



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 04:42 AM UTC

PDB ID : 5FQ8 / pdb_00005fq8
Title : Crystal structure of the SusCD complex BT2261-2264 from Bacteroides thetaiotaomicron
Authors : Glenwright, A.J.; Pothula, K.R.; Chorev, D.S.; Basle, A.; Robinson, C.V.; Kleinekathoefer, U.; Bolam, D.N.; van den Berg, B.
Deposited on : 2015-12-07
Resolution : 2.75 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

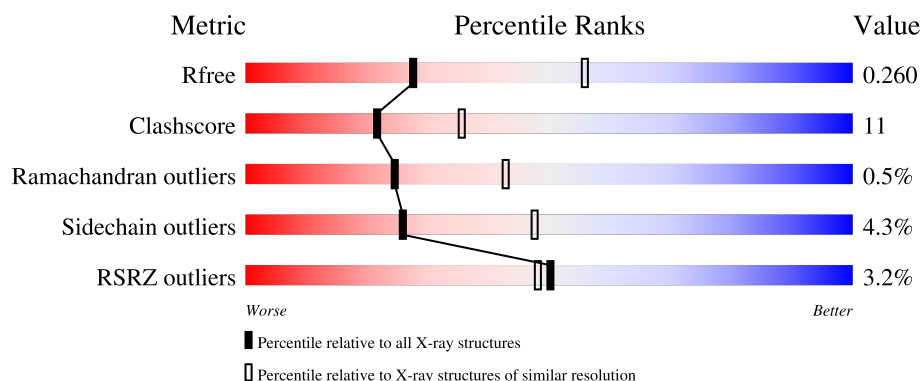
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	480	77% 22% .
1	C	480	75% 23% .
2	B	984	70% 24% .
2	D	984	68% 26% .

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Mol	Chain	Length	Quality of chain
3	E	148	80% 18%
3	F	148	% 82% 16%
4	G	212	33% 67% 29%
5	P	10	40% 60% 40%
6	Q	9	11% 78% 22%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 27220 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 PUTATIVE LIPOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	1	0
			3749	2373	616	743	17			
1	C	479	Total	C	N	O	S	0	0	0
			3734	2364	614	739	17			

- Molecule 2 is a protein called OUTER MEMBRANE PROTEIN OMP121.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	945	Total	C	N	O	S	0	0	0
			7373	4666	1230	1447	30			
2	D	941	Total	C	N	O	S	0	0	0
			7341	4646	1224	1441	30			

- Molecule 3 is a protein called UNCHARACTERIZED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	145	Total	C	N	O	S	0	0	0
			1134	717	178	234	5			
3	F	146	Total	C	N	O	S	0	0	0
			1142	721	180	236	5			

- Molecule 4 is a protein called BT_2262 (UNCHARACTERISED LIPOPROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	212	Total	C	N	O	S	0	0	0
			1646	1052	253	335	6			

- Molecule 5 is a protein called UNCHARACTERISED PROTEIN, BOUND PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	P	10	Total	C	N	O	0	0	0
			40	20	10	10			

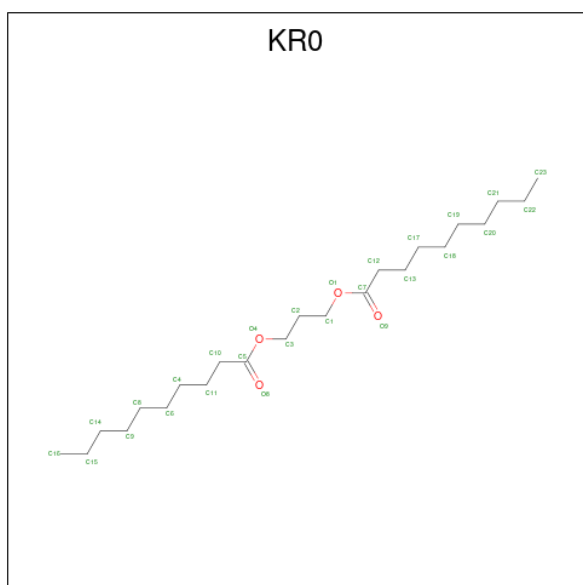
- Molecule 6 is a protein called UNCHARACTERISED PROTEIN, BOUND PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	Q	9	Total	C	N	O	0	0	0
			36	18	9	9			

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

- Molecule 8 is 3-decanoyloxypropyl decanoate (CCD ID: KR0) (formula: C₂₃H₄₄O₄).

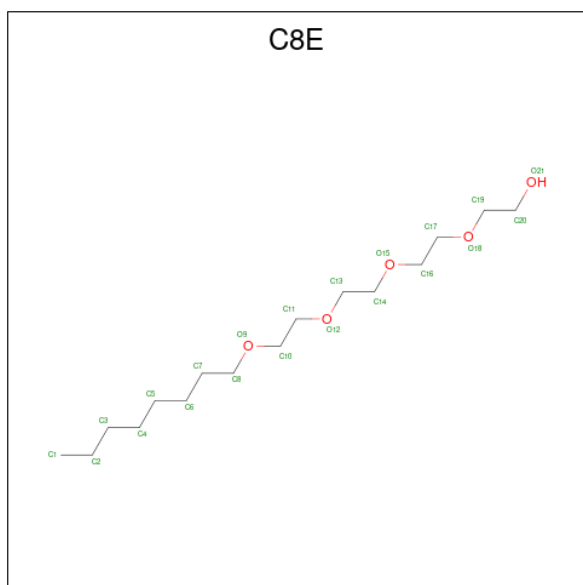


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			27	23	4		
8	D	1	Total	C	O	0	0
			27	23	4		

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	2	Total Ca 2 2	0	0
9	D	2	Total Ca 2 2	0	0

- Molecule 10 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 9 8 1	0	0
10	D	1	Total C O 9 6 3	0	0
10	D	1	Total C O 11 7 4	0	0
10	D	1	Total C 6 6	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	179	Total O 179 179	0	0
11	B	292	Total O 292 292	0	0
11	C	123	Total O 123 123	0	0

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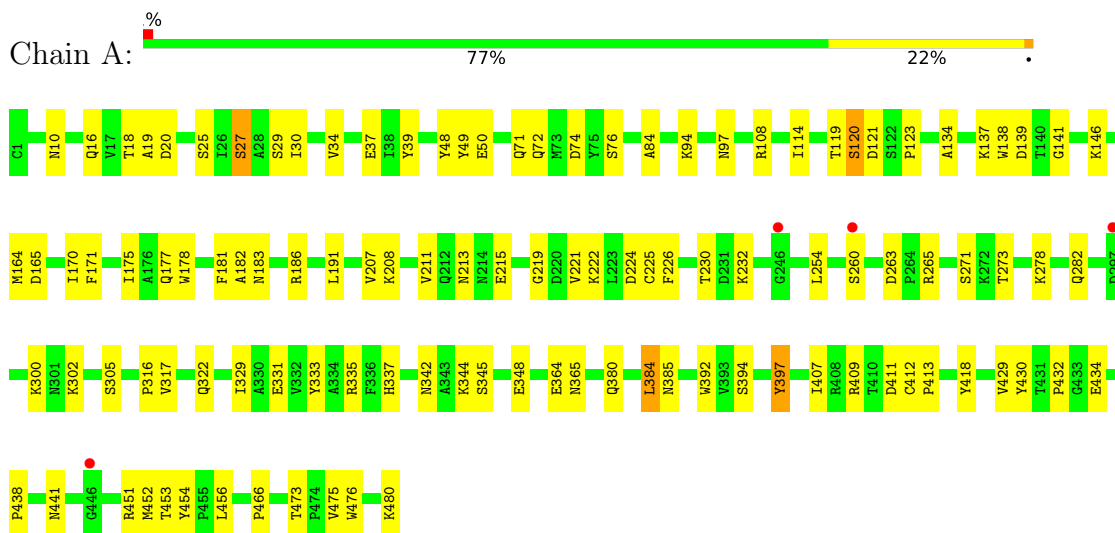
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	244	Total 244	O 244	0	0
11	E	41	Total 41	O 41	0	0
11	F	33	Total 33	O 33	0	0
11	G	15	Total 15	O 15	0	0
11	P	1	Total 1	O 1	0	0

