4	F07-C06-C08	2.85	122.61	117.96
4	C	805	NAG	O5-C1-C2	-2.83	106.82	111.29
4	A	805	NAG	O5-C5-C6	2.80	111.59	107.20
4	B	802	NAG	O3-C3-C2	2.78	115.21	109.47
4	A	804	NAG	O5-C1-C2	-2.72	107.00	111.29
4	D	806	NAG	C1-O5-C5	2.69	115.84	112.19
8	D	808	9K4	C48-N14-C15	-2.66	107.50	112.62
4	A	803	NAG	C1-C2-N2	2.63	114.98	110.49
4	B	802	NAG	C1-O5-C5	2.63	115.75	112.19
8	D	808	9K4	C18-N17-C47	2.60	115.13	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	801	NAG	C4-C3-C2	-2.60	107.21	111.02
4	A	802	NAG	O5-C5-C4	-2.59	104.53	110.83
8	D	808	9K4	C05-C06-C08	-2.54	120.65	123.98
4	A	801	NAG	O3-C3-C2	2.53	114.71	109.47
4	A	802	NAG	O5-C5-C6	2.52	111.16	107.20
4	B	801	NAG	C1-O5-C5	2.46	115.53	112.19
4	A	803	NAG	C4-C3-C2	2.44	114.60	111.02
4	D	803	NAG	C8-C7-N2	2.44	120.23	116.10
4	C	806	NAG	C1-O5-C5	2.42	115.47	112.19
8	B	806	9K4	C18-N17-C47	2.41	114.83	111.09
4	C	804	NAG	C2-N2-C7	2.39	126.31	122.90
4	A	802	NAG	O4-C4-C5	2.39	115.23	109.30
8	C	812	9K4	C48-N14-C15	-2.36	108.07	112.62
8	D	808	9K4	C18-N17-C16	2.32	114.69	111.09
4	D	805	NAG	C4-C3-C2	-2.28	107.68	111.02
4	C	805	NAG	O7-C7-C8	-2.27	117.83	122.06
8	B	806	9K4	C50-C02-C03	-2.24	118.48	121.03
8	A	813	9K4	C48-N14-C15	-2.23	108.32	112.62
8	C	812	9K4	C18-N17-C47	2.23	114.55	111.09
8	D	808	9K4	C15-C16-N17	2.22	115.20	110.64
4	D	803	NAG	C1-O5-C5	2.21	115.18	112.19
4	A	801	NAG	C4-C3-C2	-2.18	107.82	111.02
4	D	803	NAG	C2-N2-C7	2.15	125.97	122.90
8	D	808	9K4	F04-C03-C05	2.15	122.89	118.61
8	B	806	9K4	F07-C06-C08	2.12	121.41	117.96
4	D	803	NAG	O5-C5-C6	2.06	110.44	107.20
8	C	812	9K4	F07-C06-C08	2.04	121.29	117.96
4	B	802	NAG	C4-C3-C2	-2.03	108.04	111.02
4	C	804	NAG	O7-C7-N2	2.03	125.68	121.95
4	A	801	NAG	O5-C5-C4	-2.03	105.89	110.83
4	C	802	NAG	O5-C1-C2	-2.01	108.11	111.29
8	A	813	9K4	C18-N17-C47	2.01	114.20	111.09

