



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:47 PM UTC

PDB ID : 8BK2 / pdb_00008bk2
Title : X-ray structure of meningococcal factor H binding protein variant 2 in complex with a specific and bactericidal human monoclonal antibody 1B1
Authors : Veggi, D.; Bottomley, J.M.
Deposited on : 2022-11-08
Resolution : 2.41 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

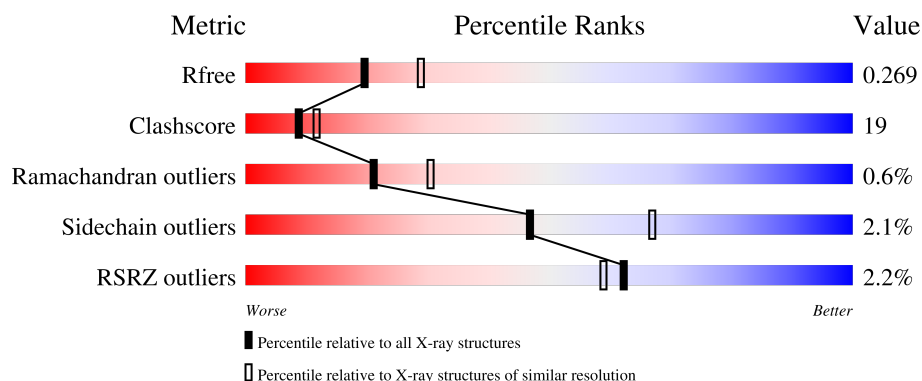
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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.



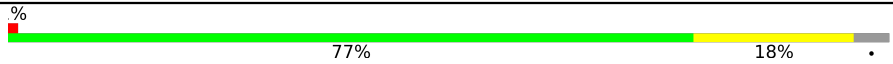
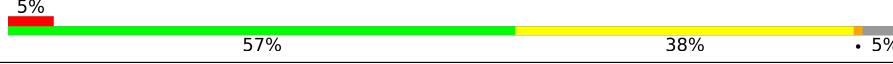
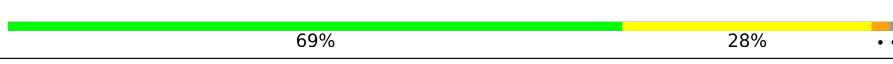
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	260	49% 18% 32%
1	B	260	48% 20% 32%
1	C	260	2% 51% 15% 33%
2	D	226	% 76% 17% 6%
2	F	226	6% 48% 42% 7%

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Mol	Chain	Length	Quality of chain
2	H	226	
3	E	216	
3	G	216	
3	L	216	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	301	-	-	X	-
8	MPD	L	302	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13902 atoms, of which 111 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 Factor H-binding protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	3	0	0
			1341	842	234	265			
1	B	176	Total	C	N	O	2	1	0
			1338	842	234	262			
1	C	173	Total	C	N	O	3	0	0
			1303	823	225	255			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP B9VX96
A	2	PRO	-	expression tag	UNP B9VX96
A	3	ASP	-	expression tag	UNP B9VX96
A	4	SER	-	expression tag	UNP B9VX96
A	5	ASP	-	expression tag	UNP B9VX96
A	6	ARG	-	expression tag	UNP B9VX96
A	7	LEU	-	expression tag	UNP B9VX96
A	8	GLN	-	expression tag	UNP B9VX96
A	9	GLN	-	expression tag	UNP B9VX96
A	10	ARG	-	expression tag	UNP B9VX96
A	11	ARG	-	expression tag	UNP B9VX96
A	259	LEU	-	expression tag	UNP B9VX96
A	260	GLU	-	expression tag	UNP B9VX96
B	1	GLY	-	expression tag	UNP B9VX96
B	2	PRO	-	expression tag	UNP B9VX96
B	3	ASP	-	expression tag	UNP B9VX96
B	4	SER	-	expression tag	UNP B9VX96
B	5	ASP	-	expression tag	UNP B9VX96
B	6	ARG	-	expression tag	UNP B9VX96
B	7	LEU	-	expression tag	UNP B9VX96
B	8	GLN	-	expression tag	UNP B9VX96
B	9	GLN	-	expression tag	UNP B9VX96
B	10	ARG	-	expression tag	UNP B9VX96

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Chain	Residue	Modelled	Actual	Comment	Reference
B	11	ARG	-	expression tag	UNP B9VX96
B	259	LEU	-	expression tag	UNP B9VX96
B	260	GLU	-	expression tag	UNP B9VX96
C	1	GLY	-	expression tag	UNP B9VX96
C	2	PRO	-	expression tag	UNP B9VX96
C	3	ASP	-	expression tag	UNP B9VX96
C	4	SER	-	expression tag	UNP B9VX96
C	5	ASP	-	expression tag	UNP B9VX96
C	6	ARG	-	expression tag	UNP B9VX96
C	7	LEU	-	expression tag	UNP B9VX96
C	8	GLN	-	expression tag	UNP B9VX96
C	9	GLN	-	expression tag	UNP B9VX96
C	10	ARG	-	expression tag	UNP B9VX96
C	11	ARG	-	expression tag	UNP B9VX96
C	259	LEU	-	expression tag	UNP B9VX96
C	260	GLU	-	expression tag	UNP B9VX96

- Molecule 2 is a protein called Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	1	0	0
			1602	1007	271	318	6			
2	D	213	Total	C	N	O	S	1	0	0
			1570	988	263	313	6			
2	F	210	Total	C	N	O	S	0	0	0
			1536	967	257	306	6			

- Molecule 3 is a protein called Fab light Chains.

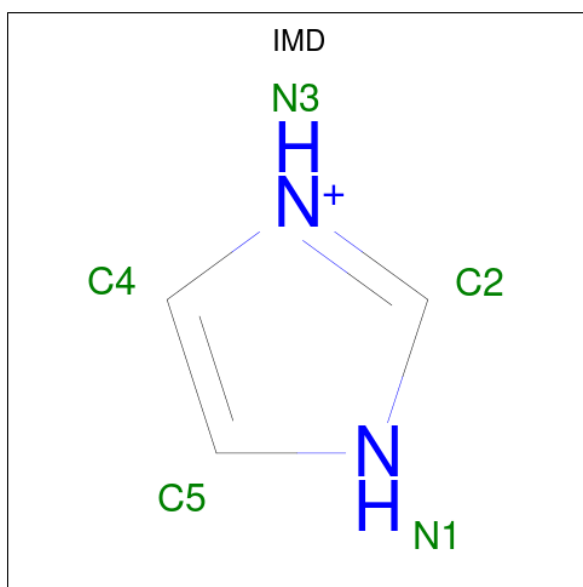
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	2	0	0
			1629	1019	276	329	5			
3	E	214	Total	C	N	O	S	0	0	0
			1618	1013	274	326	5			
3	G	206	Total	C	N	O	S	0	0	0
			1558	975	263	315	5			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



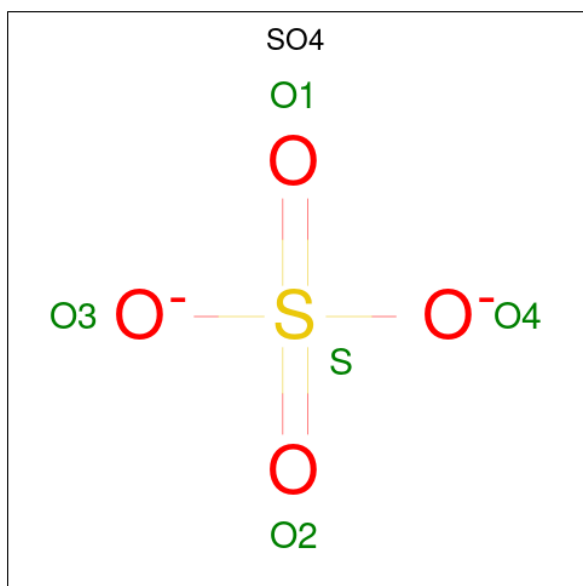
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	E	1	Total	C	H	O	0	0
			10	2	6	2		
4	F	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



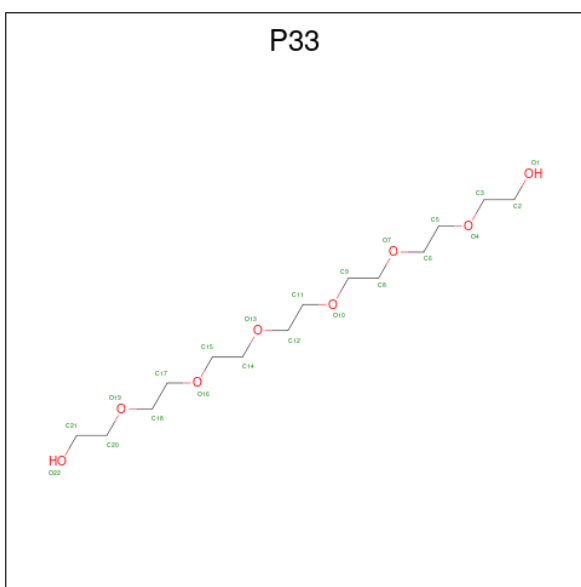
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	N	0	0
			10	3	5	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