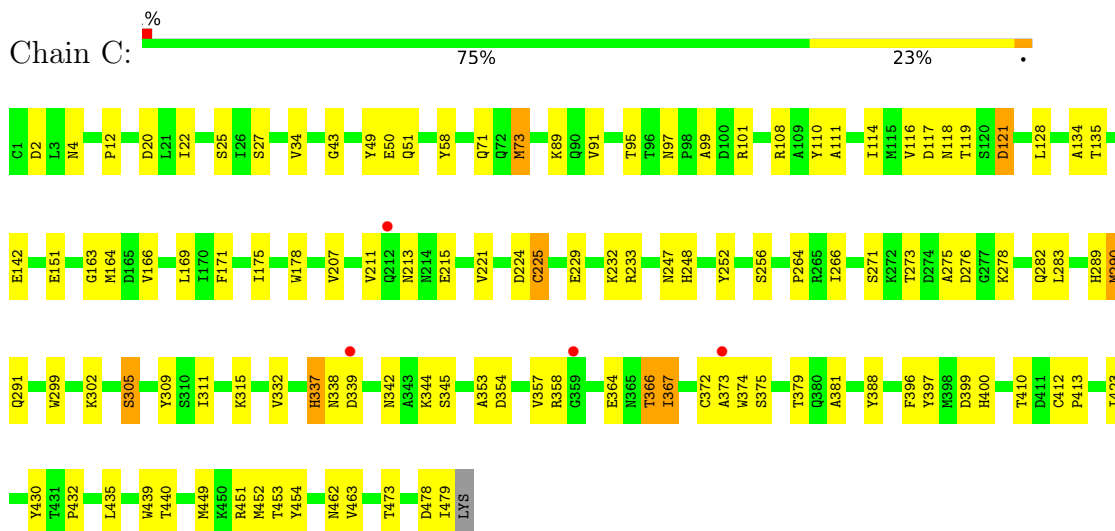
3 Residue-property plots

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: PUTATIVE LIPOPROTEIN

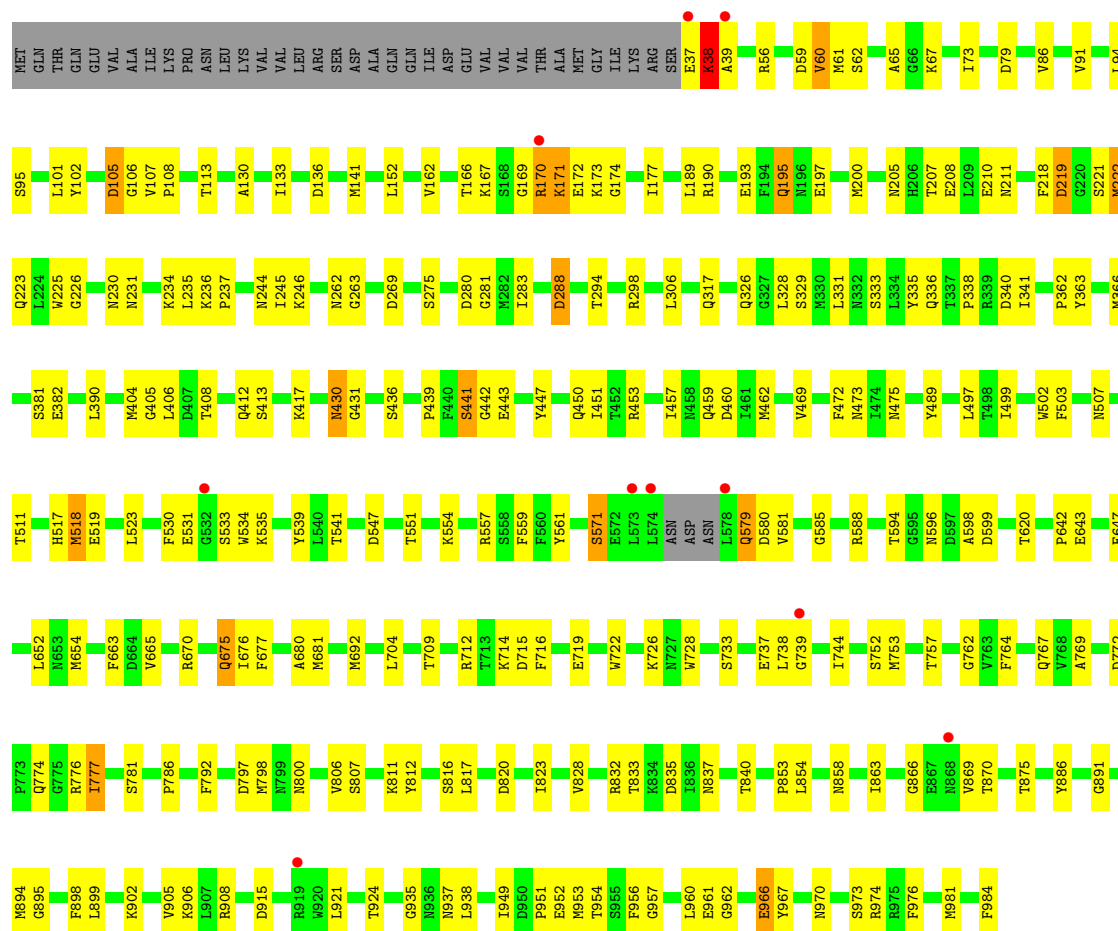


• Molecule 1: PUTATIVE LIPOPROTEIN

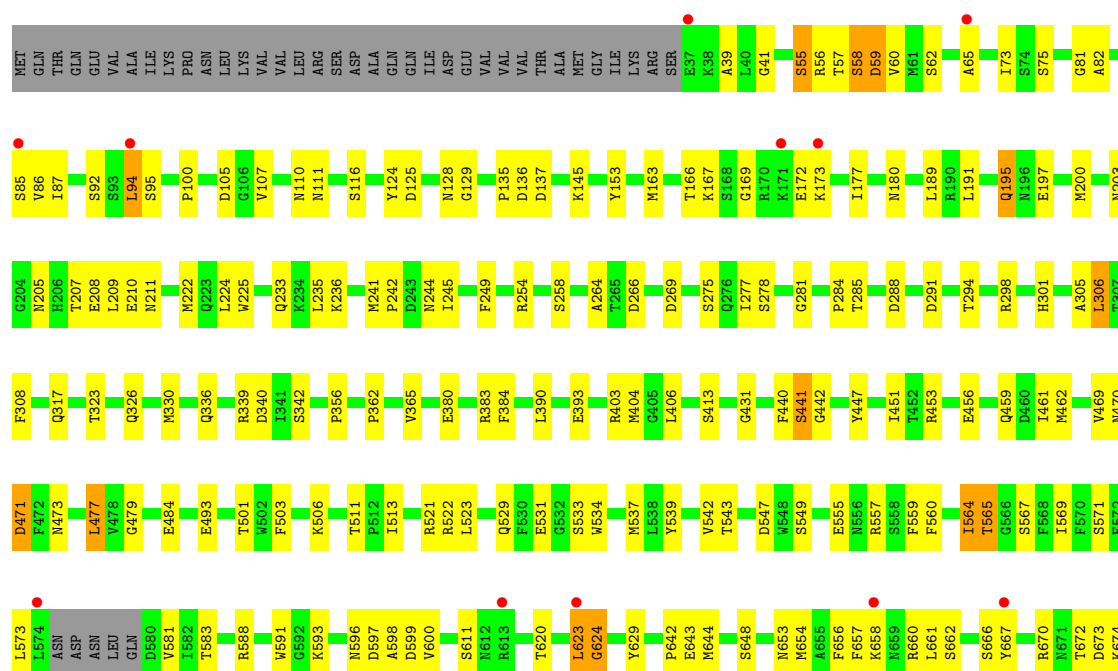


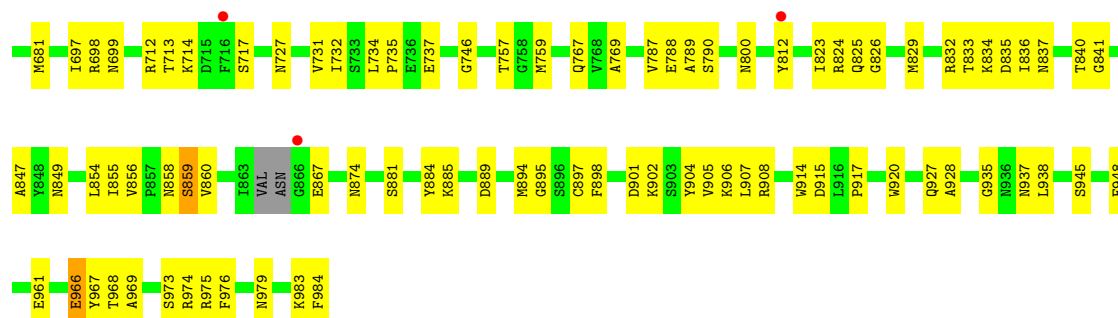
• Molecule 2: OUTER MEMBRANE PROTEIN OMP121



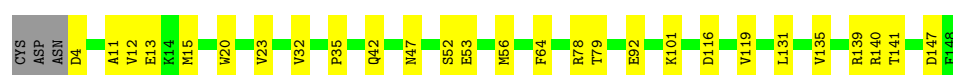
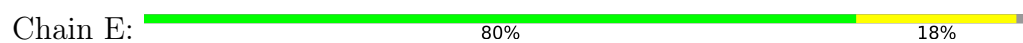


● Molecule 2: OUTER MEMBRANE PROTEIN OMP121

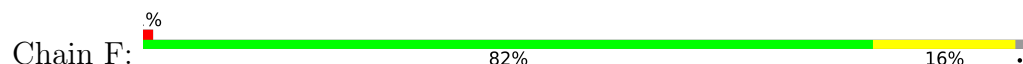




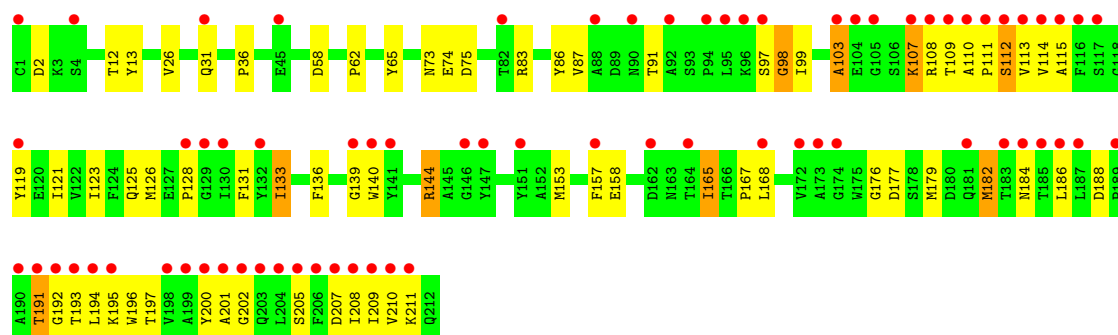
• Molecule 3: UNCHARACTERIZED PROTEIN



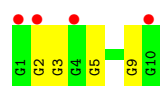
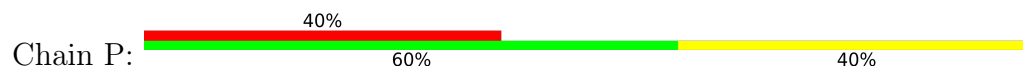
• Molecule 3: UNCHARACTERIZED PROTEIN



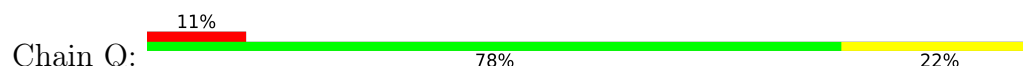
• Molecule 4: BT_2262 (UNCHARACTERISED LIPOPROTEIN)

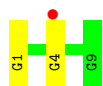


• Molecule 5: UNCHARACTERISED PROTEIN, BOUND PEPTIDE



• Molecule 6: UNCHARACTERISED PROTEIN, BOUND PEPTIDE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.11Å 122.74Å 122.83Å 111.41° 98.33° 98.51°	Depositor
Resolution (Å)	52.93 – 2.75 52.93 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.93-2.75) 93.0 (52.93-2.75)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.205 , 0.259 0.206 , 0.260	Depositor DCC
R_{free} test set	6252 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.015 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	27220	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, KR0, C8E, MG

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	0.52	0/3843	0.54	0/5231
1	C	0.46	0/3825	0.51	0/5209
2	B	0.51	0/7550	0.60	4/10237 (0.0%)
2	D	0.51	2/7517 (0.0%)	0.59	2/10190 (0.0%)
3	E	0.46	0/1162	0.53	0/1578
3	F	0.41	0/1170	0.51	0/1589
4	G	0.29	0/1685	0.48	0/2293
5	P	0.54	0/39	1.29	0/47
6	Q	0.69	0/35	0.75	0/42
All	All	0.49	2/26826 (0.0%)	0.56	6/36416 (0.0%)

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
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	812	TYR	CA-C	6.37	1.55	1.52
2	D	431	GLY	CA-C	-6.20	1.48	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	105	ASP	N-CA-C	8.79	120.78	110.41
2	B	430	ASN	N-CA-C	8.37	123.67	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	579	GLN	CA-C-N	6.27	132.99	121.70
2	B	579	GLN	C-N-CA	6.27	132.99	121.70
2	D	81	GLY	N-CA-C	-5.43	97.56	113.30
2	D	624	GLY	N-CA-C	-5.43	97.56	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	38	LYS	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	3749	0	3565	72	0
1	C	3734	0	3548	75	0
2	B	7373	0	7059	170	0
2	D	7341	0	7024	171	0
3	E	1134	0	1050	16	0
3	F	1142	0	1056	13	0
4	G	1646	0	1565	52	0
5	P	40	0	32	2	0
6	Q	36	0	29	2	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	B	27	0	0	0	0
8	D	27	0	0	0	0
9	B	2	0	0	0	0
9	D	2	0	0	0	0
10	B	9	0	17	0	0
10	D	26	0	30	3	0
11	A	179	0	0	12	0
11	B	292	0	0	18	0
11	C	123	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	244	0	0	22	0
11	E	41	0	0	3	0
11	F	33	0	0	0	0
11	G	15	0	0	4	0
11	P	1	0	0	0	0
All	All	27220	0	24975	551	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 11.