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	808	9K4	C08-C09-C10-C12
8	D	808	9K4	C09-C10-C12-C13
8	D	808	9K4	N11-C10-C12-C13
4	B	803	NAG	O5-C5-C6-O6
4	A	805	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	D	805	NAG	O5-C5-C6-O6
4	C	805	NAG	O5-C5-C6-O6
4	D	802	NAG	O5-C5-C6-O6
4	B	803	NAG	C4-C5-C6-O6
4	D	802	NAG	C4-C5-C6-O6
4	D	806	NAG	O5-C5-C6-O6
4	C	802	NAG	C4-C5-C6-O6
4	D	806	NAG	C4-C5-C6-O6
8	C	812	9K4	N20-C21-C22-O23
8	B	806	9K4	O32-C33-C34-O35
8	D	808	9K4	O29-C30-C31-O32
8	C	812	9K4	O23-C24-C25-O26
8	D	808	9K4	O32-C33-C34-O35
4	C	802	NAG	O5-C5-C6-O6
4	D	801	NAG	C4-C5-C6-O6
8	D	808	9K4	O35-C36-C37-O38
8	D	808	9K4	C43-C42-N41-C40
8	D	808	9K4	O45-C42-N41-C40
8	A	813	9K4	O26-C27-C28-O29
4	D	805	NAG	C4-C5-C6-O6
4	B	801	NAG	C8-C7-N2-C2
4	B	801	NAG	O7-C7-N2-C2
4	C	805	NAG	C8-C7-N2-C2
4	C	805	NAG	O7-C7-N2-C2
4	D	803	NAG	C8-C7-N2-C2
4	D	803	NAG	O7-C7-N2-C2
4	A	805	NAG	C4-C5-C6-O6
5	A	806	PG4	O2-C3-C4-O3
4	D	801	NAG	O5-C5-C6-O6
4	C	804	NAG	O5-C5-C6-O6
8	B	806	9K4	O38-C39-C40-N41
8	D	808	9K4	O38-C39-C40-N41
4	B	804	NAG	C4-C5-C6-O6
4	C	806	NAG	C4-C5-C6-O6
8	A	813	9K4	O35-C36-C37-O38
7	B	805	EDO	O1-C1-C2-O2
4	C	805	NAG	C4-C5-C6-O6
4	C	804	NAG	C4-C5-C6-O6
4	A	803	NAG	O5-C5-C6-O6
6	A	807	PEG	O2-C3-C4-O4
5	A	806	PG4	O4-C7-C8-O5
8	B	806	9K4	O26-C27-C28-O29

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Mol	Chain	Res	Type	Atoms
8	D	808	9K4	O26-C27-C28-O29
6	A	807	PEG	O1-C1-C2-O2
8	A	813	9K4	O29-C30-C31-O32
8	B	806	9K4	C09-C10-C12-C13
7	C	807	EDO	O1-C1-C2-O2
4	A	801	NAG	O5-C5-C6-O6
4	B	804	NAG	O5-C5-C6-O6
8	A	813	9K4	O32-C33-C34-O35
4	C	803	NAG	C4-C5-C6-O6
4	D	803	NAG	O5-C5-C6-O6
4	C	806	NAG	O5-C5-C6-O6
5	A	806	PG4	O1-C1-C2-O2
4	B	801	NAG	O5-C5-C6-O6
7	A	810	EDO	O1-C1-C2-O2
4	C	801	NAG	C4-C5-C6-O6
4	A	801	NAG	C3-C2-N2-C7
4	C	805	NAG	C3-C2-N2-C7
5	A	806	PG4	O3-C5-C6-O4
8	D	808	9K4	O23-C24-C25-O26
8	A	813	9K4	C21-C22-O23-C24
8	D	808	9K4	C10-C12-C13-O49
4	C	801	NAG	O5-C5-C6-O6
6	A	808	PEG	C4-C3-O2-C2
8	B	806	9K4	C24-C25-O26-C27
6	A	807	PEG	C4-C3-O2-C2
8	D	808	9K4	C10-C12-C13-N14
8	A	813	9K4	C24-C25-O26-C27
8	A	813	9K4	O23-C24-C25-O26
8	D	808	9K4	C08-C09-C10-N11
8	A	813	9K4	C34-C33-O32-C31
8	D	808	9K4	C28-C27-O26-C25
8	D	808	9K4	C30-C31-O32-C33
5	A	806	PG4	C6-C5-O3-C4
8	C	812	9K4	C31-C30-O29-C28
8	B	806	9K4	C40-C39-O38-C37
8	A	813	9K4	C27-C28-O29-C30
8	C	812	9K4	C24-C25-O26-C27
8	D	808	9K4	N20-C21-C22-O23
8	C	812	9K4	C25-C24-O23-C22
4	A	801	NAG	C4-C5-C6-O6
5	A	806	PG4	C5-C6-O4-C7
8	A	813	9K4	C28-C27-O26-C25