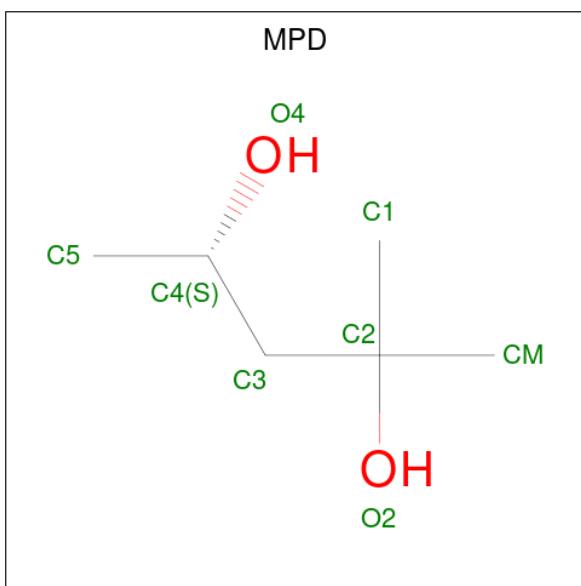
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 3,6,9,12,15,18-HEXAOSAICOSANE-1,20-DIOL (CCD ID: P33) (formula: C₁₄H₃₀O₈).



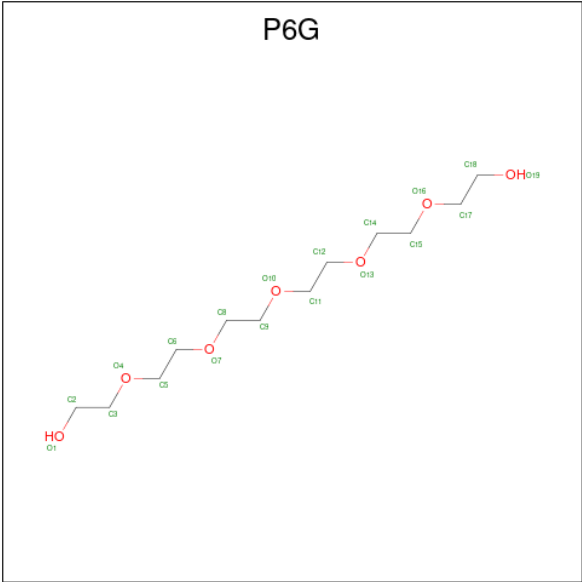
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	H	O	0	0
			52	14	30	8		

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 9 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	G	1	Total	C	H	O	0	0
			45	12	26	7		

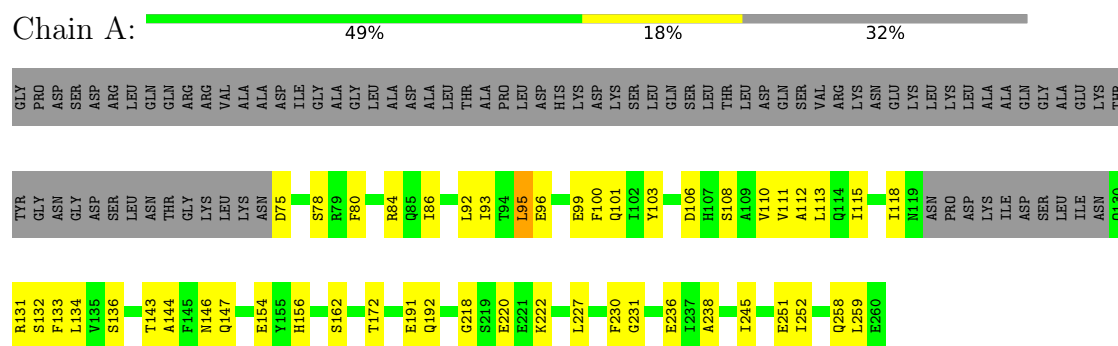
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	16	Total	O	0	0
			16	16		
10	B	7	Total	O	0	0
			7	7		
10	C	9	Total	O	0	0
			9	9		
10	H	41	Total	O	0	0
			41	41		
10	L	44	Total	O	0	0
			44	44		
10	D	28	Total	O	0	0
			28	28		
10	E	40	Total	O	0	0
			40	40		
10	F	9	Total	O	0	0
			9	9		
10	G	19	Total	O	0	0
			19	19		

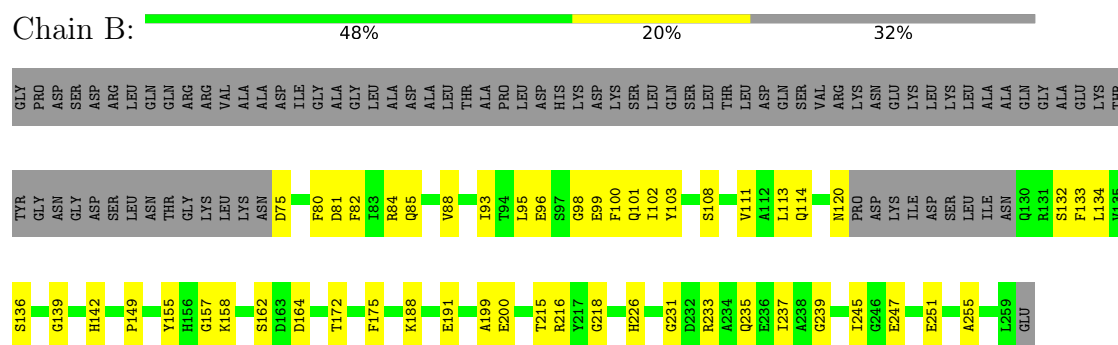
3 Residue-property plots

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.