All (551) 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:D:800:ASN:HA	2:D:826:GLY:HA3	1.53	0.90
2:B:170:ARG:HB3	2:B:171:LYS:HA	1.55	0.87
2:D:788:GLU:HA	2:D:894:MET:HE1	1.62	0.80
2:B:222:MET:HE2	2:B:237:PRO:HG3	1.63	0.78
2:B:833:THR:OG1	2:B:966:GLU:OE2	2.00	0.78
2:D:856:VAL:O	2:D:859:SER:OG	2.00	0.78
2:D:236:LYS:NZ	2:D:340:ASP:OD2	2.17	0.77
1:A:50:GLU:HG3	1:A:282:GLN:HE21	1.49	0.77
2:D:889:ASP:OD1	11:D:2235:HOH:O	2.03	0.76
2:B:170:ARG:HB3	2:B:171:LYS:CA	2.15	0.76
2:B:73:ILE:HG12	2:B:86:VAL:HG22	1.67	0.76
2:D:658:LYS:O	2:D:712:ARG:NH2	2.17	0.76
2:B:647:GLU:OE2	2:B:670:ARG:NH1	2.18	0.75
2:B:714:LYS:NZ	11:B:2219:HOH:O	2.18	0.75
1:A:385:ASN:ND2	11:A:2153:HOH:O	2.19	0.75
2:B:722:TRP:HD1	2:B:806:VAL:HG12	1.50	0.75
2:B:61:MET:HE3	2:B:102:TYR:HE2	1.51	0.74
2:B:234:LYS:NZ	11:B:2100:HOH:O	2.20	0.73
1:C:4:ASN:OD1	2:D:557:ARG:NH2	2.20	0.73
2:D:59:ASP:OD2	2:D:62:SER:OG	2.07	0.73
2:B:275:SER:HG	2:B:294:THR:HG1	1.32	0.72
2:D:264:ALA:O	11:D:2061:HOH:O	2.08	0.72
2:B:938:LEU:O	2:B:974:ARG:NH1	2.23	0.71
1:C:452:MET:HE3	1:C:453:THR:H	1.56	0.71
2:B:571:SER:OG	2:B:585:GLY:N	2.24	0.71
2:D:110:ASN:ND2	2:D:456:GLU:OE2	2.22	0.71
1:A:94:LYS:NZ	11:A:2058:HOH:O	2.15	0.71
2:B:246:LYS:NZ	11:B:2104:HOH:O	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:GLU:OE2	11:C:2049:HOH:O	2.07	0.71
1:A:335:ARG:HD2	1:A:384:LEU:HD21	1.71	0.70
2:B:417:LYS:NZ	2:B:443:GLU:OE1	2.25	0.70
2:B:739:GLY:O	11:B:2228:HOH:O	2.08	0.70
2:D:326:GLN:HE22	6:Q:4:GLY:HA2	1.56	0.70
2:D:529:GLN:HG3	2:D:543:THR:HG22	1.74	0.70
2:B:767:GLN:HG3	2:B:895:GLY:H	1.56	0.70
1:C:273:THR:HG22	1:C:276:ASP:H	1.57	0.70
2:D:145:LYS:O	2:D:670:ARG:NH2	2.24	0.70
2:D:945:SER:O	11:D:2222:HOH:O	2.09	0.70
2:D:249:PHE:O	11:D:2096:HOH:O	2.10	0.69
2:B:211:ASN:ND2	2:B:336:GLN:OE1	2.23	0.69
2:D:470:ASN:OD1	11:D:2137:HOH:O	2.10	0.69
1:A:72:GLN:OE1	11:A:2047:HOH:O	2.11	0.69
4:G:13:TYR:O	4:G:73:ASN:ND2	2.24	0.68
2:D:275:SER:HG	2:D:294:THR:HG1	1.34	0.68
2:D:591:TRP:HD1	10:D:1990:C8E:H101	1.58	0.68
2:D:128:ASN:ND2	11:D:2027:HOH:O	2.27	0.68
1:C:71:GLN:O	11:C:2014:HOH:O	2.12	0.68
2:D:961:GLU:OE1	11:D:2041:HOH:O	2.12	0.68
2:D:531:GLU:OE2	11:D:2151:HOH:O	2.11	0.67
2:B:193:GLU:O	11:B:2079:HOH:O	2.12	0.67
2:D:41:GLY:HA3	2:D:565:THR:HG23	1.76	0.67
2:D:938:LEU:O	2:D:974:ARG:NH1	2.28	0.67
2:D:167:LYS:O	2:D:298:ARG:NH1	2.28	0.67
2:D:713:THR:HG22	2:D:714:LYS:H	1.59	0.67
2:B:107:VAL:HG11	2:B:405:GLY:HA3	1.76	0.67
1:C:273:THR:HG22	1:C:275:ALA:H	1.60	0.67
2:D:834:LYS:NZ	2:D:897:CYS:O	2.25	0.67
2:D:583:THR:OG1	2:D:657:PHE:O	2.12	0.66
2:D:254:ARG:NH1	11:D:2065:HOH:O	2.29	0.66
3:E:131:LEU:O	11:E:2033:HOH:O	2.14	0.66
2:B:472:PHE:CE1	2:B:534:TRP:HD1	2.14	0.66
2:B:719:GLU:OE1	11:B:2221:HOH:O	2.14	0.65
2:B:753:MET:HE3	2:B:764:PHE:CZ	2.32	0.65
2:B:961:GLU:OE1	11:B:2289:HOH:O	2.15	0.65
2:D:95:SER:O	11:D:2030:HOH:O	2.13	0.65
2:D:859:SER:HB2	2:D:874:ASN:HB3	1.77	0.65
4:G:197:THR:HG22	4:G:207:ASP:HA	1.77	0.65
2:D:195:GLN:NE2	2:D:841:GLY:O	2.30	0.65
2:D:484:GLU:OE1	11:D:2135:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:699:ASN:OD1	2:D:727:ASN:ND2	2.18	0.65
2:B:475:ASN:HB3	2:B:531:GLU:HB3	1.77	0.65
2:D:697:ILE:HD12	2:D:731:VAL:HG22	1.78	0.65
2:D:901:ASP:OD1	11:D:2219:HOH:O	2.14	0.65
1:A:452:MET:HE3	1:A:453:THR:H	1.61	0.65
2:B:924:THR:O	11:B:2283:HOH:O	2.15	0.65
1:A:137:LYS:NZ	1:A:139:ASP:OD1	2.31	0.64
2:B:800:ASN:O	11:B:2224:HOH:O	2.13	0.64
2:B:430:ASN:N	2:B:431:GLY:HA3	2.10	0.64
2:B:554:LYS:HG2	2:B:557:ARG:NH2	2.12	0.64
2:B:167:LYS:O	2:B:298:ARG:NH1	2.30	0.64
1:C:20:ASP:HA	1:C:166:VAL:HG23	1.79	0.64
4:G:108:ARG:HD2	4:G:114:VAL:HG12	1.79	0.64
2:B:61:MET:HE3	2:B:102:TYR:CE2	2.31	0.63
2:D:654:MET:HE3	2:D:656:PHE:HZ	1.63	0.63
1:C:358:ARG:NH2	1:C:396:PHE:O	2.32	0.63
2:D:241:MET:HE3	2:D:342:SER:HB2	1.80	0.62
2:D:447:TYR:CD1	2:D:503:PHE:HB3	2.35	0.62
2:D:534:TRP:HZ3	2:D:537:MET:HE2	1.64	0.62
1:A:164:MET:HE1	1:A:178:TRP:CD1	2.36	0.61
1:C:224:ASP:OD1	11:C:2065:HOH:O	2.15	0.61
2:D:471:ASP:OD1	2:D:471:ASP:N	2.17	0.61
2:B:430:ASN:O	2:B:439:PRO:HD2	2.00	0.61
2:B:511:THR:HG23	2:D:511:THR:HG23	1.83	0.61
1:C:264:PRO:HD3	1:C:366:THR:HG21	1.83	0.61
2:D:593:LYS:HD3	2:D:644:MET:HE3	1.82	0.61
2:B:744:ILE:HD13	2:B:960:LEU:HD21	1.82	0.61
1:A:27:SER:OG	11:A:2019:HOH:O	2.02	0.61
2:B:733:SER:HA	2:B:757:THR:HG23	1.81	0.61
2:D:244:ASN:OD1	2:D:245:ILE:N	2.34	0.60
4:G:97:SER:N	11:G:2011:HOH:O	2.32	0.60
2:B:654:MET:HB2	2:B:663:PHE:CE2	2.37	0.60
2:B:95:SER:HB2	2:B:677:PHE:HE1	1.65	0.60
2:D:207:THR:HB	2:D:210:GLU:HG2	1.84	0.60
2:D:65:ALA:HB3	2:D:908:ARG:HD3	1.83	0.60
2:D:177:ILE:HB	2:D:984:PHE:HB2	1.84	0.60
2:B:283:ILE:HB	2:B:288:ASP:OD1	2.02	0.60
4:G:193:THR:HG22	4:G:211:LYS:HB2	1.83	0.60
2:B:65:ALA:HB3	2:B:908:ARG:HD3	1.84	0.60
2:D:55:SER:HB3	2:D:57:THR:HG23	1.84	0.60
2:D:902:LYS:NZ	11:D:2221:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:447:TYR:CD1	2:B:503:PHE:HB3	2.37	0.59
1:C:344:LYS:HD2	1:C:374:TRP:CD1	2.38	0.59
2:D:829:MET:HE2	2:D:902:LYS:HG3	1.85	0.59
1:C:271:SER:O	1:C:305:SER:OG	2.17	0.59
2:B:753:MET:HE2	2:B:798:MET:HB3	1.83	0.59
1:C:108:ARG:NH1	1:C:151:GLU:OE2	2.36	0.58
4:G:108:ARG:NH1	4:G:112:SER:H	2.01	0.58
2:B:722:TRP:CD1	2:B:806:VAL:HG12	2.35	0.58
1:A:394:SER:OG	11:A:2140:HOH:O	2.14	0.58
2:D:823:ILE:HG12	2:D:905:VAL:HG22	1.86	0.58
2:B:588:ARG:NE	11:B:2186:HOH:O	2.31	0.58
2:D:559:PHE:HB3	2:D:642:PRO:HG2	1.86	0.57
2:B:937:ASN:ND2	2:B:973:SER:O	2.37	0.57
2:D:200:MET:HG3	2:D:210:GLU:HB2	1.86	0.57
2:B:413:SER:HB3	11:B:2139:HOH:O	2.04	0.57
1:C:163:GLY:HA2	1:C:175:ILE:HD11	1.87	0.57
2:D:413:SER:HB2	11:D:2124:HOH:O	2.05	0.57
4:G:167:PRO:HG3	4:G:182:MET:SD	2.45	0.57
1:A:171:PHE:HZ	1:A:221:VAL:HG22	1.69	0.57
2:D:110:ASN:HB3	2:D:383:ARG:HH21	1.70	0.57
1:A:119:THR:O	1:A:121:ASP:N	2.38	0.57
2:B:675:GLN:HB3	11:B:2210:HOH:O	2.04	0.57
2:B:451:ILE:HG21	2:D:451:ILE:HG21	1.85	0.57
2:B:219:ASP:HB3	2:B:221:SER:H	1.70	0.56
2:B:599:ASP:O	11:B:2178:HOH:O	2.17	0.56
2:D:284:PRO:O	2:D:285:THR:OG1	2.22	0.56
2:B:195:GLN:HG2	2:B:197:GLU:H	1.71	0.56
4:G:191:THR:HB	4:G:193:THR:HG23	1.87	0.56
3:F:140:ARG:NH1	3:F:147:ASP:OD1	2.39	0.56
2:D:746:GLY:O	6:Q:1:GLY:HA3	2.05	0.56
2:D:523:LEU:HD11	2:D:547:ASP:HB3	1.87	0.55
1:C:89:LYS:NZ	1:C:128:LEU:O	2.27	0.55
11:D:2079:HOH:O	3:E:141:THR:O	2.18	0.55
1:C:111:ALA:HA	1:C:114:ILE:HD12	1.88	0.55
3:E:140:ARG:NH1	3:E:147:ASP:OD1	2.40	0.55
2:B:177:ILE:HB	2:B:984:PHE:HB2	1.87	0.55
2:B:262:ASN:OD1	2:B:263:GLY:N	2.39	0.55
2:B:596:ASN:HB3	2:B:643:GLU:HB3	1.88	0.55
2:B:762:GLY:HA3	2:B:798:MET:HE3	1.88	0.55
2:B:767:GLN:HB3	2:B:792:PHE:CE1	2.41	0.55
2:D:462:MET:HB3	2:D:477:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:549:SER:O	2:D:557:ARG:HD3	2.07	0.55
1:A:181:PHE:CE1	1:A:221:VAL:HG11	2.42	0.55
1:A:191:LEU:HB3	1:A:409:ARG:NH1	2.22	0.55
1:C:379:THR:HG22	1:C:381:ALA:H	1.72	0.54
2:B:807:SER:OG	2:B:820:ASP:OD2	2.18	0.54
4:G:176:GLY:N	4:G:177:ASP:HB2	2.23	0.54
2:D:555:GLU:H	2:D:555:GLU:CD	2.16	0.54
1:A:407:ILE:HG12	1:A:413:PRO:HD2	1.89	0.54
2:B:665:VAL:HG22	2:B:704:LEU:HD13	1.89	0.54
2:B:317:GLN:HG2	2:B:381:SER:HB3	1.88	0.54
3:F:15:MET:HE1	3:F:73:VAL:HG13	1.89	0.54
2:B:170:ARG:HD2	2:B:172:GLU:HB2	1.90	0.54
1:C:50:GLU:HG3	1:C:51:GLN:N	2.22	0.54
2:B:61:MET:HE1	2:B:162:VAL:HG11	1.90	0.54
2:B:207:THR:HG21	2:B:210:GLU:OE2	2.07	0.54
2:B:207:THR:HB	2:B:210:GLU:HG2	1.90	0.54
1:C:164:MET:HE1	1:C:178:TRP:HD1	1.74	0.53
1:C:229:GLU:O	1:C:233:ARG:HG3	2.08	0.53
1:C:367:ILE:HG23	1:C:372:CYS:HB2	1.89	0.53
2:D:207:THR:HG22	2:D:209:LEU:H	1.74	0.53
1:C:50:GLU:HG3	1:C:51:GLN:H	1.74	0.53
2:D:116:SER:O	11:D:2042:HOH:O	2.18	0.53
2:D:116:SER:HB2	2:D:124:TYR:CE2	2.43	0.53
2:B:205:ASN:OD1	3:F:140:ARG:NH2	2.41	0.53
1:C:232:LYS:NZ	11:C:2071:HOH:O	2.41	0.53
1:C:134:ALA:HB2	2:D:681:MET:HE3	1.91	0.53
2:D:591:TRP:CD1	10:D:1990:C8E:H101	2.42	0.53
1:A:34:VAL:O	1:A:39:TYR:HB2	2.08	0.53
1:A:232:LYS:NZ	2:B:620:THR:HG23	2.24	0.53
2:B:823:ILE:HG13	2:B:905:VAL:HG13	1.90	0.53
2:B:170:ARG:HG3	2:B:262:ASN:ND2	2.23	0.53
2:B:469:VAL:O	2:B:472:PHE:N	2.42	0.53
1:C:164:MET:HE1	1:C:178:TRP:CD1	2.43	0.52
2:D:403:ARG:HD2	11:D:2035:HOH:O	2.09	0.52
2:D:904:TYR:CE1	2:D:906:LYS:HE3	2.44	0.52
2:D:565:THR:HG22	11:D:2152:HOH:O	2.09	0.52
2:D:653:ASN:ND2	11:D:2164:HOH:O	2.28	0.52
2:B:130:ALA:O	2:B:133:ILE:HG22	2.09	0.52
2:B:331:LEU:HD22	2:B:970:ASN:HA	1.92	0.52
1:C:399:ASP:OD2	11:C:2042:HOH:O	2.19	0.52
2:D:767:GLN:HG2	2:D:894:MET:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:HIS:HD1	1:C:309:TYR:HH	1.56	0.52
2:D:205:ASN:OD1	3:E:140:ARG:NH2	2.42	0.52
2:D:599:ASP:OD1	2:D:600:VAL:N	2.36	0.52
2:D:837:ASN:HA	2:D:840:THR:HG22	1.91	0.52
1:A:30:ILE:O	1:A:34:VAL:HG23	2.10	0.52
2:D:173:LYS:HB3	2:D:927:GLN:OE1	2.10	0.52
2:D:169:GLY:HA3	2:D:269:ASP:HB2	1.92	0.52
3:E:23:VAL:HG11	3:E:64:PHE:CZ	2.44	0.52
2:B:382:GLU:OE1	2:D:453:ARG:NH2	2.43	0.52
2:D:180:ASN:HB2	2:D:258:SER:HB3	1.92	0.52
2:B:105:ASP:OD2	2:B:166:THR:OG1	2.26	0.51
2:B:105:ASP:N	2:B:106:GLY:HA2	2.23	0.51
2:D:135:PRO:O	2:D:136:ASP:HB2	2.09	0.51
1:A:263:ASP:OD2	1:A:265:ARG:NH2	2.40	0.51
1:C:339:ASP:CB	1:C:342:ASN:HB2	2.40	0.51
4:G:58:ASP:HB3	4:G:65:TYR:OH	2.09	0.51
2:B:715:ASP:O	2:B:812:TYR:HA	2.10	0.51
2:D:767:GLN:NE2	2:D:788:GLU:OE1	2.29	0.51
4:G:119:TYR:CE2	4:G:144:ARG:HG2	2.46	0.51
1:A:19:ALA:HB2	1:A:94:LYS:HB2	1.93	0.51
2:D:906:LYS:HD3	2:D:937:ASN:OD1	2.10	0.51
1:A:16:GLN:NE2	11:A:2014:HOH:O	2.44	0.50
2:B:579:GLN:HA	2:B:580:ASP:CB	2.41	0.50
4:G:121:ILE:HD11	4:G:210:VAL:HG11	1.92	0.50
2:D:698:ARG:HD3	2:D:732:ILE:HD11	1.92	0.50
1:A:225:CYS:HB3	11:A:2085:HOH:O	2.10	0.50
2:B:906:LYS:NZ	2:B:952:GLU:OE1	2.44	0.50
4:G:103:ALA:HB3	4:G:209:ILE:HG23	1.93	0.50
1:A:141:GLY:HA3	1:A:476:TRP:CD1	2.47	0.50
1:C:430:TYR:CE2	1:C:432:PRO:HA	2.46	0.50
2:D:767:GLN:HB3	2:D:895:GLY:HA3	1.92	0.50
4:G:131:PHE:HB2	4:G:157:PHE:CE1	2.46	0.50
1:A:20:ASP:OD1	1:A:20:ASP:N	2.42	0.50
1:A:208:LYS:HG2	1:A:337:HIS:NE2	2.27	0.50
2:B:170:ARG:HG3	2:B:262:ASN:CG	2.36	0.50
2:B:333:SER:OG	2:B:366:MET:O	2.17	0.50
2:D:224:LEU:HD23	2:D:235:LEU:HG	1.93	0.50
2:D:596:ASN:HB3	2:D:643:GLU:HB3	1.92	0.50
2:D:967:TYR:O	2:D:968:THR:OG1	2.23	0.50
1:A:224:ASP:HA	1:A:316:PRO:HB3	1.93	0.50
2:D:829:MET:CE	2:D:902:LYS:HG3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:673:ASP:OD1	2:D:674:LYS:N	2.45	0.50
2:D:82:ALA:HB1	2:D:125:ASP:HB3	1.94	0.49
2:B:223:GLN:O	2:B:235:LEU:HD12	2.13	0.49
2:D:39:ALA:HB1	2:D:539:TYR:CG	2.47	0.49
4:G:110:ALA:HA	11:G:2014:HOH:O	2.11	0.49
1:C:110:TYR:CE2	1:C:114:ILE:HD11	2.47	0.49
1:C:423:ILE:HG23	1:C:430:TYR:HB2	1.93	0.49
1:C:213:ASN:HB3	1:C:215:GLU:HG3	1.93	0.49
1:A:430:TYR:OH	1:A:434:GLU:O	2.19	0.49
2:B:95:SER:HB2	2:B:677:PHE:CE1	2.47	0.49
2:B:473:ASN:HB3	2:B:533:SER:HB3	1.93	0.49
1:C:110:TYR:CZ	1:C:114:ILE:HD11	2.47	0.49
1:C:135:THR:HG22	1:C:462:ASN:HA	1.94	0.49
1:C:282:GLN:NE2	1:C:299:TRP:HE1	2.11	0.49
1:C:339:ASP:HB3	1:C:342:ASN:HB2	1.94	0.49
3:E:11:ALA:HB1	3:E:53:GLU:HB3	1.93	0.49
2:B:737:GLU:H	2:B:737:GLU:CD	2.21	0.49
2:D:73:ILE:HA	2:D:85:SER:O	2.13	0.49
4:G:196:TRP:CZ2	4:G:208:ILE:HD11	2.48	0.49
2:D:266:ASP:OD1	2:D:266:ASP:N	2.39	0.49
1:A:164:MET:HE2	1:A:175:ILE:HG12	1.94	0.48
1:C:283:LEU:HD12	1:C:290:MET:HE1	1.95	0.48
1:A:271:SER:O	1:A:305:SER:HB2	2.13	0.48
2:B:113:THR:HG22	11:B:2046:HOH:O	2.12	0.48
2:B:406:LEU:HD12	2:B:457:ILE:HG12	1.94	0.48
2:B:949:ILE:O	2:B:951:PRO:HD3	2.13	0.48
1:C:91:VAL:O	1:C:95:THR:HG22	2.12	0.48
1:A:48:TYR:HD1	1:A:254:LEU:HD22	1.79	0.48
2:B:328:LEU:HD22	2:B:366:MET:HG3	1.96	0.48
1:A:48:TYR:OH	1:A:392:TRP:O	2.29	0.48
1:A:300:LYS:HE3	1:A:302:LYS:HE2	1.95	0.48
1:A:412:CYS:HA	1:A:413:PRO:C	2.38	0.48
2:B:956:PHE:HB2	2:B:962:GLY:HA2	1.96	0.48
2:D:86:VAL:O	2:D:100:PRO:HD3	2.14	0.48
1:A:108:ARG:NH1	11:A:2052:HOH:O	2.40	0.48
1:C:452:MET:HE3	1:C:453:THR:HG23	1.95	0.48
1:A:10:ASN:O	2:D:506:LYS:NZ	2.30	0.48
1:A:364:GLU:OE1	11:A:2151:HOH:O	2.20	0.48
1:C:34:VAL:HG11	1:C:114:ILE:HD13	1.95	0.48
1:C:289:HIS:CD2	1:C:439:TRP:CG	3.02	0.48
1:C:51:GLN:NE2	1:C:58:TYR:H	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:ASP:C	1:C:479:ILE:HG13	2.39	0.48
1:A:18:THR:OG1	1:A:20:ASP:OD1	2.22	0.48
2:B:502:TRP:CZ3	1:C:12:PRO:HD3	2.49	0.48
2:B:837:ASN:HA	2:B:840:THR:HG22	1.96	0.48
1:C:119:THR:O	1:C:121:ASP:N	2.47	0.48
4:G:125:GLN:HB3	4:G:131:PHE:CE2	2.49	0.48