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Mol	Chain	Res	Type	Atoms
4	C	803	NAG	O5-C5-C6-O6
8	B	806	9K4	C36-C37-O38-C39
6	A	808	PEG	O1-C1-C2-O2
5	A	806	PG4	C4-C3-O2-C2
7	A	812	EDO	O1-C1-C2-O2
4	A	803	NAG	C4-C5-C6-O6
8	C	812	9K4	C30-C31-O32-C33
8	A	813	9K4	C30-C31-O32-C33
7	C	811	EDO	O1-C1-C2-O2
8	B	806	9K4	C27-C28-O29-C30
8	A	813	9K4	C09-C10-C12-C13
6	D	807	PEG	C4-C3-O2-C2
8	A	813	9K4	C37-C36-O35-C34
8	C	812	9K4	C21-C22-O23-C24
8	C	812	9K4	C34-C33-O32-C31
8	C	812	9K4	O26-C27-C28-O29
7	C	809	EDO	O1-C1-C2-O2
7	A	809	EDO	O1-C1-C2-O2
6	A	808	PEG	O2-C3-C4-O4
4	D	804	NAG	C3-C2-N2-C7
6	A	808	PEG	C1-C2-O2-C3
5	A	806	PG4	C8-C7-O4-C6
8	B	806	9K4	N11-C10-C12-C13
8	C	812	9K4	N17-C18-C19-N20
8	B	806	9K4	O23-C24-C25-O26
8	B	806	9K4	O35-C36-C37-O38
8	D	808	9K4	N17-C18-C19-N20

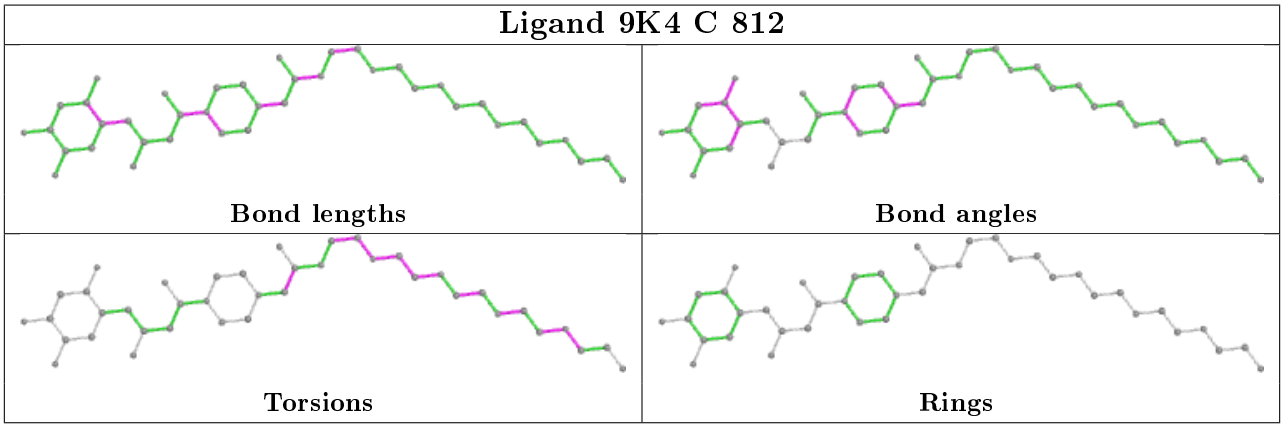
There are no ring outliers.

9 monomers are involved in 10 short contacts:

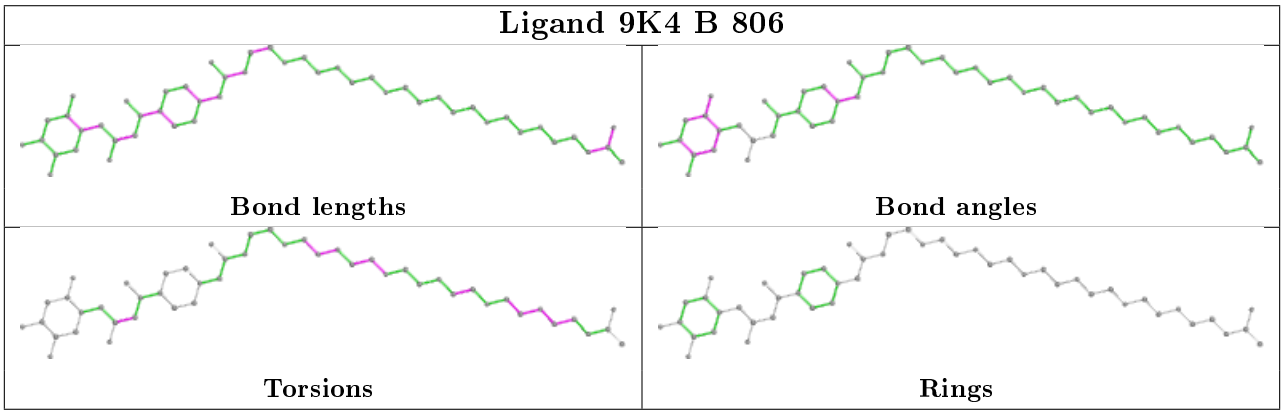
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	807	PEG	1	0
4	D	806	NAG	1	0
4	B	801	NAG	1	0
8	C	812	9K4	2	0
8	B	806	9K4	1	0
4	A	801	NAG	1	0
4	C	805	NAG	1	0
7	B	805	EDO	1	0
7	A	811	EDO	1	0

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 then 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.