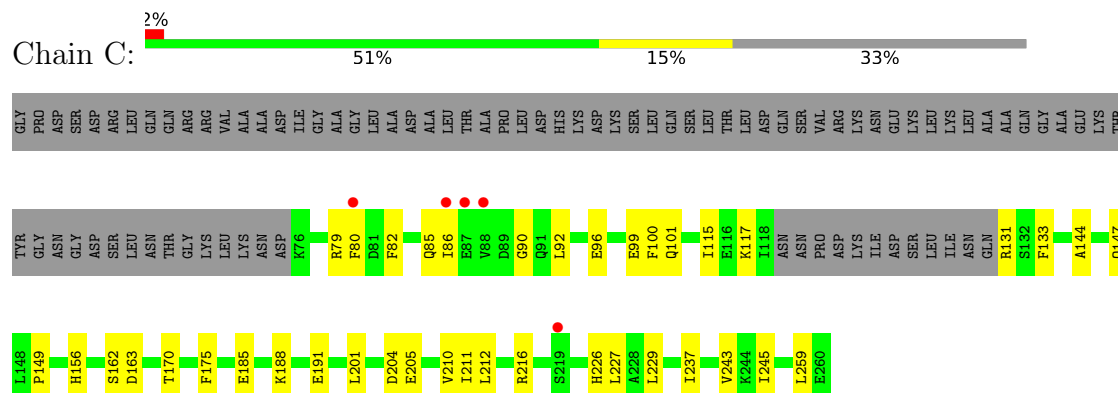
• Molecule 1: Factor H-binding protein



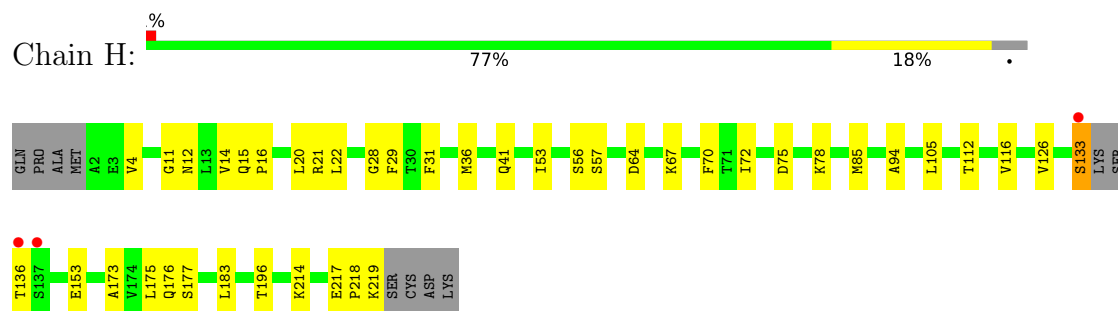
• Molecule 1: Factor H-binding protein



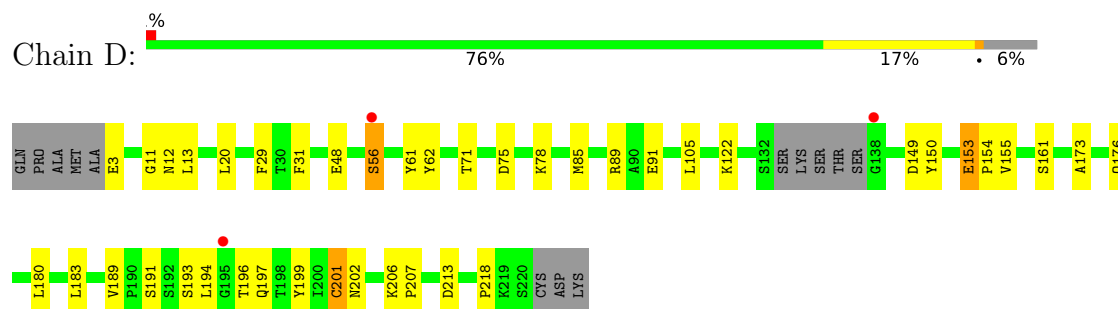
• Molecule 1: Factor H-binding protein



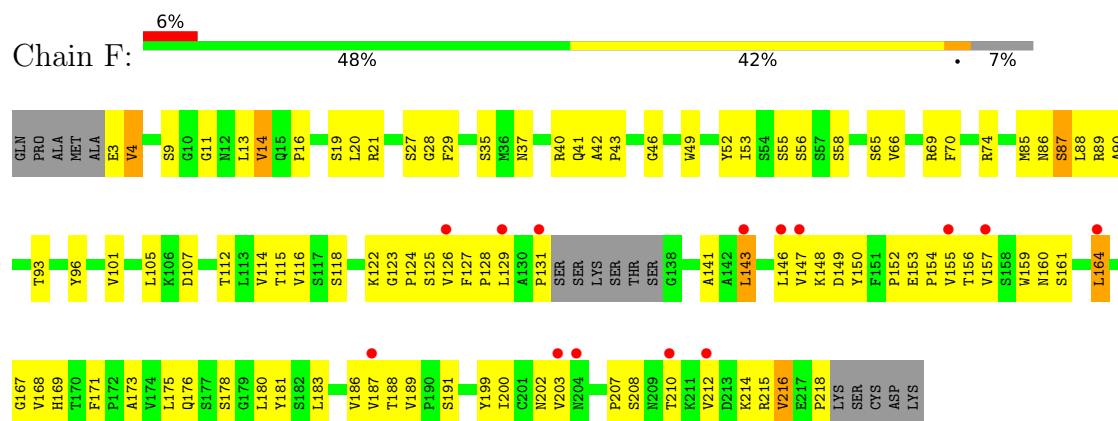
- Molecule 2: Fab Heavy chain



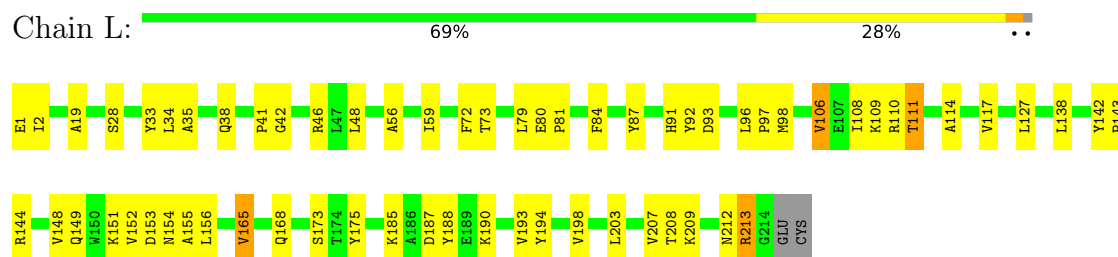
- Molecule 2: Fab Heavy chain



- Molecule 2: Fab Heavy chain

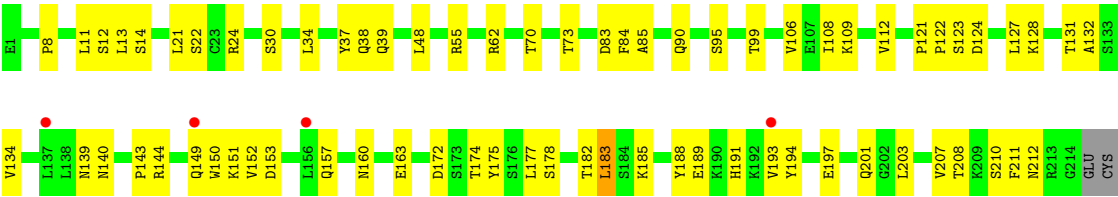


- Molecule 3: Fab light Chains

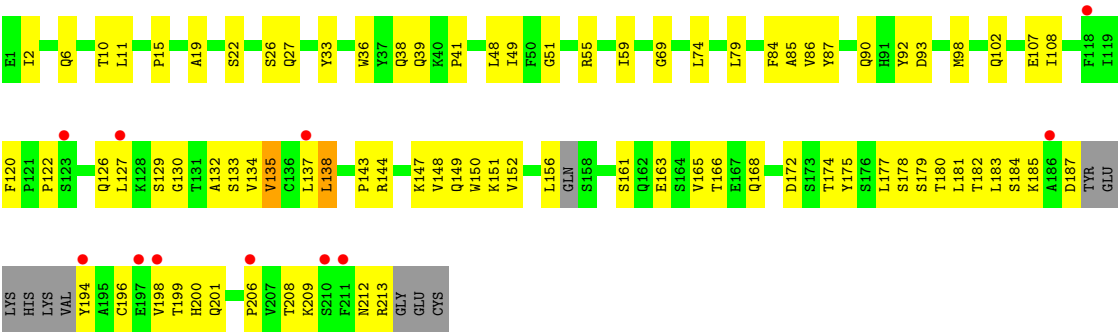


- Molecule 3: Fab light Chains





● Molecule 3: Fab light Chains



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.15Å 135.64Å 121.53Å 90.00° 105.18° 90.00°	Depositor
Resolution (Å)	49.66 – 2.41 49.66 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.66-2.41) 99.6 (49.66-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.204 , 0.270 (Not available) , 0.269	Depositor DCC
R_{free} test set	4734 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	62.0	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13902	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: P33, SO4, P6G, MPD, EDO, IMD

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	0.35	0/1362	0.54	0/1831
1	B	0.33	0/1362	0.56	0/1831
1	C	0.36	0/1324	0.54	0/1781
2	D	0.39	0/1605	0.60	0/2189
2	F	0.32	0/1571	0.52	0/2147
2	H	0.43	0/1637	0.61	0/2229
3	E	0.35	0/1654	0.55	0/2249
3	G	0.35	0/1590	0.54	0/2159
3	L	0.41	0/1665	0.59	0/2262
All	All	0.37	0/13770	0.56	0/18678

There are no bond length outliers.

There are no bond angle outliers.

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	1341	0	1298	39	0
1	B	1338	0	1294	40	0
1	C	1303	0	1261	36	0
2	D	1570	0	1522	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1536	0	1465	118	0
2	H	1602	0	1572	48	0
3	E	1618	0	1556	65	0
3	G	1558	0	1505	83	0
3	L	1629	0	1575	60	0
4	A	4	6	6	1	0
4	B	4	6	6	5	0
4	D	8	12	12	4	0
4	E	4	6	6	0	0
4	F	4	6	6	2	0
5	B	5	5	5	2	0
6	C	5	0	0	0	0
7	L	22	30	30	3	0
8	L	8	14	14	8	0
9	G	19	26	26	3	0
10	A	16	0	0	1	0
10	B	7	0	0	3	0
10	C	9	0	0	4	0
10	D	28	0	0	1	0
10	E	40	0	0	2	0
10	F	9	0	0	0	0
10	G	19	0	0	2	0
10	H	41	0	0	1	0
10	L	44	0	0	1	0
All	All	13791	111	13159	500	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 19.