2:B:326:GLN:HE22	5:P:5:GLY:HA2	1.78	0.47
1:C:388:TYR:CE2	1:C:410:THR:HB	2.48	0.47
2:D:404:MET:HG3	2:D:459:GLN:HG3	1.96	0.47
1:C:121:ASP:OD1	1:C:454:TYR:OH	2.32	0.47
2:D:107:VAL:HG23	2:D:403:ARG:HD3	1.96	0.47
2:D:236:LYS:HE3	2:D:236:LYS:HB3	1.61	0.47
2:D:306:LEU:HD11	2:D:390:LEU:HD11	1.95	0.47
1:A:418:TYR:CZ	1:A:429:VAL:HB	2.48	0.47
2:B:726:LYS:HE2	2:B:728:TRP:CZ2	2.49	0.47
2:D:493:GLU:HB3	2:D:513:ILE:HB	1.96	0.47
4:G:157:PHE:HB2	4:G:165:ILE:HD12	1.95	0.47
1:C:366:THR:HG23	1:C:367:ILE:HD13	1.95	0.47
2:D:667:TYR:HB3	10:D:1990:C8E:H202	1.97	0.47
11:D:2226:HOH:O	3:E:47:ASN:OD1	2.20	0.47
1:A:331:GLU:OE1	11:A:2144:HOH:O	2.20	0.47
2:B:579:GLN:HA	2:B:580:ASP:HB3	1.96	0.47
2:D:56:ARG:O	2:D:254:ARG:NH2	2.46	0.47
3:F:107:ALA:HB2	3:F:117:SER:HB2	1.97	0.47
2:B:798:MET:HE1	2:B:960:LEU:HD11	1.96	0.47
2:D:560:PHE:O	2:D:644:MET:HE1	2.15	0.47
2:B:412:GLN:HA	2:B:450:GLN:O	2.16	0.47
2:D:135:PRO:C	2:D:137:ASP:H	2.23	0.47
2:D:928:ALA:HB3	2:D:983:LYS:HB2	1.96	0.46
2:B:281:GLY:H	2:B:288:ASP:HB2	1.80	0.46
4:G:182:MET:HE2	4:G:196:TRP:HB2	1.97	0.46
2:B:200:MET:HE1	2:B:225:TRP:HB2	1.97	0.46
2:B:709:THR:HG23	2:B:719:GLU:HG2	1.98	0.46
2:D:539:TYR:HB2	2:D:567:SER:HB3	1.97	0.46
4:G:97:SER:HA	4:G:98:GLY:HA2	1.75	0.46
2:B:61:MET:CE	2:B:162:VAL:HG11	2.45	0.46
1:C:412:CYS:HA	1:C:413:PRO:C	2.41	0.46
2:D:301:HIS:HB3	2:D:308:PHE:CZ	2.51	0.46
1:A:27:SER:HB3	1:A:170:ILE:HD11	1.97	0.46
2:B:170:ARG:CB	2:B:171:LYS:HA	2.37	0.46
2:B:499:ILE:O	2:B:507:ASN:ND2	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:195:GLN:HG3	2:D:847:ALA:HB2	1.97	0.46
4:G:108:ARG:HB3	4:G:113:VAL:HA	1.98	0.46
4:G:139:GLY:O	4:G:144:ARG:HB2	2.16	0.46
1:A:182:ALA:O	1:A:186:ARG:HG3	2.15	0.46
1:A:333:TYR:CD2	1:A:342:ASN:HB3	2.51	0.46
2:D:935:GLY:HA2	2:D:976:PHE:HA	1.97	0.46
2:D:961:GLU:HG3	11:D:2031:HOH:O	2.16	0.46
1:A:430:TYR:CE2	1:A:432:PRO:HA	2.51	0.46
2:B:173:LYS:HA	2:B:174:GLY:HA2	1.64	0.46
2:B:460:ASP:HB3	2:B:462:MET:HE3	1.98	0.46
2:D:734:LEU:O	2:D:735:PRO:C	2.59	0.46
2:D:907:LEU:HD23	2:D:938:LEU:HB2	1.98	0.46
4:G:125:GLN:HA	4:G:131:PHE:HA	1.98	0.46
2:B:280:ASP:HA	2:B:288:ASP:O	2.16	0.46
2:B:489:TYR:CE2	2:B:517:HIS:HB3	2.51	0.46
2:D:484:GLU:HG3	2:D:522:ARG:HG2	1.97	0.46
2:D:832:ARG:HH11	2:D:968:THR:HG21	1.80	0.46
4:G:108:ARG:CB	4:G:113:VAL:HA	2.46	0.46
1:C:232:LYS:HE3	2:D:620:THR:O	2.15	0.45
1:C:247:ASN:HB2	11:C:2073:HOH:O	2.16	0.45
2:D:588:ARG:NH1	11:D:2002:HOH:O	2.35	0.45
2:B:218:PHE:HE1	2:B:340:ASP:HB3	1.81	0.45
2:B:559:PHE:HB3	2:B:642:PRO:HG2	1.98	0.45
2:D:356:PRO:O	2:D:440:PHE:HZ	1.98	0.45
2:D:713:THR:HG22	2:D:714:LYS:N	2.28	0.45
2:D:833:THR:OG1	2:D:966:GLU:OE2	2.28	0.45
3:E:116:ASP:OD2	3:E:139:ARG:NE	2.39	0.45
1:A:34:VAL:HG21	1:A:114:ILE:HD13	1.98	0.45
2:B:769:ALA:HB3	2:B:777:ILE:HD11	1.98	0.45
1:A:411:ASP:OD2	1:A:480:LYS:OXT	2.34	0.45
2:B:832:ARG:HD2	2:B:967:TYR:CE2	2.51	0.45
1:C:99:ALA:HB1	1:C:164:MET:HG3	1.98	0.45
1:C:273:THR:HG22	1:C:276:ASP:N	2.28	0.45
1:A:451:ARG:HD3	1:A:473:THR:HB	1.98	0.45
2:B:441:SER:HA	2:B:442:GLY:HA2	1.60	0.45
2:D:737:GLU:H	2:D:737:GLU:CD	2.25	0.45
3:F:62:GLY:HA2	3:F:66:GLU:HA	1.98	0.45
4:G:133:ILE:HB	4:G:157:PHE:HE2	1.81	0.45
2:B:329:SER:O	2:B:333:SER:HB2	2.16	0.45
2:D:973:SER:HB2	2:D:975:ARG:NH1	2.31	0.45
4:G:194:LEU:HD22	4:G:196:TRP:HE3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:875:THR:HG23	3:F:57:TRP:CZ2	2.51	0.45
2:D:105:ASP:OD2	2:D:166:THR:OG1	2.23	0.45
2:D:611:SER:HB2	2:D:620:THR:HG22	1.99	0.45
2:B:338:PRO:HB2	2:B:341:ILE:HG12	1.98	0.45
2:B:39:ALA:HB1	2:B:539:TYR:CG	2.52	0.45
2:D:834:LYS:HG3	2:D:948:PHE:CZ	2.51	0.45
3:F:94:LYS:HB2	3:F:125:ASP:CG	2.42	0.45
4:G:62:PRO:HA	4:G:87:VAL:HB	1.98	0.45
4:G:103:ALA:O	11:G:2013:HOH:O	2.21	0.45
2:D:384:PHE:HE2	2:D:406:LEU:HD23	1.82	0.45
4:G:191:THR:N	4:G:192:GLY:HA2	2.32	0.45
1:A:123:PRO:HD3	1:A:138:TRP:CD2	2.52	0.44
1:C:449:MET:HE2	1:C:449:MET:HB2	1.82	0.44
2:D:521:ARG:NH2	2:D:598:ALA:O	2.50	0.44
4:G:2:ASP:HB2	11:G:2002:HOH:O	2.16	0.44
4:G:188:ASP:HB3	4:G:191:THR:OG1	2.17	0.44
2:B:170:ARG:HB3	2:B:171:LYS:C	2.41	0.44
2:B:453:ARG:NH2	2:D:380:GLU:OE2	2.31	0.44
1:C:273:THR:HG23	1:C:302:LYS:O	2.16	0.44
1:C:289:HIS:NE2	1:C:440:THR:OG1	2.40	0.44
3:F:21:VAL:HA	3:F:137:GLY:HA3	1.99	0.44
1:A:37:GLU:HG2	1:A:76:SER:OG	2.18	0.44
2:B:231:ASN:HB3	11:B:2097:HOH:O	2.17	0.44
2:B:716:PHE:HA	2:B:811:LYS:O	2.17	0.44
1:C:34:VAL:HG12	1:C:114:ILE:HG21	1.99	0.44
2:D:200:MET:HE1	2:D:225:TRP:HB2	1.99	0.44
2:D:855:ILE:HG23	2:D:874:ASN:ND2	2.32	0.44
2:D:966:GLU:HG2	2:D:969:ALA:H	1.83	0.44
4:G:158:GLU:HB2	4:G:168:LEU:HD21	1.99	0.44
2:B:244:ASN:OD1	2:B:245:ILE:N	2.50	0.44
2:B:797:ASP:O	2:B:828:VAL:HG12	2.16	0.44
1:C:171:PHE:HZ	1:C:221:VAL:HG22	1.83	0.44
1:A:219:GLY:O	1:A:322:GLN:HB2	2.17	0.44
2:B:218:PHE:CE1	2:B:340:ASP:HB3	2.52	0.44
2:B:774:GLN:OE1	2:B:776:ARG:NE	2.51	0.44
2:B:863:ILE:HB	2:B:870:THR:HB	1.99	0.44
1:C:252:TYR:HE1	1:C:430:TYR:CD2	2.35	0.44
2:D:336:GLN:NE2	2:D:836:ILE:HD11	2.32	0.44
2:D:884:TYR:CG	2:D:885:LYS:N	2.85	0.44
1:A:134:ALA:HB2	2:B:681:MET:HE3	1.99	0.44
4:G:108:ARG:HH12	4:G:111:PRO:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ILE:HA	2:D:629:TYR:O	2.18	0.44
2:D:917:PRO:HG2	2:D:920:TRP:CD1	2.52	0.44
1:A:211:VAL:HG13	1:A:329:ILE:HG12	2.00	0.44
2:D:57:THR:C	2:D:59:ASP:H	2.25	0.44
2:D:111:ASN:HA	2:D:129:GLY:HA3	1.99	0.44
2:D:789:ALA:O	2:D:790:SER:HB3	2.18	0.44
2:B:166:THR:HB	2:B:298:ARG:NH1	2.33	0.44
2:D:542:VAL:HG22	2:D:564:ILE:HD12	2.00	0.44
3:E:12:VAL:HG21	3:E:56:MET:HB3	1.99	0.44
1:A:222:LYS:HE2	1:A:224:ASP:HB2	1.99	0.43
4:G:107:LYS:HG3	4:G:115:ALA:HA	2.00	0.43
2:B:598:ALA:HB2	2:B:676:ILE:HD13	2.00	0.43
3:E:79:THR:HA	3:E:101:LYS:HA	2.00	0.43
4:G:107:LYS:N	4:G:207:ASP:OD1	2.49	0.43
1:A:451:ARG:HD2	1:A:473:THR:O	2.18	0.43
2:B:953:MET:HB3	2:B:966:GLU:HB2	2.00	0.43
1:C:413:PRO:HB2	1:C:435:LEU:HG	2.01	0.43
4:G:188:ASP:OD2	4:G:191:THR:HG23	2.18	0.43
2:B:67:LYS:HE3	2:B:820:ASP:OD2	2.19	0.43
2:B:101:LEU:HD11	2:B:108:PRO:HB3	2.00	0.43
1:C:73:MET:HE3	1:C:73:MET:HB2	1.86	0.43
4:G:114:VAL:HG11	4:G:140:TRP:CH2	2.53	0.43
2:B:404:MET:SD	2:B:459:GLN:NE2	2.92	0.43
2:D:207:THR:HG22	2:D:208:GLU:N	2.34	0.43
2:B:141:MET:HE3	2:B:141:MET:HB2	1.84	0.43
2:B:786:PRO:HG2	2:B:894:MET:HE3	2.01	0.43
2:D:242:PRO:HA	2:D:339:ARG:NH2	2.33	0.43
2:B:828:VAL:CG2	2:B:899:LEU:HB3	2.49	0.43
2:B:869:VAL:O	11:B:2270:HOH:O	2.22	0.43
2:D:92:SER:HB3	2:D:672:THR:OG1	2.19	0.43
2:D:94:LEU:HA	2:D:95:SER:HA	1.80	0.43
2:D:195:GLN:HG2	2:D:197:GLU:H	1.83	0.43
1:A:226:PHE:CE2	1:A:317:VAL:HG23	2.54	0.43
2:B:91:VAL:HG11	2:B:960:LEU:HD13	2.01	0.43
1:C:169:LEU:HD23	1:C:225:CYS:SG	2.59	0.43
2:D:56:ARG:HG3	2:D:979:ASN:HB2	2.00	0.43
2:B:306:LEU:HD11	2:B:390:LEU:HD11	2.01	0.43
2:B:680:ALA:O	2:B:738:LEU:HD23	2.18	0.43
2:B:853:PRO:HD2	3:F:17:GLY:HA2	2.01	0.43
1:C:373:ALA:C	1:C:375:SER:H	2.26	0.43
3:F:123:GLN:NE2	3:F:132:THR:OG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:12:THR:OG1	4:G:75:ASP:OD2	2.26	0.43
4:G:153:MET:HE1	4:G:179:MET:HB3	2.01	0.43
2:B:200:MET:HE1	2:B:225:TRP:CB	2.49	0.42
2:B:523:LEU:HD11	2:B:547:ASP:HB3	2.01	0.42
2:D:623:LEU:HA	2:D:624:GLY:HA2	1.74	0.42
2:D:849:ASN:ND2	2:D:854:LEU:HB3	2.33	0.42
3:E:4:ASP:N	11:E:2001:HOH:O	2.51	0.42
4:G:26:VAL:HG22	4:G:86:TYR:HB2	2.01	0.42
2:B:169:GLY:HA3	2:B:269:ASP:HB2	2.01	0.42
2:B:518:MET:HG2	2:B:519:GLU:N	2.31	0.42
2:B:776:ARG:HB3	2:B:858:ASN:O	2.19	0.42
2:B:954:THR:HG21	2:B:957:GLY:O	2.18	0.42
2:D:153:TYR:OH	2:D:163:MET:HE2	2.19	0.42
2:D:203:ASN:O	2:D:881:SER:HA	2.19	0.42
1:A:50:GLU:HG3	1:A:282:GLN:NE2	2.24	0.42
1:A:71:GLN:HG2	1:A:456:LEU:HB3	2.01	0.42
4:G:157:PHE:HA	4:G:168:LEU:HD23	2.01	0.42
4:G:200:TYR:O	4:G:202:GLY:N	2.52	0.42
1:A:94:LYS:HG2	11:A:2058:HOH:O	2.19	0.42
1:A:97:ASN:ND2	1:A:165[B]:ASP:OD1	2.51	0.42
2:B:208:GLU:O	2:B:226:GLY:N	2.52	0.42
2:B:230:ASN:ND2	11:B:2095:HOH:O	2.52	0.42
1:C:43:GLY:HA3	1:C:400:HIS:HD1	1.83	0.42
2:D:110:ASN:HB3	2:D:383:ARG:NH2	2.35	0.42
2:D:759:MET:HE2	2:D:759:MET:HB3	1.97	0.42
2:D:291:ASP:O	2:D:317:GLN:HA	2.19	0.42
2:D:835:ASP:HA	2:D:898:PHE:CE1	2.53	0.42
2:B:886:TYR:CE1	2:B:891:GLY:HA2	2.54	0.42
2:B:935:GLY:HA2	2:B:976:PHE:HA	2.02	0.42
1:A:171:PHE:CD1	1:A:177:GLN:HG2	2.55	0.42
2:B:37:GLU:O	2:B:38:LYS:HB2	2.19	0.42
2:D:829:MET:HE3	2:D:902:LYS:HA	2.02	0.42
2:D:867:GLU:O	2:D:867:GLU:HG2	2.20	0.42
1:A:29:SER:HB2	1:A:84:ALA:HB2	2.02	0.42
3:E:32:VAL:O	3:E:35:PRO:HD3	2.19	0.42
2:B:59:ASP:OD2	2:B:62:SER:N	2.52	0.41
2:B:335:TYR:CE2	2:B:833:THR:HG23	2.54	0.41
2:B:835:ASP:HA	2:B:898:PHE:CE1	2.55	0.41
2:D:224:LEU:HD13	2:D:233:GLN:OE1	2.20	0.41
2:D:441:SER:HA	2:D:442:GLY:HA2	1.62	0.41
1:A:418:TYR:CE2	1:A:429:VAL:HB	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:534:TRP:CH2	2:B:535:LYS:HD2	2.55	0.41
2:D:207:THR:CB	2:D:210:GLU:HG2	2.50	0.41
2:D:569:ILE:HG22	2:D:571:SER:H	1.85	0.41
4:G:194:LEU:HD22	4:G:196:TRP:CE3	2.55	0.41
2:D:855:ILE:HG23	2:D:874:ASN:HD22	1.85	0.41
3:E:15:MET:SD	3:E:78:ARG:HA	2.60	0.41
1:A:34:VAL:CG2	1:A:114:ILE:HD13	2.49	0.41
1:A:409:ARG:HG3	11:A:2090:HOH:O	2.20	0.41
2:B:497:LEU:HA	2:B:507:ASN:O	2.20	0.41
1:C:2:ASP:O	2:D:522:ARG:HD2	2.21	0.41
1:C:451:ARG:HD2	1:C:473:THR:O	2.20	0.41
4:G:36:PRO:HD2	4:G:83:ARG:NH1	2.35	0.41
1:A:213:ASN:HB3	1:A:215:GLU:HG3	2.02	0.41
2:D:211:ASN:HB2	2:D:336:GLN:HB3	2.03	0.41
2:B:94:LEU:HD12	2:B:94:LEU:HA	1.67	0.41
1:C:311:ILE:O	1:C:315:LYS:HB2	2.21	0.41
3:E:119:VAL:HA	3:E:135:VAL:O	2.21	0.41
4:G:108:ARG:HB2	4:G:114:VAL:H	1.86	0.41
2:B:79:ASP:OD1	2:B:970:ASN:ND2	2.43	0.41
2:B:152:LEU:HD12	2:B:152:LEU:HA	1.89	0.41
2:B:561:TYR:CD2	2:B:594:THR:HA	2.56	0.41
1:C:353:ALA:O	1:C:357:VAL:HG23	2.21	0.41
2:D:599:ASP:OD1	2:D:600:VAL:HG22	2.20	0.41
1:A:183:ASN:OD1	1:A:186:ARG:NH1	2.54	0.41
2:B:551:THR:HB	11:B:2178:HOH:O	2.21	0.41
2:D:461:ILE:O	2:D:479:GLY:HA2	2.21	0.41
4:G:194:LEU:O	4:G:209:ILE:HG13	2.21	0.41
1:A:39:TYR:OH	1:A:397:TYR:HA	2.20	0.41
1:A:344:LYS:O	1:A:348:GLU:HG3	2.21	0.41
2:B:817:LEU:HD12	2:B:817:LEU:HA	1.89	0.41
1:C:116:VAL:C	1:C:118:ASN:H	2.28	0.41
1:C:211:VAL:HG21	1:C:332:VAL:HG11	2.03	0.41
2:D:473:ASN:HB3	2:D:533:SER:HB3	2.03	0.41
2:D:769:ALA:C	2:D:789:ALA:HB2	2.46	0.41
3:F:15:MET:HB3	3:F:56:MET:HE1	2.02	0.41
4:G:123:ILE:HG12	4:G:133:ILE:HD12	2.02	0.41
1:A:454:TYR:CZ	1:A:466:PRO:HB2	2.56	0.41
2:B:221:SER:HB3	3:F:113:MET:HE3	2.03	0.41
2:B:363:TYR:HB3	5:P:9:GLY:HA3	2.03	0.41
1:C:337:HIS:HB3	1:C:338:ASN:H	1.77	0.41
2:D:330:MET:HB3	2:D:330:MET:HE3	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:20:TRP:CZ3	3:E:42:GLN:HG3	2.56	0.41
4:G:91:THR:HG21	4:G:128:PRO:HB3	2.04	0.41
4:G:176:GLY:CA	4:G:177:ASP:HB2	2.51	0.41
2:B:472:PHE:CE1	2:B:534:TRP:CD1	3.03	0.40
2:B:762:GLY:HA3	2:B:798:MET:HG2	2.02	0.40
2:B:798:MET:HE1	2:B:960:LEU:CD1	2.50	0.40
2:D:58:SER:HB2	2:D:277:ILE:HD13	2.03	0.40
4:G:109:THR:HB	4:G:205:SER:OG	2.20	0.40
1:A:273:THR:HG23	1:A:278:LYS:O	2.21	0.40
2:B:60:VAL:HG13	2:B:141:MET:HE1	2.03	0.40
2:B:530:PHE:O	2:B:541:THR:HA	2.22	0.40
2:B:953:MET:HE2	2:B:970:ASN:O	2.21	0.40
2:D:254:ARG:HA	2:D:278:SER:O	2.22	0.40
2:B:772:ASP:C	2:B:774:GLN:H	2.28	0.40
1:C:97:ASN:O	1:C:101:ARG:HG3	2.22	0.40
2:D:305:ALA:HB1	2:D:393:GLU:O	2.21	0.40
2:D:384:PHE:CE2	2:D:406:LEU:HD23	2.56	0.40
3:E:140:ARG:HG3	11:E:2040:HOH:O	2.21	0.40
1:A:181:PHE:CZ	1:A:221:VAL:HG11	2.57	0.40
2:B:56:ARG:NH1	2:B:136:ASP:OD1	2.43	0.40
1:C:354:ASP:OD1	1:C:358:ARG:NH1	2.53	0.40
4:G:136:PHE:CB	4:G:153:MET:HE2	2.51	0.40
4:G:165:ILE:HD13	4:G:165:ILE:HA	1.60	0.40
1:A:438:PRO:HD2	1:A:441:ASN:ND2	2.37	0.40
2:B:189:LEU:HD13	2:B:974:ARG:HG3	2.03	0.40
2:B:652:LEU:HD11	2:B:654:MET:HE3	2.04	0.40
1:C:364:GLU:H	1:C:364:GLU:CD	2.27	0.40
2:D:281:GLY:C	2:D:288:ASP:OD2	2.65	0.40
2:D:597:ASP:OD1	2:D:597:ASP:N	2.50	0.40
3:F:12:VAL:HA	3:F:75:TYR:CE1	2.56	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	479/480 (100%)	448 (94%)	30 (6%)	1 (0%)	43	64
1	C	477/480 (99%)	442 (93%)	32 (7%)	3 (1%)	21	38
2	B	941/984 (96%)	886 (94%)	51 (5%)	4 (0%)	30	50
2	D	935/984 (95%)	870 (93%)	64 (7%)	1 (0%)	48	71
3	E	143/148 (97%)	137 (96%)	4 (3%)	2 (1%)	9	17
3	F	144/148 (97%)	138 (96%)	6 (4%)	0	100	100
4	G	210/212 (99%)	187 (89%)	20 (10%)	3 (1%)	9	17
5	P	8/10 (80%)	6 (75%)	0	2 (25%)	0	0
6	Q	7/9 (78%)	7 (100%)	0	0	100	100
All	All	3344/3455 (97%)	3121 (93%)	207 (6%)	16 (0%)	24	43