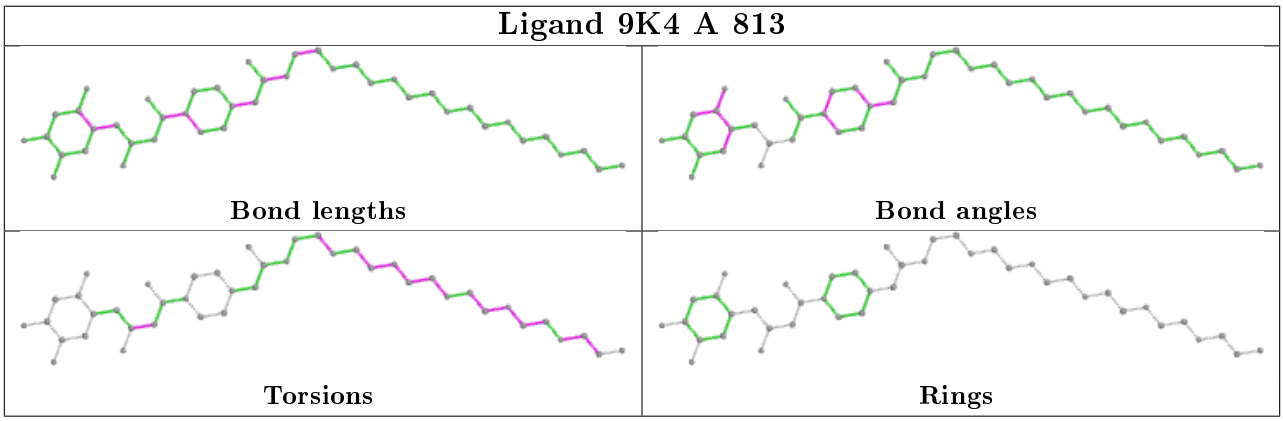
Ligand 9K4 C 812

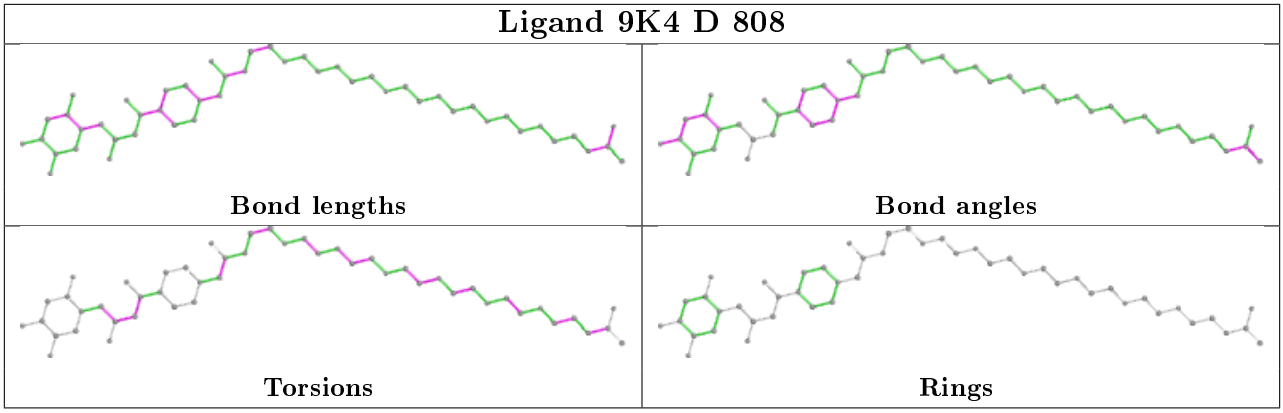


Ligand 9K4 B 806



Ligand 9K4 A 813





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	728/739 (98%)	-0.55	0 100 100	19, 40, 62, 100	0
1	B	718/739 (97%)	-0.49	0 100 100	19, 43, 70, 86	0
1	C	728/739 (98%)	-0.47	1 (0%) 95 95	27, 51, 72, 98	0
1	D	727/739 (98%)	-0.42	3 (0%) 92 91	28, 50, 74, 103	0
2	E	204/213 (95%)	-0.18	2 (0%) 82 77	35, 65, 88, 102	0
2	G	100/213 (46%)	0.03	1 (1%) 82 77	32, 72, 102, 116	0
2	J	89/213 (41%)	-0.07	1 (1%) 80 75	37, 70, 104, 126	0
2	L	208/213 (97%)	-0.23	0 100 100	35, 62, 85, 91	0
3	F	217/217 (100%)	-0.42	1 (0%) 91 88	30, 47, 67, 78	0
3	H	217/217 (100%)	-0.56	0 100 100	25, 44, 62, 77	0
3	I	115/217 (52%)	-0.23	0 100 100	50, 70, 86, 98	0
3	K	110/217 (50%)	0.23	1 (0%) 84 80	47, 77, 101, 111	0
All	All	4161/4676 (88%)	-0.41	10 (0%) 95 94	19, 49, 81, 126	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	203	PRO	5.4
1	D	278	THR	3.5
1	D	277	THR	3.1
2	G	57	VAL	3.1
1	C	277	THR	2.9
2	J	7	SER	2.6
1	D	333	LEU	2.6
2	E	107	ARG	2.3
3	F	44	SER	2.1
3	K	17	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	D	804	14/15	0.68	0.19	90,97,104,104	0
4	NAG	D	802	14/15	0.73	0.27	92,105,108,109	0
4	NAG	C	801	14/15	0.81	0.17	63,70,80,80	0
4	NAG	C	803	14/15	0.82	0.25	60,77,83,85	0
4	NAG	B	801	14/15	0.84	0.14	77,81,84,86	0
4	NAG	A	805	14/15	0.85	0.14	70,74,77,77	0
4	NAG	D	805	14/15	0.85	0.15	79,84,89,90	0
4	NAG	D	803	14/15	0.85	0.23	69,77,78,78	0
4	NAG	B	804	14/15	0.86	0.15	60,66,70,71	0
4	NAG	A	801	14/15	0.86	0.15	67,71,73,73	0
8	9K4	D	808	49/49	0.86	0.25	55,91,95,98	0
4	NAG	B	802	14/15	0.87	0.16	52,53,58,58	0
4	NAG	C	806	14/15	0.87	0.16	87,92,95,96	0
4	NAG	A	802	14/15	0.88	0.19	53,57,64,66	0
7	EDO	C	807	4/4	0.88	0.19	68,72,74,77	0
6	PEG	A	808	7/7	0.89	0.20	49,55,66,67	0
8	9K4	C	812	40/49	0.90	0.23	49,80,98,103	0
4	NAG	C	802	14/15	0.90	0.15	53,64,69,71	0
7	EDO	B	805	4/4	0.91	0.19	60,62,63,65	0
8	9K4	B	806	49/49	0.92	0.25	36,83,108,111	0
7	EDO	C	811	4/4	0.92	0.12	52,54,55,56	0
4	NAG	C	805	14/15	0.92	0.22	63,67,70,73	0
6	PEG	A	807	7/7	0.92	0.14	52,56,60,61	0
4	NAG	D	806	14/15	0.92	0.16	53,55,61,70	0
5	PG4	A	806	13/13	0.92	0.14	54,57,60,60	0
4	NAG	A	804	14/15	0.92	0.14	61,66,73,78	0
4	NAG	A	803	14/15	0.93	0.12	32,34,35,36	0