All (500) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:PHE:HB3	1:A:113:LEU:HD13	1.33	1.10
2:F:52:TYR:HB2	3:G:98:MET:HE1	1.28	1.08
3:E:193:VAL:HG22	3:E:212:ASN:HA	1.36	1.07
2:F:183:LEU:HA	4:F:301:EDO:H11	1.40	0.99
2:H:11:GLY:H	2:H:112:THR:HG21	1.29	0.97
2:F:126:VAL:HG21	2:F:212:VAL:HG21	1.46	0.96
3:L:203:LEU:HD13	3:L:207:VAL:HG23	1.47	0.95
3:L:149:GLN:HG2	3:L:156:LEU:HD11	1.46	0.94
3:G:127:LEU:HD21	3:G:132:ALA:HB2	1.48	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:75:ASP:OD2	2:H:78:LYS:HE2	1.70	0.91
3:E:122:PRO:HB2	3:E:127:LEU:HD11	1.54	0.90
3:G:177:LEU:HD23	3:G:178:SER:N	1.87	0.90
3:E:203:LEU:HD13	3:E:207:VAL:HG23	1.53	0.89
8:L:302:MPD:O4	8:L:302:MPD:H12	1.71	0.88
2:H:11:GLY:HA3	2:H:112:THR:HG22	1.55	0.87
1:B:88:VAL:HG21	1:B:93:ILE:HD12	1.56	0.85
2:F:126:VAL:CG2	2:F:212:VAL:HG21	2.06	0.84
3:L:2:ILE:HB	8:L:302:MPD:H13	1.60	0.84
1:A:100:PHE:HB3	1:A:113:LEU:CD1	2.10	0.82
1:B:191:GLU:HB2	1:B:245:ILE:HD13	1.62	0.81
2:F:52:TYR:CB	3:G:98:MET:HE1	2.07	0.81
3:G:151:LYS:HG2	3:G:156:LEU:HD13	1.62	0.81
2:H:133:SER:HA	2:H:136:THR:HG22	1.63	0.81
3:E:121:PRO:HB3	3:E:211:PHE:CE2	2.16	0.80
2:H:219:LYS:N	10:H:301:HOH:O	2.09	0.80
1:B:100:PHE:HE1	1:B:102:ILE:HD11	1.47	0.80
2:F:13:LEU:HA	2:F:115:THR:O	1.82	0.79
2:F:126:VAL:HG21	2:F:212:VAL:CG2	2.13	0.79
2:F:131:PRO:HG3	2:F:143:LEU:HD21	1.63	0.79
3:G:120:PHE:HB2	3:G:135:VAL:HG13	1.64	0.79
1:C:170:THR:OG1	10:C:401:HOH:O	2.00	0.79
1:B:101:GLN:NE2	1:B:162:SER:O	2.15	0.78
2:H:64:ASP:HA	2:H:67:LYS:HD3	1.66	0.78
2:D:201:CYS:O	2:D:213:ASP:HA	1.82	0.78
2:F:131:PRO:HD2	2:F:218:PRO:HA	1.65	0.78
1:B:88:VAL:CG2	1:B:93:ILE:HD12	2.13	0.77
2:F:131:PRO:HG3	2:F:143:LEU:CD2	2.14	0.77
2:F:147:VAL:HB	2:F:183:LEU:HD23	1.66	0.76
1:A:86:ILE:HD13	1:A:95:LEU:HD11	1.65	0.76
2:F:14:VAL:O	2:F:116:VAL:HA	1.84	0.76
2:F:200:ILE:HD12	2:F:200:ILE:O	1.85	0.76
3:G:51:GLY:O	10:G:401:HOH:O	2.02	0.76
2:F:93:THR:HG23	2:F:116:VAL:HG12	1.66	0.76
3:E:185:LYS:O	3:E:189:GLU:HG3	1.85	0.75
4:D:302:EDO:H21	3:E:99:THR:HA	1.67	0.75
2:F:93:THR:HG22	2:F:115:THR:HA	1.68	0.75
1:C:156:HIS:CE1	1:C:259:LEU:HD11	2.22	0.74
2:D:75:ASP:OD2	2:D:78:LYS:HD2	1.86	0.74
1:B:85:GLN:NE2	10:B:401:HOH:O	2.11	0.74
2:F:70:PHE:CZ	2:F:85:MET:HG2	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:96:LEU:HA	4:D:301:EDO:H21	1.68	0.73
3:E:152:VAL:HG22	3:E:157:GLN:OE1	1.87	0.73
3:L:149:GLN:CG	3:L:156:LEU:HD11	2.18	0.73
3:L:41:PRO:HA	7:L:301:P33:H171	1.70	0.72
2:H:126:VAL:O	2:H:214:LYS:HE3	1.90	0.72
2:F:9:SER:HA	2:F:112:THR:HG21	1.70	0.72
3:E:157:GLN:HG2	3:E:160:ASN:HD21	1.52	0.72
1:A:86:ILE:CD1	1:A:95:LEU:HD11	2.20	0.71
1:B:82:PHE:CE1	1:B:98:GLY:HA3	2.25	0.71
2:F:167:GLY:O	2:F:187:VAL:HA	1.91	0.71
1:C:205:GLU:CD	1:C:205:GLU:H	1.95	0.71
2:F:152:PRO:HD2	2:F:207:PRO:HB2	1.73	0.70
2:F:93:THR:CG2	2:F:116:VAL:H	2.04	0.70
3:G:150:TRP:CD2	3:G:181:LEU:HD12	2.26	0.70
1:C:204:ASP:OD2	10:C:402:HOH:O	2.09	0.70
2:F:52:TYR:HB2	3:G:98:MET:CE	2.16	0.69
2:F:89:ARG:O	2:F:116:VAL:HG11	1.92	0.69
3:G:143:PRO:HD2	3:G:200:HIS:HE1	1.58	0.69
2:H:11:GLY:H	2:H:112:THR:CG2	2.05	0.69
3:E:123:SER:O	3:E:127:LEU:HD12	1.93	0.68
2:F:9:SER:CA	2:F:112:THR:HG21	2.23	0.68
3:E:121:PRO:HB3	3:E:211:PHE:CZ	2.27	0.68
2:D:176:GLN:HG2	2:D:180:LEU:O	1.95	0.67
2:H:11:GLY:N	2:H:112:THR:HG21	2.05	0.67
3:G:120:PHE:HB2	3:G:135:VAL:CG1	2.24	0.67
2:F:69:ARG:CD	2:F:87:SER:HB2	2.24	0.67
1:B:199:ALA:HA	4:B:301:EDO:H12	1.77	0.67
3:E:55:ARG:HG3	10:E:417:HOH:O	1.95	0.67
2:F:69:ARG:HG2	2:F:87:SER:HB2	1.77	0.67
3:G:41:PRO:HA	9:G:301:P6G:H22	1.77	0.66
2:F:40:ARG:HD3	2:F:96:TYR:CE2	2.31	0.66
2:F:200:ILE:HD13	2:F:202:ASN:OD1	1.94	0.66
1:C:229:LEU:HD12	1:C:237:ILE:HG22	1.78	0.66
2:F:3:GLU:O	2:F:4:VAL:HB	1.94	0.66
2:F:141:ALA:HB2	2:F:191:SER:HB3	1.77	0.66
1:A:218:GLY:HA3	10:A:401:HOH:O	1.95	0.66
1:C:144:ALA:HB3	1:C:147:GLN:HG3	1.77	0.66
3:L:97:PRO:HD2	8:L:302:MPD:H4	1.78	0.66
3:G:165:VAL:HG12	3:G:166:THR:O	1.96	0.66
1:A:191:GLU:HB2	1:A:245:ILE:CD1	2.26	0.66
3:E:185:LYS:NZ	3:E:189:GLU:OE1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:127:LEU:O	3:E:185:LYS:HD2	1.96	0.65
2:H:67:LYS:HD2	2:D:56:SER:HB2	1.77	0.65
2:D:91:GLU:CD	2:D:91:GLU:H	2.04	0.65
2:F:153:GLU:O	2:F:155:VAL:N	2.30	0.65
3:G:172:ASP:OD1	3:G:174:THR:HG23	1.96	0.65
3:E:122:PRO:CB	3:E:127:LEU:HD11	2.27	0.65
3:L:109:LYS:HA	3:L:142:TYR:OH	1.96	0.65
1:C:90:GLY:N	10:C:403:HOH:O	2.20	0.64
1:C:156:HIS:HE1	1:C:259:LEU:HD11	1.60	0.64
3:L:48:LEU:HD11	3:L:87:TYR:HE2	1.62	0.64
2:F:148:LYS:HD3	2:F:149:ASP:OD2	1.96	0.64