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	38	LYS
4	G	201	ALA
1	A	120	SER
3	E	92	GLU
5	P	2	GLY
5	P	3	GLY
3	E	13	GLU
2	B	866	GLY
2	D	362	PRO
4	G	98	GLY
2	B	571	SER
1	C	117	ASP
4	G	103	ALA
1	C	225	CYS
1	C	337	HIS
2	B	362	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	393/392 (100%)	378 (96%)	15 (4%)	29	52
1	C	391/392 (100%)	374 (96%)	17 (4%)	26	47
2	B	800/836 (96%)	773 (97%)	27 (3%)	32	57
2	D	796/836 (95%)	755 (95%)	41 (5%)	21	39
3	E	121/124 (98%)	120 (99%)	1 (1%)	73	84
3	F	122/124 (98%)	118 (97%)	4 (3%)	33	57
4	G	176/177 (99%)	162 (92%)	14 (8%)	11	20
All	All	2799/2881 (97%)	2680 (96%)	119 (4%)	26	47

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	27	SER
1	A	49	TYR
1	A	74	ASP
1	A	120	SER
1	A	146	LYS
1	A	207	VAL
1	A	230	THR
1	A	260	SER
1	A	345	SER
1	A	365	ASN
1	A	380	GLN
1	A	384	LEU
1	A	397	TYR
1	A	475	VAL
2	B	60	VAL
2	B	170	ARG
2	B	171	LYS
2	B	190	ARG
2	B	195	GLN
2	B	219	ASP
2	B	222	MET
2	B	236	LYS
2	B	288	ASP
2	B	408	THR
2	B	436	SER