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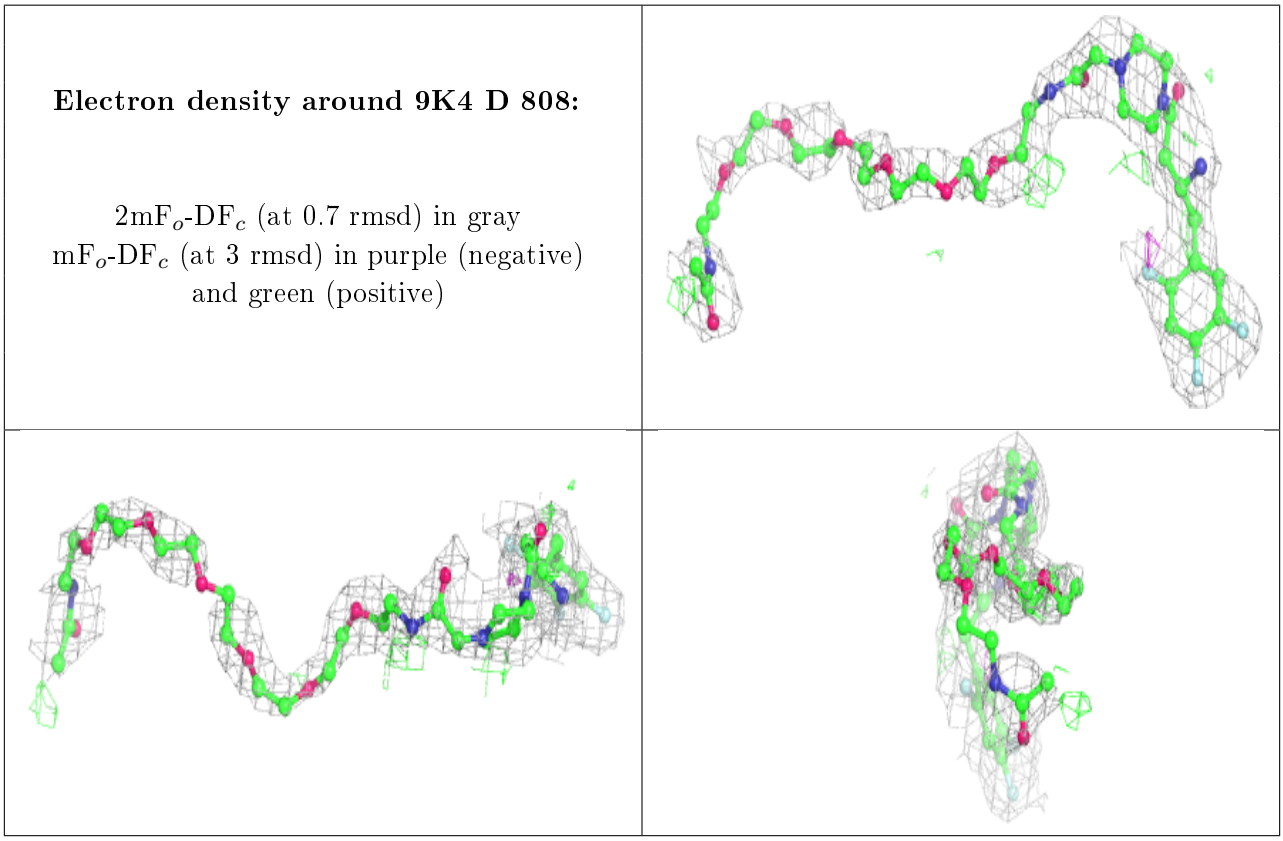
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	9K4	A	813	43/49	0.93	0.20	33,56,87,90	0
7	EDO	C	810	4/4	0.93	0.14	43,47,48,49	0
7	EDO	C	808	4/4	0.93	0.13	57,57,58,59	0
6	PEG	D	807	7/7	0.94	0.12	48,51,53,53	0
4	NAG	B	803	14/15	0.94	0.15	42,45,50,55	0
7	EDO	C	809	4/4	0.94	0.14	52,57,60,62	0
7	EDO	A	810	4/4	0.95	0.24	53,54,54,56	0
4	NAG	D	801	14/15	0.95	0.10	46,53,60,65	0
4	NAG	C	804	14/15	0.96	0.11	38,39,40,44	0
7	EDO	A	811	4/4	0.96	0.15	40,41,41,42	0
7	EDO	A	812	4/4	0.96	0.28	37,39,40,40	0
7	EDO	A	809	4/4	0.96	0.17	28,28,28,28	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.