1:A:136:SER:HB3	1:A:251:GLU:OE2	1.96	0.64
1:C:101:GLN:NE2	1:C:162:SER:O	2.31	0.63
3:L:80:GLU:OE1	2:F:21:ARG:NH2	2.31	0.63
2:F:116:VAL:O	2:F:116:VAL:HG13	1.98	0.63
2:F:160:ASN:H	2:F:200:ILE:HD12	1.64	0.63
3:G:48:LEU:O	3:G:49:ILE:HD13	1.98	0.63
1:B:172:THR:HG21	5:B:302:IMD:H4	1.81	0.63
3:E:152:VAL:HG12	3:E:194:TYR:CD2	2.34	0.62
1:C:86:ILE:CG2	1:C:92:LEU:HD22	2.29	0.62
3:E:172:ASP:OD1	3:E:174:THR:HG23	1.99	0.62
2:F:11:GLY:HA2	2:F:114:VAL:HG12	1.81	0.62
2:F:69:ARG:HD2	2:F:87:SER:HB2	1.82	0.62
1:B:84:ARG:NH1	1:B:96:GLU:OE2	2.33	0.61
3:L:153:ASP:HA	3:L:193:VAL:HG23	1.82	0.61
2:H:133:SER:HA	2:H:136:THR:CG2	2.31	0.61
2:H:22:LEU:HG	2:H:85:MET:HE2	1.82	0.61
3:E:124:ASP:O	3:E:128:LYS:HG2	2.00	0.61
3:G:148:VAL:HG11	3:G:179:SER:HB2	1.81	0.61
2:F:124:PRO:HA	2:F:150:TYR:HB3	1.83	0.60
1:C:191:GLU:OE1	1:C:191:GLU:N	2.32	0.60
3:L:84:PHE:CD1	3:L:108:ILE:HG13	2.36	0.60
2:F:93:THR:HG22	2:F:116:VAL:H	1.65	0.60
2:H:21:ARG:HG3	2:H:21:ARG:HH11	1.67	0.60
2:H:133:SER:CA	2:H:136:THR:HG22	2.32	0.60
3:L:114:ALA:HB1	3:L:203:LEU:CD2	2.32	0.60
2:F:90:ALA:HA	2:F:116:VAL:HG13	1.84	0.60
1:B:233:ARG:HD3	3:L:1:GLU:OE2	2.02	0.60
2:F:128:PRO:HB3	2:F:216:VAL:HA	1.82	0.60
2:F:129:LEU:HB3	3:G:120:PHE:CD2	2.36	0.60
3:L:84:PHE:CG	3:L:108:ILE:HG13	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:208:SER:OG	2:F:210:THR:OG1	2.20	0.59
1:B:95:LEU:HD22	1:B:120:ASN:HB2	1.84	0.59
3:G:6:GLN:O	3:G:102:GLN:NE2	2.35	0.59
1:C:210:VAL:HG23	1:C:227:LEU:O	2.02	0.59
3:G:150:TRP:CE3	3:G:181:LEU:HD12	2.37	0.59
2:F:164:LEU:O	2:F:168:VAL:HG21	2.02	0.59
1:C:149:PRO:HG2	1:C:175:PHE:CE2	2.38	0.59
2:F:178:SER:OG	2:F:180:LEU:HD12	2.02	0.58
3:L:48:LEU:HD11	3:L:87:TYR:CE2	2.38	0.58
2:F:4:VAL:HG22	2:F:29:PHE:CD1	2.38	0.58
1:C:86:ILE:HG21	1:C:92:LEU:HD13	1.84	0.58
1:A:144:ALA:HB3	1:A:147:GLN:HG3	1.84	0.58
3:G:39:GLN:HA	10:G:416:HOH:O	2.02	0.58
3:G:19:ALA:HB2	3:G:79:LEU:HD11	1.83	0.58
1:B:191:GLU:HB2	1:B:245:ILE:CD1	2.34	0.58
3:G:147:LYS:HB3	3:G:199:THR:HB	1.86	0.57
3:G:212:ASN:O	3:G:213:ARG:HB2	2.04	0.57
2:D:61:TYR:OH	3:E:95:SER:HA	2.04	0.57
3:E:39:GLN:O	3:E:85:ALA:HB1	2.04	0.57
2:D:12:ASN:OD1	2:D:13:LEU:N	2.33	0.57
2:F:69:ARG:CG	2:F:87:SER:HB2	2.35	0.57
3:L:212:ASN:O	3:L:213:ARG:HB2	2.03	0.57
1:B:136:SER:OG	1:B:251:GLU:OE2	2.23	0.57
1:B:199:ALA:HB1	4:B:301:EDO:H11	1.87	0.56
3:E:139:ASN:ND2	3:E:140:ASN:OD1	2.38	0.56
2:F:203:VAL:HB	2:F:212:VAL:HG23	1.87	0.56
3:G:86:VAL:HG21	9:G:301:P6G:H61	1.87	0.56
3:G:127:LEU:HD21	3:G:132:ALA:CB	2.28	0.56
2:F:171:PHE:CZ	3:G:178:SER:HB3	2.40	0.56
3:E:24:ARG:HA	3:E:70:THR:O	2.04	0.56
2:F:14:VAL:HG11	2:F:20:LEU:HD13	1.87	0.56
2:F:85:MET:HB3	2:F:88:LEU:HD21	1.86	0.56
3:G:148:VAL:HG11	3:G:179:SER:CB	2.36	0.56
2:F:41:GLN:HG3	2:F:46:GLY:O	2.06	0.56
1:B:157:GLY:HA3	1:B:255:ALA:O	2.06	0.55
2:H:11:GLY:HA3	2:H:112:THR:CG2	2.33	0.55
3:G:184:SER:HB2	3:G:187:ASP:HB2	1.87	0.55
1:C:115:ILE:HG13	1:C:133:PHE:CZ	2.41	0.55
2:F:152:PRO:HD2	2:F:207:PRO:CB	2.35	0.55
1:C:117:LYS:HD2	1:C:131:ARG:HG3	1.87	0.55
3:E:21:LEU:HD12	3:E:21:LEU:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:138:LEU:N	3:G:138:LEU:HD12	2.22	0.55
1:A:131:ARG:HA	1:A:131:ARG:NE	2.20	0.55
2:D:11:GLY:O	2:D:12:ASN:HB2	2.07	0.55
2:F:143:LEU:HD12	2:F:189:VAL:CG2	2.37	0.55
1:A:100:PHE:CB	1:A:113:LEU:HD13	2.23	0.55
1:B:199:ALA:HA	4:B:301:EDO:C1	2.36	0.55
2:H:75:ASP:OD2	2:H:78:LYS:CE	2.50	0.55
3:E:153:ASP:OD2	3:E:191:HIS:HB3	2.07	0.55
3:L:114:ALA:HB1	3:L:203:LEU:HD21	1.90	0.54
4:F:301:EDO:HO2	3:G:178:SER:HG	1.52	0.54
3:G:122:PRO:HD3	3:G:134:VAL:HG22	1.88	0.54
2:F:129:LEU:CD2	3:G:135:VAL:HG11	2.38	0.54
3:G:143:PRO:HD2	3:G:200:HIS:CE1	2.41	0.54
1:A:156:HIS:HE1	1:A:259:LEU:HD11	1.71	0.54
1:B:100:PHE:CE2	1:B:113:LEU:HD11	2.41	0.54
3:L:96:LEU:HD22	8:L:302:MPD:H4	1.89	0.54
3:G:127:LEU:CD2	3:G:132:ALA:HB2	2.30	0.54
2:F:9:SER:HA	2:F:112:THR:CG2	2.37	0.54
3:G:92:TYR:HA	3:G:98:MET:HG3	1.89	0.54
1:A:92:LEU:O	1:A:93:ILE:HD13	2.07	0.54
2:F:186:VAL:HG11	3:G:137:LEU:CD1	2.38	0.54
8:L:302:MPD:O4	8:L:302:MPD:C1	2.47	0.53
2:D:150:TYR:CE1	2:D:155:VAL:HG13	2.43	0.53
2:F:129:LEU:HD22	3:G:135:VAL:HG11	1.90	0.53
2:F:157:VAL:HA	2:F:202:ASN:O	2.08	0.53
1:A:134:LEU:HD13	1:A:251:GLU:HB2	1.90	0.53
2:H:173:ALA:HA	2:H:183:LEU:HB3	1.89	0.53
3:E:134:VAL:HG12	3:E:150:TRP:CH2	2.43	0.53
3:G:2:ILE:CD1	3:G:27:GLN:HB2	2.39	0.53
1:A:172:THR:HG22	4:A:301:EDO:H11	1.90	0.53
2:F:150:TYR:CZ	2:F:181:TYR:HB2	2.43	0.53
1:B:102:ILE:HD13	1:B:111:VAL:HB	1.89	0.53
1:C:85:GLN:HB3	1:C:96:GLU:HG3	1.91	0.53