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Mol	Chain	Res	Type
2	B	441	SER
2	B	518	MET
2	B	581	VAL
2	B	675	GLN
2	B	692	MET
2	B	712	ARG
2	B	752	SER
2	B	777	ILE
2	B	781	SER
2	B	816	SER
2	B	854	LEU
2	B	902	LYS
2	B	915	ASP
2	B	921	LEU
2	B	966	GLU
2	B	981	MET
1	C	25	SER
1	C	27	SER
1	C	49	TYR
1	C	73	MET
1	C	121	ASP
1	C	207	VAL
1	C	256	SER
1	C	266	ILE
1	C	278	LYS
1	C	290	MET
1	C	291	GLN
1	C	305	SER
1	C	345	SER
1	C	366	THR
1	C	367	ILE
1	C	397	TYR
1	C	463	VAL
2	D	55	SER
2	D	58	SER
2	D	59	ASP
2	D	60	VAL
2	D	75	SER
2	D	87	ILE
2	D	94	LEU
2	D	172	GLU
2	D	189	LEU

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Mol	Chain	Res	Type
2	D	191	LEU
2	D	195	GLN
2	D	222	MET
2	D	306	LEU
2	D	323	THR
2	D	365	VAL
2	D	441	SER
2	D	469	VAL
2	D	471	ASP
2	D	477	LEU
2	D	501	THR
2	D	564	ILE
2	D	565	THR
2	D	573	LEU
2	D	581	VAL
2	D	623	LEU
2	D	648	SER
2	D	660	ARG
2	D	661	LEU
2	D	662	SER
2	D	666	SER
2	D	717	SER
2	D	757	THR
2	D	787	VAL
2	D	824	ARG
2	D	825	GLN
2	D	858	ASN
2	D	859	SER
2	D	860	VAL
2	D	914	TRP
2	D	915	ASP
2	D	966	GLU
3	E	52	SER
3	F	3	ASN
3	F	52	SER
3	F	60	ASP
3	F	89	VAL
4	G	31	GLN
4	G	74	GLU
4	G	99	ILE
4	G	107	LYS
4	G	112	SER

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Mol	Chain	Res	Type
4	G	126	MET
4	G	133	ILE
4	G	144	ARG
4	G	165	ILE
4	G	182	MET
4	G	184	ASN
4	G	186	LEU
4	G	191	THR
4	G	195	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	322	GLN
1	A	380	GLN
2	B	110	ASN
2	B	180	ASN
2	B	227	ASN
2	B	464	ASN
2	B	475	ASN
2	B	579	GLN
2	B	604	ASN
2	B	653	ASN
2	B	690	GLN
2	B	800	ASN
2	B	979	ASN
1	C	326	GLN
1	C	385	ASN
2	D	257	ASN
2	D	609	GLN
2	D	671	ASN
2	D	748	ASN
2	D	774	GLN
2	D	861	ASN
2	D	874	ASN
3	F	123	GLN
4	G	160	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 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	$\# Z > 2$
10	C8E	D	1991	-	5,5,20	0.22	0	4,4,19	0.50	0
10	C8E	D	1989	-	8,8,20	0.42	0	7,7,19	0.45	0
8	KR0	B	1985	1	26,26,26	1.24	2 (7%)	27,27,27	1.26	3 (11%)
10	C8E	D	1990	-	9,9,20	0.40	0	7,7,19	0.55	0
10	C8E	B	1989	-	8,8,20	0.26	0	7,7,19	0.43	0
8	KR0	D	1985	1	26,26,26	1.26	2 (7%)	27,27,27	1.27	4 (14%)

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
10	C8E	D	1991	-	-	1/3/3/18	-
10	C8E	D	1989	-	-	2/6/6/18	-
8	KR0	B	1985	1	-	7/26/26/26	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	C8E	D	1990	-	-	1/5/5/18	-
10	C8E	B	1989	-	-	2/6/6/18	-
8	KR0	D	1985	1	-	7/26/26/26	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	1985	KR0	O4-C5	4.37	1.46	1.33
8	B	1985	KR0	O1-C7	4.29	1.45	1.33
8	B	1985	KR0	O4-C5	4.29	1.45	1.33
8	D	1985	KR0	O1-C7	4.20	1.45	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1985	KR0	O4-C5-C10	3.69	123.10	111.83
8	D	1985	KR0	O4-C5-C10	3.39	122.17	111.83
8	B	1985	KR0	O1-C7-C12	3.06	121.18	111.83
8	D	1985	KR0	O1-C7-C12	2.82	120.42	111.83
8	B	1985	KR0	O4-C5-O8	-2.43	117.56	123.63
8	D	1985	KR0	O4-C5-O8	-2.38	117.66	123.63
8	D	1985	KR0	C1-O1-C7	2.33	124.20	116.90

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	1985	KR0	C12-C7-O1-C1
8	D	1985	KR0	O9-C7-O1-C1
10	D	1989	C8E	O9-C10-C11-O12
10	D	1990	C8E	O9-C10-C11-O12
8	B	1985	KR0	C12-C7-O1-C1
10	B	1989	C8E	C5-C6-C7-C8
8	B	1985	KR0	O9-C7-O1-C1
8	D	1985	KR0	C13-C17-C18-C19
8	D	1985	KR0	C17-C18-C19-C20
8	B	1985	KR0	O1-C1-C2-C3
8	B	1985	KR0	C12-C13-C17-C18
10	B	1989	C8E	C3-C4-C5-C6
8	D	1985	KR0	C12-C13-C17-C18
8	B	1985	KR0	C10-C11-C4-C6

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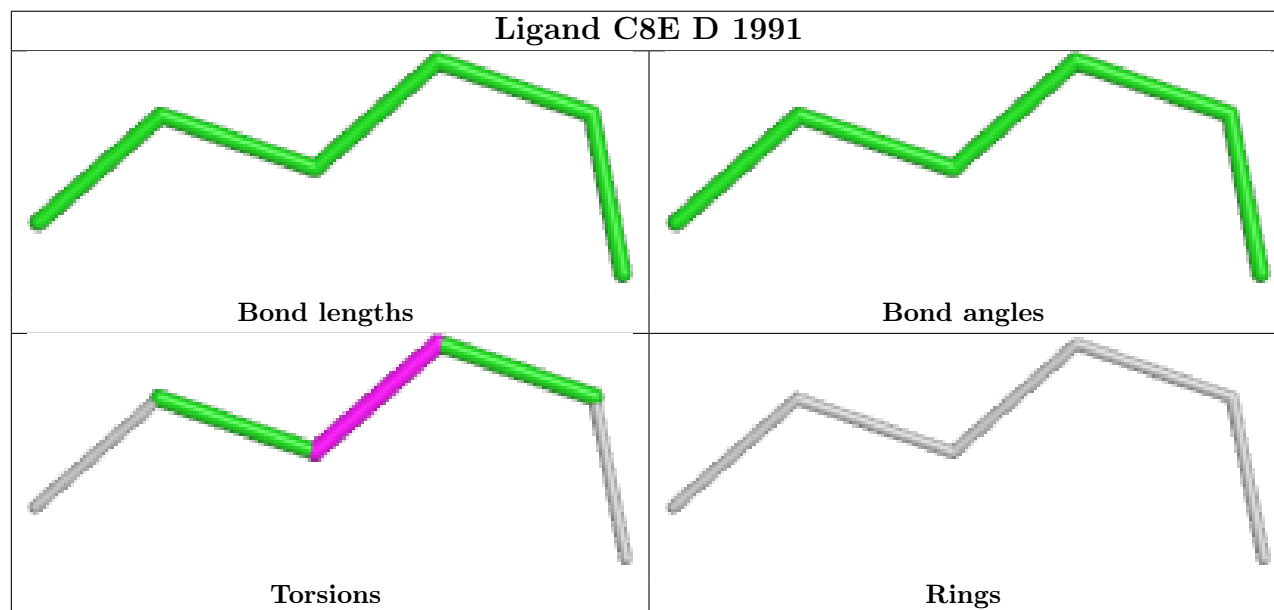
Mol	Chain	Res	Type	Atoms
8	D	1985	KR0	C9-C14-C15-C16
10	D	1989	C8E	C11-C10-O9-C8
10	D	1991	C8E	C2-C3-C4-C5
8	B	1985	KR0	C11-C10-C5-O4
8	B	1985	KR0	C11-C10-C5-O8
8	D	1985	KR0	C13-C12-C7-O1