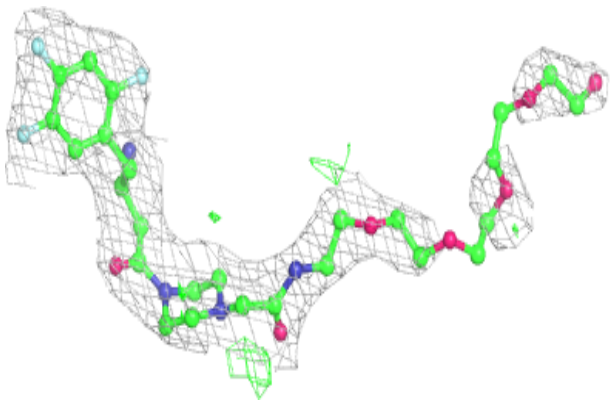
Electron density around 9K4 D 808:

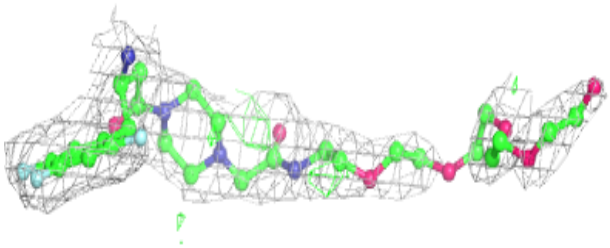
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

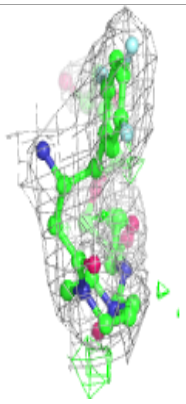


Electron density around 9K4 C 812:

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

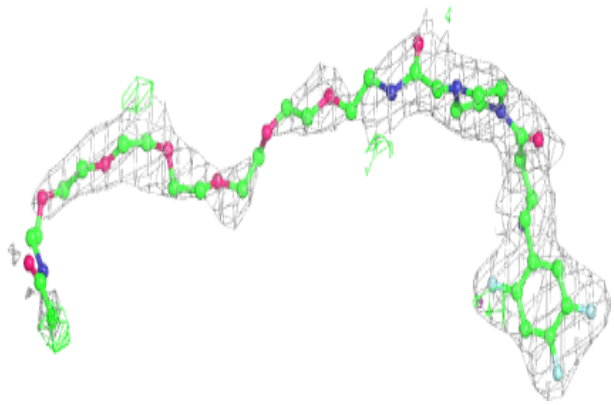


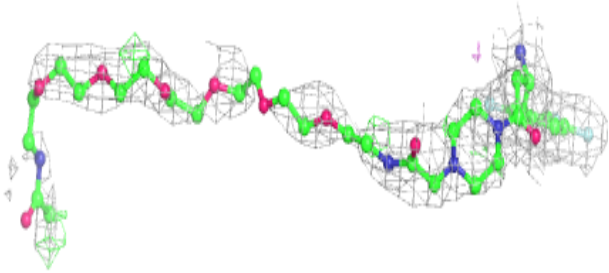


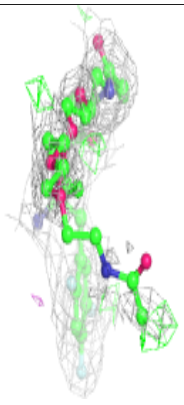


Electron density around 9K4 B 806:

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

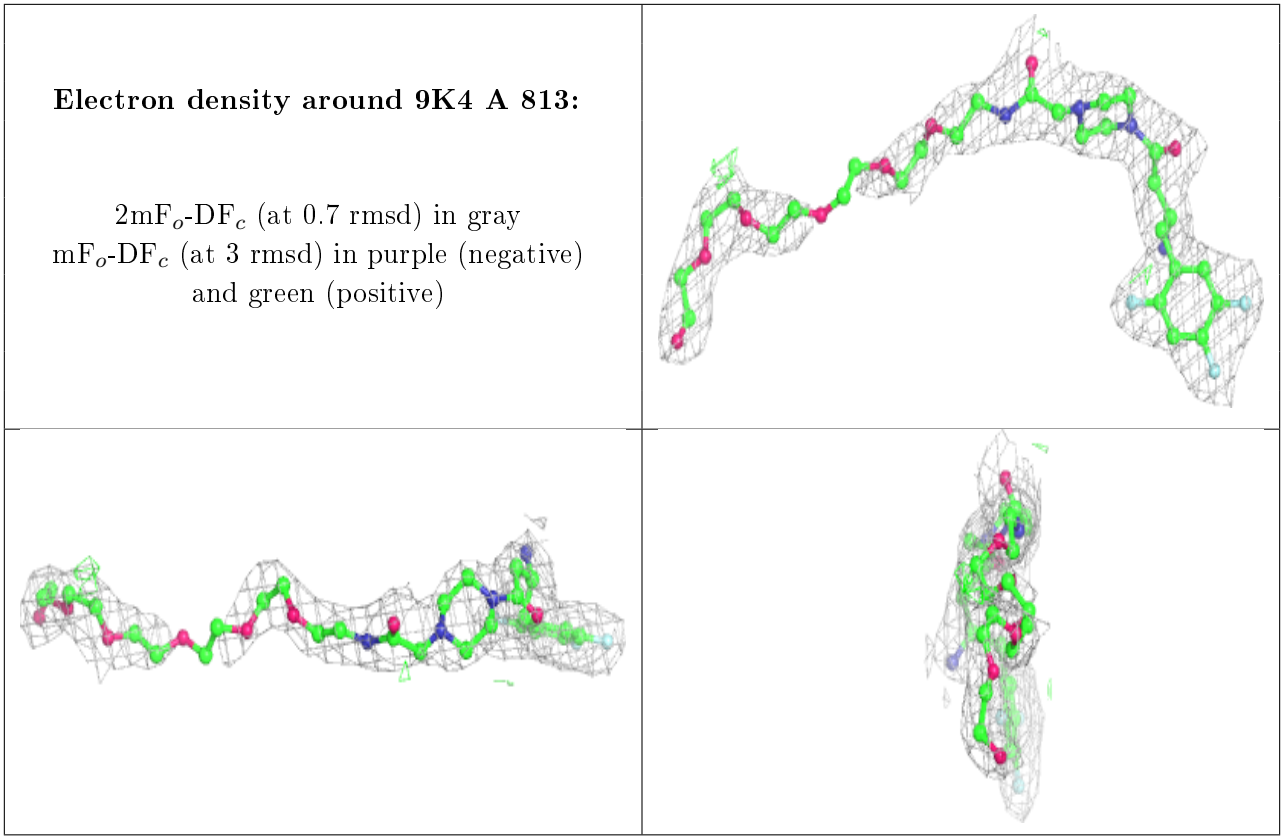






Electron density around 9K4 A 813:

$2mF_o$-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 (i)

There are no such residues in this entry.