2:D:48:GLU:HG2	4:D:302:EDO:H12	1.90	0.53
3:E:193:VAL:HG13	3:E:211:PHE:O	2.09	0.53
2:F:186:VAL:HG21	3:G:137:LEU:HD11	1.91	0.53
2:D:149:ASP:OD1	2:D:176:GLN:NE2	2.42	0.53
3:L:2:ILE:CB	8:L:302:MPD:H13	2.37	0.52
3:L:153:ASP:O	3:L:154:ASN:HB2	2.08	0.52
2:H:183:LEU:C	2:H:183:LEU:HD12	2.35	0.52
2:D:191:SER:HA	2:D:194:LEU:HG	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:171:PHE:CE2	3:G:178:SER:HB3	2.45	0.52
3:G:163:GLU:HA	3:G:178:SER:O	2.08	0.52
2:F:66:VAL:HB	2:F:70:PHE:HB2	1.91	0.52
3:E:207:VAL:HG12	3:E:208:THR:N	2.24	0.52
3:L:73:THR:OG1	10:L:401:HOH:O	2.18	0.52
2:H:53:ILE:HG22	2:H:72:ILE:CD1	2.38	0.52
3:E:122:PRO:HB2	3:E:127:LEU:CD1	2.34	0.52
2:H:64:ASP:HA	2:H:67:LYS:CD	2.38	0.52
2:D:62:TYR:OH	2:D:71:THR:HA	2.10	0.51
3:E:203:LEU:HD13	3:E:207:VAL:CG2	2.33	0.51
2:F:70:PHE:CE1	2:F:85:MET:HG2	2.45	0.51
1:B:149:PRO:HG2	1:B:175:PHE:CE2	2.45	0.51
2:H:75:ASP:HB3	2:H:78:LYS:HE3	1.91	0.51
3:L:80:GLU:HB3	3:L:81:PRO:HD2	1.91	0.51
3:E:84:PHE:CD2	3:E:108:ILE:HG13	2.44	0.51
1:C:191:GLU:HB2	1:C:245:ILE:CD1	2.40	0.51
2:F:49:TRP:CE2	3:G:98:MET:HE2	2.45	0.51
3:L:152:VAL:HG13	3:L:194:TYR:CE2	2.46	0.51
1:B:103:TYR:HD2	1:B:255:ALA:HB3	1.75	0.51
3:L:42:GLY:H	7:L:301:P33:H212	1.76	0.51
3:G:198:VAL:O	3:G:206:PRO:HA	2.10	0.51
3:L:153:ASP:HA	3:L:193:VAL:CG2	2.40	0.51
2:H:173:ALA:HB2	2:H:183:LEU:HD23	1.93	0.51
3:L:110:ARG:NH1	3:L:111:THR:O	2.44	0.51
2:F:200:ILE:HD12	2:F:200:ILE:C	2.35	0.51
2:H:20:LEU:HD12	2:H:21:ARG:H	1.76	0.51
3:E:106:VAL:O	10:E:401:HOH:O	2.20	0.51
1:C:144:ALA:HB3	1:C:147:GLN:CG	2.41	0.51
3:L:187:ASP:HA	3:L:190:LYS:HD2	1.91	0.51
3:E:140:ASN:HA	3:E:174:THR:OG1	2.11	0.51
1:A:106:ASP:HB2	1:A:236:GLU:OE2	2.10	0.50
3:G:144:ARG:O	3:G:144:ARG:HG2	2.10	0.50
2:D:197:GLN:HA	2:D:197:GLN:OE1	2.11	0.50
3:E:149:GLN:OE1	3:E:197:GLU:HG2	2.11	0.50
3:E:152:VAL:CG1	3:E:194:TYR:CD2	2.93	0.50
2:F:49:TRP:NE1	3:G:98:MET:HE2	2.26	0.50
1:B:80:PHE:HB2	1:B:100:PHE:HB3	1.94	0.50
2:H:153:GLU:OE2	2:H:173:ALA:HB3	2.12	0.50
4:D:302:EDO:H11	10:D:401:HOH:O	2.12	0.50
3:E:38:GLN:HB2	3:E:48:LEU:HD11	1.94	0.50
3:E:188:TYR:O	3:E:194:TYR:OH	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:HIS:ND1	1:C:259:LEU:HD21	2.26	0.50
3:L:144:ARG:O	3:L:144:ARG:HG2	2.12	0.49
2:F:35:SER:HB2	2:F:101:VAL:HB	1.94	0.49
3:L:144:ARG:HB2	3:L:175:TYR:CE2	2.46	0.49
2:F:16:PRO:HA	2:F:88:LEU:O	2.13	0.49
1:A:110:VAL:CG2	1:A:238:ALA:HB1	2.43	0.49
1:B:75:ASP:O	1:B:158:LYS:NZ	2.41	0.49
1:C:210:VAL:HG21	1:C:226:HIS:NE2	2.27	0.49
3:L:203:LEU:HD13	3:L:207:VAL:CG2	2.30	0.49
1:B:81:ASP:OD1	1:B:99:GLU:HG3	2.12	0.49
3:E:24:ARG:HB2	3:E:24:ARG:NH1	2.28	0.49
1:C:80:PHE:CD2	1:C:82:PHE:CE1	3.00	0.49
1:C:163:ASP:N	1:C:163:ASP:OD1	2.44	0.49
2:H:11:GLY:N	2:H:112:THR:CG2	2.72	0.49
3:L:127:LEU:O	3:L:185:LYS:HD2	2.13	0.49
2:D:193:SER:O	2:D:196:THR:HG22	2.13	0.49
3:E:183:LEU:HD21	3:E:188:TYR:HA	1.95	0.49
2:D:89:ARG:CB	2:D:91:GLU:OE2	2.61	0.49
1:A:192:GLN:HB3	1:A:252:ILE:HD11	1.94	0.49
2:H:75:ASP:CB	2:H:78:LYS:HE3	2.42	0.49
3:E:177:LEU:HD23	3:E:178:SER:N	2.28	0.49
2:F:20:LEU:O	2:F:85:MET:HB2	2.13	0.49
3:G:149:GLN:OE1	3:G:149:GLN:HA	2.13	0.49
3:L:38:GLN:OE1	3:L:46:ARG:NH1	2.44	0.49
3:G:152:VAL:HG22	3:G:194:TYR:CD1	2.47	0.49
1:C:201:LEU:HD13	1:C:211:ILE:HD11	1.95	0.48
2:D:161:SER:HA	2:D:202:ASN:OD1	2.13	0.48
3:E:131:THR:HG22	3:E:132:ALA:N	2.28	0.48
2:H:21:ARG:HG3	2:H:21:ARG:NH1	2.27	0.48
3:E:163:GLU:HA	3:E:178:SER:O	2.13	0.48
2:F:52:TYR:CG	3:G:98:MET:HE1	2.47	0.48
3:E:24:ARG:HB2	3:E:24:ARG:HH11	1.78	0.48
2:F:4:VAL:HG11	2:F:107:ASP:OD2	2.14	0.48
2:F:127:PHE:HD2	2:F:146:LEU:HD23	1.79	0.48
3:E:84:PHE:CG	3:E:108:ILE:HG13	2.49	0.48
2:H:175:LEU:HD12	2:H:176:GLN:N	2.29	0.48
1:C:210:VAL:HG22	1:C:211:ILE:N	2.29	0.48
2:F:20:LEU:HB3	2:F:85:MET:HE3	1.96	0.48
3:G:150:TRP:CG	3:G:181:LEU:HD12	2.48	0.48
1:A:75:ASP:HB3	1:A:103:TYR:HE1	1.78	0.47
2:H:56:SER:O	2:H:57:SER:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:161:SER:HA	2:F:202:ASN:ND2	2.29	0.47
2:H:29:PHE:CE2	2:H:31:PHE:HA	2.49	0.47
3:L:34:LEU:HD22	3:L:72:PHE:CG	2.50	0.47
2:D:183:LEU:HD12	2:D:183:LEU:C	2.40	0.47
2:F:4:VAL:HG22	2:F:29:PHE:HD1	1.78	0.47
2:F:175:LEU:HD13	2:F:175:LEU:C	2.39	0.47
2:H:36:MET:HE3	2:H:36:MET:HB3	1.69	0.47
2:D:3:GLU:HA	2:D:3:GLU:OE1	2.15	0.47
3:E:21:LEU:O	3:E:73:THR:HA	2.15	0.47
2:F:143:LEU:HD12	2:F:189:VAL:HG21	1.95	0.47
2:F:159:TRP:HA	2:F:200:ILE:O	2.15	0.47
3:G:36:TRP:CE2	3:G:74:LEU:HB2	2.50	0.47
3:E:163:GLU:HB2	3:E:177:LEU:HD21	1.95	0.47
1:B:82:PHE:CZ	1:B:98:GLY:HA3	2.50	0.47
3:L:207:VAL:HG12	3:L:208:THR:N	2.29	0.47