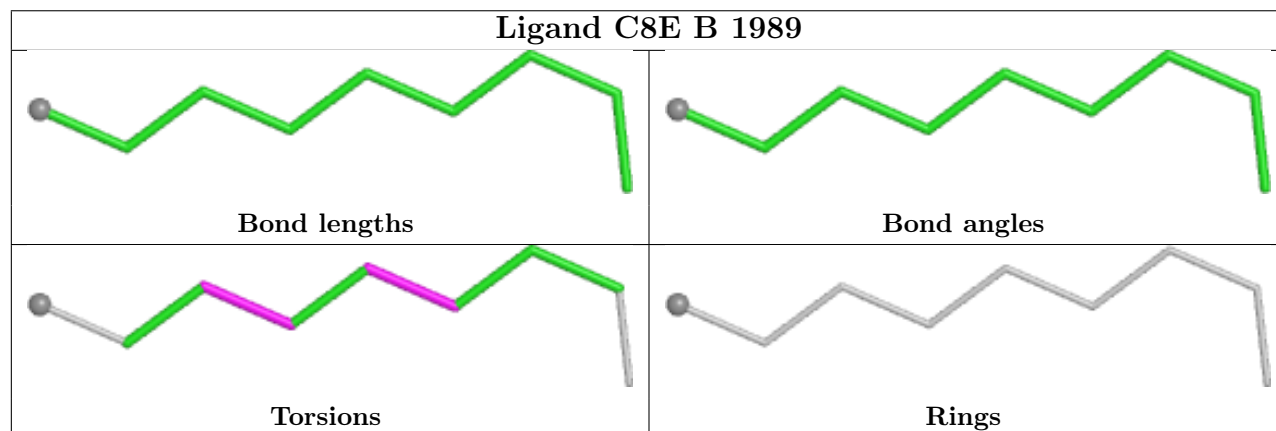
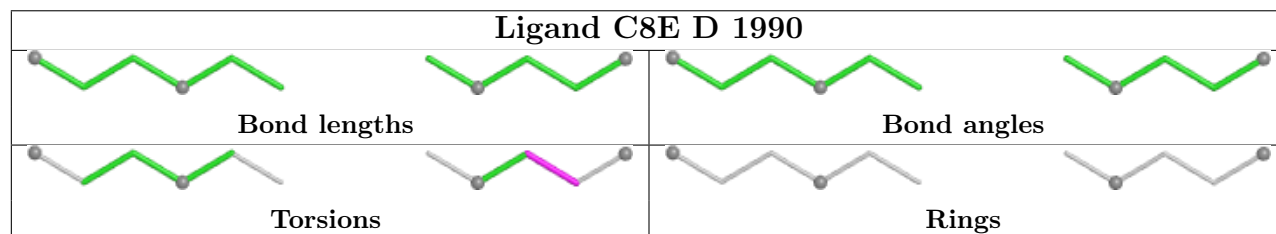
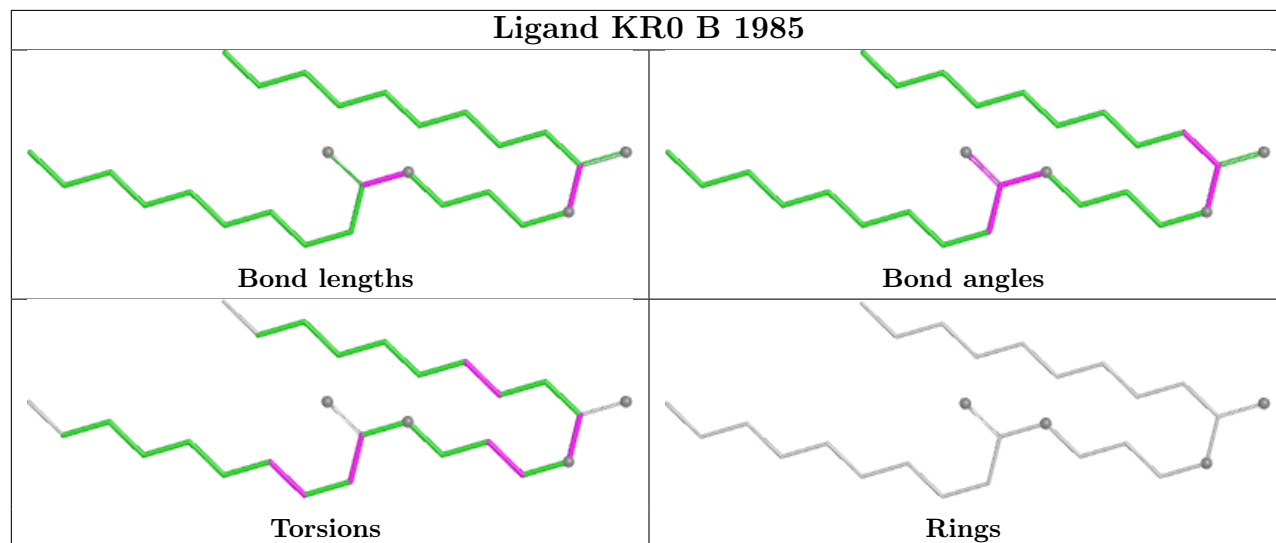
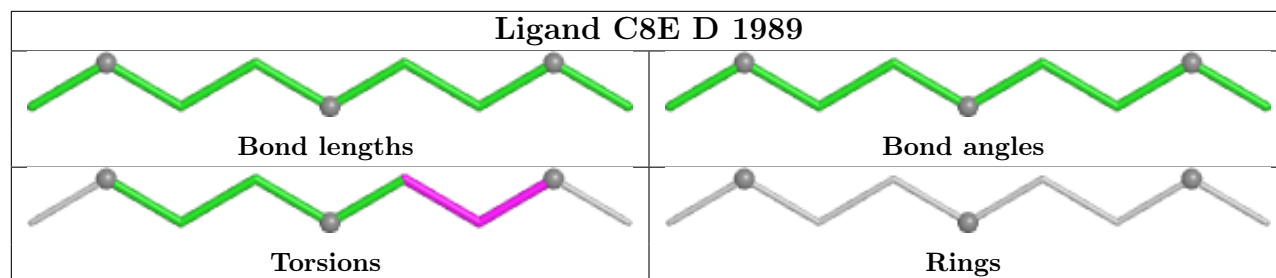
There are no ring outliers.

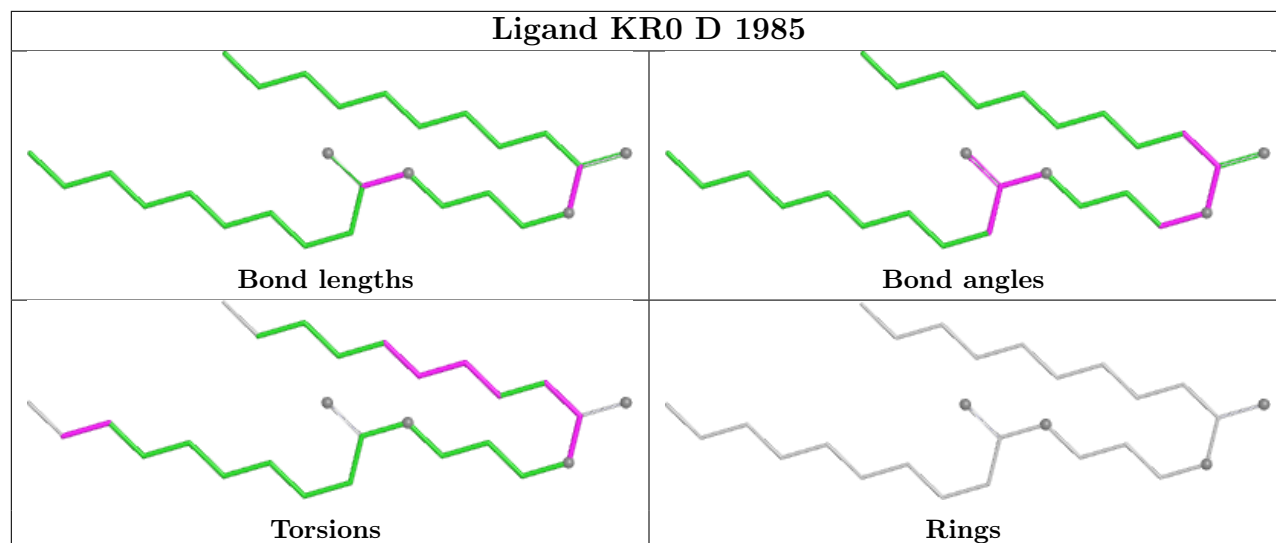
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	1990	C8E	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	480/480 (100%)	0.01	4 (0%)	82 82	22, 29, 41, 60	1 (0%)
1	C	479/480 (99%)	0.29	4 (0%)	82 82	25, 39, 61, 81	0
2	B	945/984 (96%)	0.12	10 (1%)	78 77	22, 31, 48, 86	0
2	D	941/984 (95%)	0.26	14 (1%)	72 71	26, 34, 54, 85	0
3	E	145/148 (97%)	0.02	0	100 100	29, 35, 49, 58	0
3	F	146/148 (98%)	0.24	1 (0%)	84 84	27, 40, 61, 88	0
4	G	212/212 (100%)	1.62	71 (33%)	1 0	32, 74, 115, 130	0
5	P	10/10 (100%)	1.81	4 (40%)	1 0	28, 29, 50, 67	0
6	Q	9/9 (100%)	1.25	1 (11%)	10 9	26, 27, 31, 34	0
All	All	3367/3455 (97%)	0.27	109 (3%)	50 48	22, 34, 66, 130	1 (0%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	573	LEU	5.6
4	G	111	PRO	5.4
4	G	110	ALA	4.8
4	G	128	PRO	4.7
2	D	574	LEU	4.4
4	G	115	ALA	4.3
4	G	210	VAL	4.3
4	G	1	CYS	4.2
4	G	189	PRO	4.2
5	P	1	GLY	4.2
4	G	186	LEU	4.2
4	G	140	TRP	4.2
4	G	192	GLY	4.2
2	B	574	LEU	3.9
2	D	812	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
4	G	108	ARG	3.7
4	G	112	SER	3.7
4	G	208	ILE	3.5
2	D	866	GLY	3.5
4	G	90	ASN	3.4
4	G	201	ALA	3.4
4	G	4	SER	3.4
2	D	613	ARG	3.4
2	D	173	LYS	3.3
5	P	2	GLY	3.3
4	G	103	ALA	3.3
4	G	114	VAL	3.2
4	G	88	ALA	3.1
4	G	206	PHE	3.1
4	G	207	ASP	3.1
4	G	162	ASP	3.0
4	G	199	ALA	3.0
4	G	113	VAL	3.0
4	G	92	ALA	3.0
4	G	139	GLY	3.0
4	G	191	THR	3.0
2	B	578	LEU	2.9
4	G	94	PRO	2.8
2	D	65	ALA	2.8
4	G	184	ASN	2.8
4	G	105	GLY	2.8
4	G	209	ILE	2.7
2	B	39	ALA	2.7
4	G	172	VAL	2.7
2	D	85	SER	2.7
2	B	532	GLY	2.6
4	G	109	THR	2.6
2	D	716	PHE	2.6
4	G	190	ALA	2.6
4	G	193	THR	2.6
1	A	246	GLY	2.6
4	G	187	LEU	2.5
4	G	129	GLY	2.5
3	F	3	ASN	2.5
4	G	181	GLN	2.5
2	B	170	ARG	2.5
4	G	132	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
4	G	198	VAL	2.5
2	D	658	LYS	2.5
4	G	96	LYS	2.5
4	G	202	GLY	2.5
2	B	919	ARG	2.4
5	P	4	GLY	2.4
4	G	203	GLN	2.4
4	G	164	THR	2.4
2	D	37	GLU	2.4
2	B	739	GLY	2.4
6	Q	4	GLY	2.4
4	G	173	ALA	2.4
4	G	107	LYS	2.4
5	P	10	GLY	2.3
2	D	94	LEU	2.3
2	D	623	LEU	2.3
2	D	667	TYR	2.3
4	G	174	GLY	2.3
4	G	185	THR	2.3
4	G	104	GLU	2.3
4	G	31	GLN	2.3
4	G	157	PHE	2.3
4	G	147	TYR	2.3
4	G	97	SER	2.2
4	G	146	GLY	2.2
4	G	194	LEU	2.2
1	C	373	ALA	2.2
4	G	211	LYS	2.2
4	G	200	TYR	2.2
1	C	212	GLN	2.2
1	A	297	ASP	2.2
4	G	204	LEU	2.2
4	G	116	PHE	2.2
4	G	119	TYR	2.2
1	A	260	SER	2.1
4	G	117	SER	2.1
4	G	82	THR	2.1
4	G	183	THR	2.1
4	G	95	LEU	2.1
4	G	168	LEU	2.1
1	C	339	ASP	2.1
4	G	45	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	171	LYS	2.1
4	G	195	LYS	2.1
1	A	446	GLY	2.1
4	G	141	TYR	2.1
2	B	37	GLU	2.0
2	B	868	ASN	2.0
4	G	151	TYR	2.0
4	G	205	SER	2.0
1	C	359	GLY	2.0
4	G	130	ILE	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.