3:E:8:PRO:HG3	3:E:11:LEU:HD13	1.95	0.47
3:L:91:HIS:O	3:L:98:MET:HB3	2.14	0.47
3:E:194:TYR:HB2	3:E:211:PHE:CE1	2.50	0.47
2:F:19:SER:OG	2:F:86:ASN:OD1	2.24	0.47
2:F:69:ARG:HD2	2:F:87:SER:O	2.15	0.47
2:F:160:ASN:HA	2:F:200:ILE:HD11	1.96	0.47
3:G:122:PRO:HB2	3:G:127:LEU:HG	1.97	0.47
1:C:191:GLU:HB2	1:C:245:ILE:HD13	1.96	0.47
2:F:122:LYS:NZ	2:F:123:GLY:O	2.47	0.47
3:G:33:TYR:CD1	3:G:93:ASP:HA	2.50	0.47
1:B:103:TYR:CD2	1:B:255:ALA:HB3	2.50	0.47
3:L:34:LEU:HD22	3:L:72:PHE:CB	2.45	0.47
3:E:183:LEU:HD21	3:E:188:TYR:CA	2.45	0.46
2:F:55:SER:HA	2:F:74:ARG:NH1	2.30	0.46
1:B:142:HIS:HD2	10:B:402:HOH:O	1.97	0.46
1:B:215:THR:O	1:B:216:ARG:HG3	2.15	0.46
2:F:96:TYR:CE1	2:F:114:VAL:CG2	2.98	0.46
3:G:161:SER:HA	3:G:180:THR:O	2.15	0.46
1:B:155:TYR:CE2	1:B:237:ILE:HG23	2.49	0.46
3:L:19:ALA:HB2	3:L:79:LEU:HD11	1.97	0.46
3:G:144:ARG:HB2	3:G:175:TYR:CE2	2.50	0.46
1:A:118:ILE:HG22	1:A:118:ILE:O	2.15	0.46
1:C:117:LYS:CD	1:C:131:ARG:HG3	2.45	0.46
2:F:69:ARG:HG2	2:F:87:SER:CB	2.44	0.46
3:G:138:LEU:N	3:G:138:LEU:CD1	2.79	0.46
3:E:14:SER:HB3	3:E:109:LYS:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:110:ARG:HD2	3:L:173:SER:HB2	1.98	0.46
3:L:117:VAL:HG12	3:L:209:LYS:HG3	1.98	0.46
3:E:201:GLN:O	3:E:201:GLN:HG2	2.15	0.46
3:G:39:GLN:O	3:G:85:ALA:HB1	2.15	0.46
3:G:86:VAL:HG21	9:G:301:P6G:C6	2.45	0.46
3:L:114:ALA:HB1	3:L:203:LEU:HD23	1.96	0.46
2:F:70:PHE:CE2	2:F:85:MET:HG2	2.51	0.46
2:F:93:THR:HG22	2:F:116:VAL:N	2.31	0.46
3:G:2:ILE:HD11	3:G:27:GLN:HB2	1.97	0.46
3:G:38:GLN:HB2	3:G:48:LEU:HD11	1.97	0.45
3:G:55:ARG:HD2	3:G:59:ILE:O	2.17	0.45
3:G:196:CYS:O	3:G:208:THR:HA	2.16	0.45
1:A:75:ASP:HB3	1:A:103:TYR:CE1	2.50	0.45
1:A:156:HIS:ND1	1:A:259:LEU:HG	2.31	0.45
2:F:89:ARG:O	2:F:116:VAL:CG1	2.63	0.45
3:E:144:ARG:HB2	3:E:175:TYR:CE2	2.51	0.45
2:F:150:TYR:CE1	2:F:181:TYR:HB2	2.52	0.45
1:A:132:SER:C	1:A:133:PHE:CD1	2.94	0.45
3:L:97:PRO:HB2	8:L:302:MPD:H31	1.99	0.45
2:F:176:GLN:HG3	2:F:180:LEU:O	2.17	0.45
3:G:130:GLY:HA2	3:G:185:LYS:HB3	1.97	0.45
1:A:156:HIS:CE1	1:A:259:LEU:HD21	2.51	0.45
1:B:199:ALA:CB	4:B:301:EDO:H11	2.46	0.45
3:L:96:LEU:HD22	8:L:302:MPD:C4	2.46	0.45
1:A:101:GLN:NE2	1:A:162:SER:O	2.50	0.45
3:G:15:PRO:HD3	3:G:108:ILE:HG23	1.98	0.45
2:H:14:VAL:CG2	2:H:116:VAL:HG22	2.47	0.45
1:A:95:LEU:N	1:A:95:LEU:CD1	2.79	0.45
1:C:216:ARG:NH1	10:C:405:HOH:O	2.47	0.45
2:H:70:PHE:CE1	2:H:85:MET:HB3	2.52	0.45
3:E:34:LEU:HD22	3:E:90:GLN:O	2.16	0.45
1:A:154:GLU:O	1:A:258:GLN:HA	2.17	0.45
2:H:53:ILE:HG22	2:H:72:ILE:HD11	1.99	0.45
2:D:89:ARG:HB2	2:D:91:GLU:OE2	2.18	0.44
3:G:36:TRP:CD2	3:G:74:LEU:HB2	2.52	0.44
2:H:14:VAL:HG23	2:H:116:VAL:HG22	2.00	0.44
2:H:53:ILE:HG22	2:H:72:ILE:HD13	1.99	0.44
3:L:142:TYR:CG	3:L:143:PRO:HA	2.52	0.44
3:E:12:SER:O	3:E:13:LEU:HD23	2.18	0.44
3:G:152:VAL:HG22	3:G:194:TYR:CE1	2.52	0.44
1:A:143:THR:OG1	1:A:231:GLY:O	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:11:GLY:CA	2:H:112:THR:CG2	2.94	0.44
3:E:151:LYS:HE2	3:E:151:LYS:HB3	1.67	0.44
3:E:201:GLN:O	3:E:201:GLN:CG	2.66	0.44
3:L:84:PHE:HA	3:L:106:VAL:HG23	1.99	0.44
3:E:188:TYR:CD2	3:E:194:TYR:CZ	3.05	0.44
3:G:127:LEU:HD23	3:G:127:LEU:HA	1.71	0.44
2:H:11:GLY:O	2:H:12:ASN:HB2	2.17	0.44
2:F:128:PRO:HB3	2:F:216:VAL:CA	2.47	0.44
1:A:78:SER:HB3	1:A:80:PHE:HE1	1.82	0.44
3:L:34:LEU:HG	3:L:35:ALA:N	2.29	0.44
3:E:122:PRO:CG	3:E:127:LEU:HD11	2.47	0.44
2:F:53:ILE:O	2:F:53:ILE:HG23	2.17	0.44
1:A:131:ARG:HA	1:A:131:ARG:HE	1.83	0.44
2:F:56:SER:OG	2:F:58:SER:OG	2.36	0.44
3:G:181:LEU:HD21	3:G:183:LEU:HD21	1.99	0.44
1:B:231:GLY:HA3	1:B:235:GLN:OE1	2.18	0.44
2:F:66:VAL:HG11	2:F:70:PHE:CD2	2.53	0.44
2:F:105:LEU:HD13	3:G:90:GLN:HE22	1.82	0.44
1:A:191:GLU:HB2	1:A:245:ILE:HD11	2.00	0.43
3:L:110:ARG:NH1	3:L:110:ARG:HG3	2.33	0.43
1:A:220:GLU:OE1	1:A:222:LYS:NZ	2.50	0.43
1:C:212:LEU:HD21	1:C:226:HIS:CD2	2.53	0.43
3:G:163:GLU:HB2	3:G:177:LEU:HD21	2.00	0.43
3:L:151:LYS:HA	3:L:155:ALA:O	2.18	0.43
2:D:122:LYS:HD3	2:D:149:ASP:O	2.18	0.43
3:L:96:LEU:O	3:L:97:PRO:C	2.62	0.43
2:D:173:ALA:HA	2:D:183:LEU:HB3	2.00	0.43
2:F:14:VAL:CG1	2:F:20:LEU:HD13	2.48	0.43
1:C:80:PHE:HD2	1:C:82:PHE:CE1	2.37	0.43
2:H:105:LEU:HD12	2:H:105:LEU:N	2.33	0.43
2:D:189:VAL:HG11	2:D:199:TYR:CE1	2.53	0.43
1:B:114:GLN:OE1	1:B:162:SER:HB2	2.19	0.43
3:E:157:GLN:HE21	3:E:157:GLN:HB2	1.69	0.43
2:F:143:LEU:CD1	2:F:189:VAL:HG21	2.48	0.43
1:B:133:PHE:C	1:B:134:LEU:HD22	2.44	0.43
2:F:4:VAL:HA	2:F:28:GLY:HA3	1.99	0.43
2:F:160:ASN:N	2:F:200:ILE:HD12	2.32	0.43
3:G:129:SER:O	3:G:185:LYS:HB2	2.19	0.43