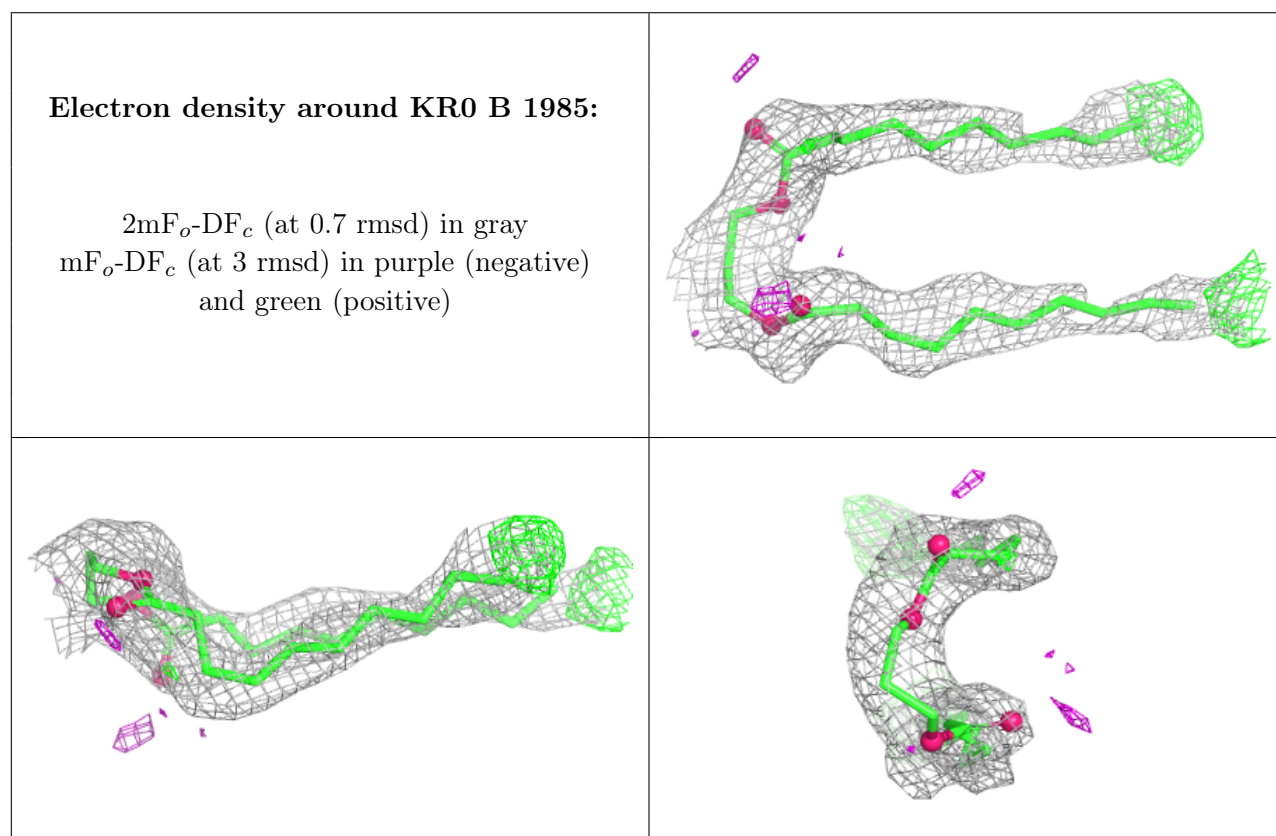
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	KR0	B	1985	27/27	0.76	0.23	41,46,54,57	0
8	KR0	D	1985	27/27	0.83	0.20	37,43,54,74	0
10	C8E	D	1989	9/21	0.83	0.20	23,38,41,42	0
10	C8E	D	1990	11/21	0.85	0.14	26,31,36,37	0
9	CA	D	1987	1/1	0.89	0.16	67,67,67,67	0
9	CA	B	1988	1/1	0.90	0.10	46,46,46,46	0
9	CA	B	1987	1/1	0.90	0.27	107,107,107,107	0
10	C8E	D	1991	6/21	0.90	0.15	18,21,24,25	0
10	C8E	B	1989	9/21	0.91	0.13	19,26,27,29	0
9	CA	D	1988	1/1	0.94	0.08	35,35,35,35	0
7	MG	A	1481	1/1	0.95	0.05	23,23,23,23	0
7	MG	C	1480	1/1	0.96	0.06	27,27,27,27	0
7	MG	D	1986	1/1	0.96	0.05	10,10,10,10	0

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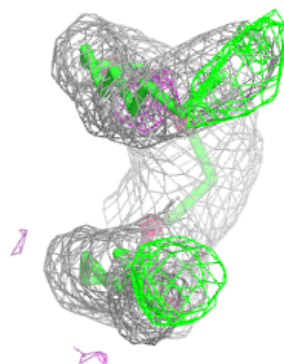
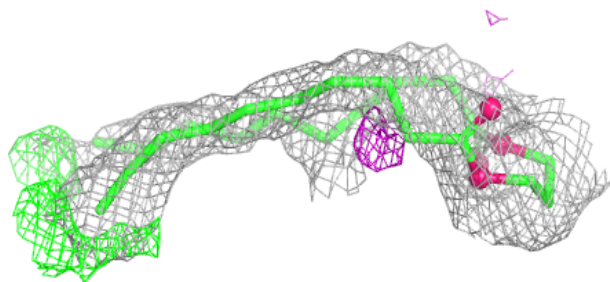
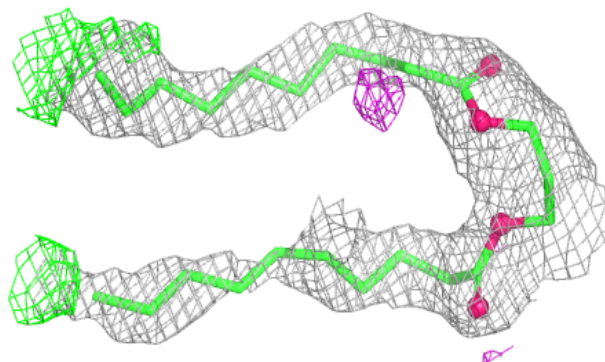
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	B	1986	1/1	0.98	0.04	13,13,13,13	0

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.

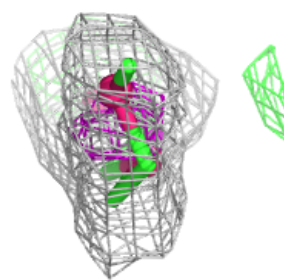
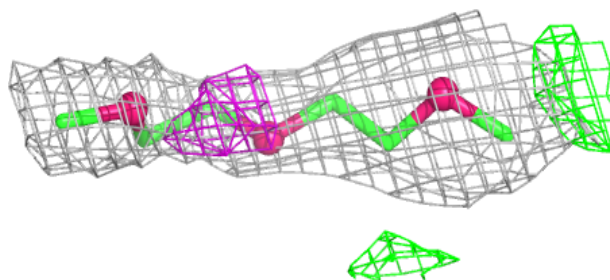
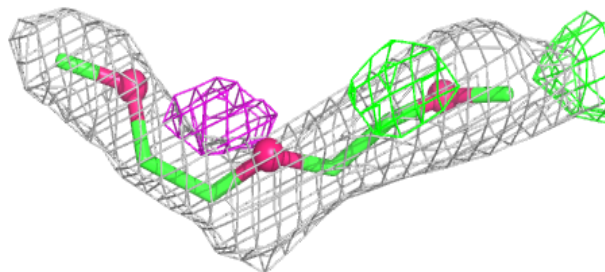


Electron density around KR0 D 1985:

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

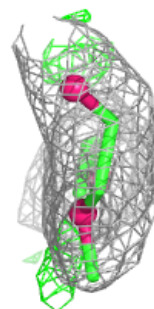
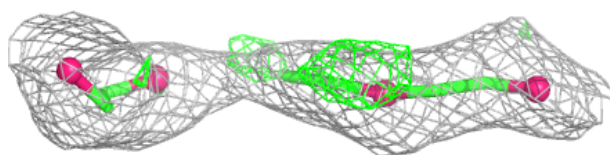
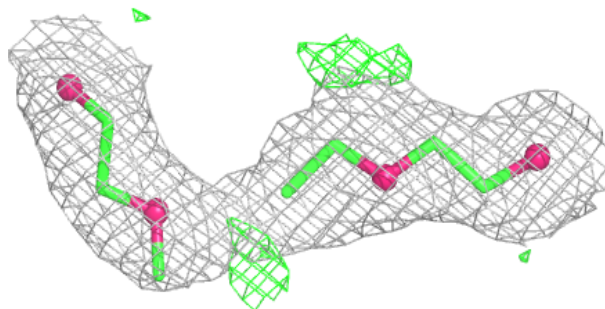
**Electron density around C8E D 1989:**

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

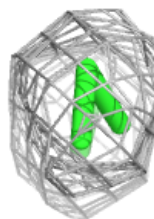
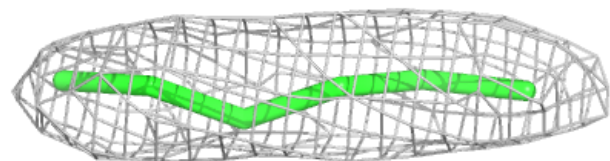
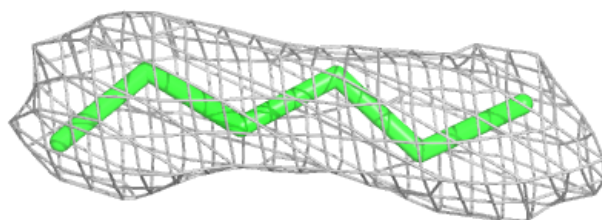


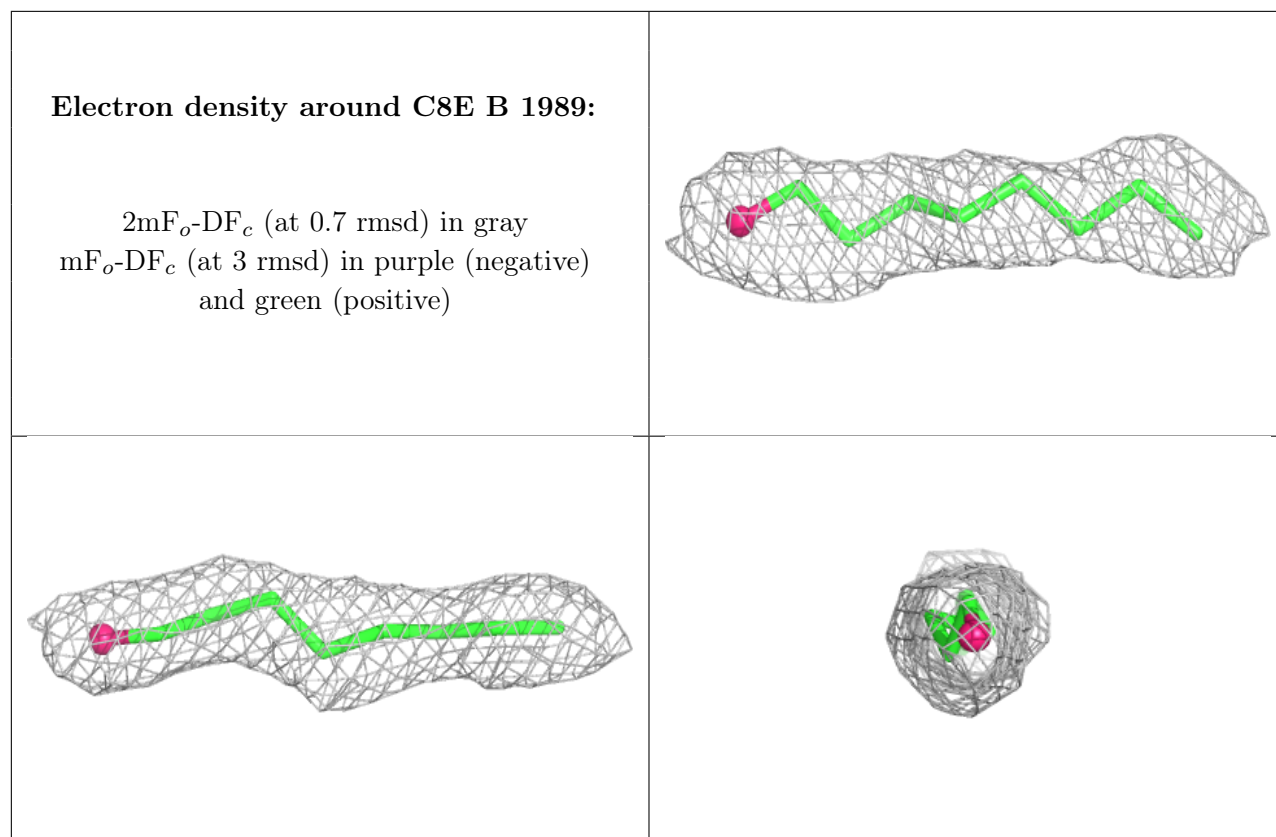
Electron density around C8E D 1990:

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

**Electron density around C8E D 1991:**

$2mF_o-DF_c$ (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.