1:B:200:GLU:H	4:B:301:EDO:C1	2.31	0.43
2:H:11:GLY:CA	2:H:112:THR:HG22	2.36	0.43
3:L:110:ARG:HG3	3:L:110:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:150:TYR:CZ	2:F:155:VAL:HG11	2.53	0.43
2:F:14:VAL:HG21	2:F:88:LEU:HD12	2.00	0.43
2:F:4:VAL:HA	2:F:27:SER:O	2.18	0.43
2:F:40:ARG:HD3	2:F:96:TYR:CZ	2.54	0.43
3:G:126:GLN:OE1	3:G:133:SER:HB2	2.19	0.43
3:G:208:THR:O	3:G:209:LYS:HG2	2.19	0.43
2:H:41:GLN:C	2:H:94:ALA:HB1	2.43	0.42
2:D:206:LYS:N	2:D:207:PRO:CD	2.81	0.42
1:A:99:GLU:O	1:A:113:LEU:HD12	2.19	0.42
1:B:100:PHE:CE2	1:B:113:LEU:CD1	3.02	0.42
2:H:217:GLU:HB2	2:H:218:PRO:CD	2.49	0.42
2:F:169:HIS:HB2	2:F:186:VAL:HG23	2.01	0.42
1:C:82:PHE:CZ	1:C:99:GLU:OE1	2.72	0.42
3:G:107:GLU:HG3	3:G:175:TYR:OH	2.19	0.42
5:B:302:IMD:N1	3:E:30:SER:OG	2.48	0.42
2:H:14:VAL:O	2:H:116:VAL:HA	2.19	0.42
2:F:40:ARG:HB3	2:F:96:TYR:CD2	2.54	0.42
2:F:216:VAL:O	2:F:216:VAL:HG22	2.19	0.42
1:A:99:GLU:OE2	1:A:162:SER:HB3	2.18	0.42
1:A:100:PHE:HB2	1:A:112:ALA:O	2.20	0.42
2:H:133:SER:C	2:H:136:THR:HG22	2.44	0.42
3:G:84:PHE:CG	3:G:108:ILE:HG12	2.55	0.42
3:L:33:TYR:CD1	3:L:93:ASP:HA	2.55	0.42
3:L:144:ARG:CZ	3:L:165:VAL:HG21	2.49	0.42
1:A:110:VAL:HG12	1:A:111:VAL:N	2.33	0.42
3:L:168:GLN:HG2	3:L:173:SER:HA	2.01	0.42
3:E:185:LYS:HZ3	3:E:189:GLU:CD	2.27	0.42
3:L:56:ALA:HB3	3:L:59:ILE:HG13	2.02	0.42
2:F:42:ALA:O	2:F:43:PRO:C	2.62	0.42
2:F:160:ASN:H	2:F:200:ILE:CD1	2.31	0.42
3:G:151:LYS:HG2	3:G:156:LEU:CD1	2.41	0.42
3:G:177:LEU:HD23	3:G:178:SER:CA	2.50	0.42
3:G:181:LEU:CD2	3:G:183:LEU:HD21	2.50	0.42
2:F:199:TYR:O	2:F:215:ARG:O	2.38	0.42
3:G:2:ILE:HD13	3:G:27:GLN:HB2	2.01	0.42
3:L:148:VAL:HG22	3:L:198:VAL:HG22	2.01	0.42
2:D:153:GLU:HG3	2:D:154:PRO:N	2.34	0.42
2:F:156:THR:O	2:F:203:VAL:HA	2.19	0.42
2:F:160:ASN:CA	2:F:200:ILE:HD11	2.49	0.42
3:G:38:GLN:HB2	3:G:87:TYR:CE2	2.55	0.42
3:L:153:ASP:OD1	3:L:193:VAL:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:LEU:HB3	2:D:85:MET:HE3	2.02	0.41
2:D:29:PHE:CE2	2:D:31:PHE:HA	2.54	0.41
1:A:108:SER:HB3	1:A:230:PHE:CG	2.55	0.41
1:B:142:HIS:CD2	10:B:402:HOH:O	2.72	0.41
2:D:105:LEU:HB2	3:E:37:TYR:OH	2.20	0.41
2:F:173:ALA:HB1	2:F:181:TYR:HB3	2.03	0.41
1:C:243:VAL:O	1:C:243:VAL:HG13	2.21	0.41
2:F:203:VAL:HB	2:F:212:VAL:CG2	2.50	0.41
1:B:133:PHE:O	1:B:134:LEU:HD22	2.20	0.41
2:H:53:ILE:CG2	2:H:72:ILE:HD13	2.50	0.41
3:E:194:TYR:O	3:E:210:SER:HA	2.21	0.41
2:F:37:ASN:OD1	3:G:98:MET:HE3	2.20	0.41
1:B:108:SER:HA	1:B:139:GLY:O	2.21	0.41
3:L:42:GLY:N	7:L:301:P33:H212	2.35	0.41
1:A:146:ASN:C	1:A:147:GLN:HG2	2.45	0.41
1:C:80:PHE:HA	1:C:100:PHE:O	2.20	0.41
1:C:149:PRO:HG2	1:C:175:PHE:CD2	2.56	0.41
3:L:138:LEU:HD12	3:L:138:LEU:N	2.36	0.41
3:E:112:VAL:HG22	3:E:143:PRO:HD3	2.03	0.41
2:F:169:HIS:HB2	2:F:186:VAL:CG2	2.51	0.41
3:G:107:GLU:HG2	3:G:168:GLN:OE1	2.21	0.41
3:G:177:LEU:HD23	3:G:177:LEU:C	2.45	0.41
2:H:4:VAL:HA	2:H:28:GLY:HA3	2.03	0.41
3:E:207:VAL:CG1	3:E:208:THR:N	2.84	0.41
2:F:147:VAL:HB	2:F:183:LEU:CD2	2.45	0.41
1:C:79:ARG:HA	1:C:79:ARG:HD3	1.94	0.40
1:A:84:ARG:HE	1:A:96:GLU:CD	2.30	0.40
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.92	0.40
1:B:226:HIS:O	1:B:239:GLY:HA3	2.21	0.40
1:C:80:PHE:HB2	1:C:101:GLN:HG2	2.03	0.40
3:L:188:TYR:HA	3:L:194:TYR:OH	2.21	0.40
3:E:193:VAL:HA	3:E:211:PHE:O	2.22	0.40
2:F:65:SER:O	2:F:69:ARG:NH2	2.50	0.40
2:H:15:GLN:O	2:H:16:PRO:C	2.63	0.40
3:E:62:ARG:NE	3:E:83:ASP:OD2	2.39	0.40
2:F:124:PRO:CA	2:F:150:TYR:HB3	2.48	0.40
1:B:164:ASP:OD2	1:B:188:LYS:HB2	2.20	0.40
2:H:20:LEU:HD12	2:H:21:ARG:N	2.37	0.40
3:L:35:ALA:HB2	3:L:92:TYR:CE1	2.56	0.40
3:G:10:THR:HG22	3:G:11:LEU:N	2.35	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	172/260 (66%)	164 (95%)	8 (5%)	0	100	100
1	B	173/260 (66%)	167 (96%)	5 (3%)	1 (1%)	21	30
1	C	169/260 (65%)	162 (96%)	6 (4%)	1 (1%)	21	30
2	D	209/226 (92%)	198 (95%)	10 (5%)	1 (0%)	24	35
2	F	206/226 (91%)	187 (91%)	15 (7%)	4 (2%)	6	7
2	H	212/226 (94%)	207 (98%)	5 (2%)	0	100	100
3	E	212/216 (98%)	197 (93%)	15 (7%)	0	100	100
3	G	200/216 (93%)	187 (94%)	11 (6%)	2 (1%)	12	18
3	L	212/216 (98%)	204 (96%)	7 (3%)	1 (0%)	24	35
All	All	1765/2106 (84%)	1673 (95%)	82 (5%)	10 (1%)	21	30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	154	PRO
2	F	214	LYS
3	L	213	ARG
2	F	216	VAL
3	G	201	GLN
2	F	4	VAL
1	C	188	LYS
2	D	218	PRO
1	B	218	GLY
3	G	69	GLY

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	135/207 (65%)	133 (98%)	2 (2%)	57	75
1	B	133/207 (64%)	131 (98%)	2 (2%)	57	75
1	C	129/207 (62%)	128 (99%)	1 (1%)	73	85
2	D	175/189 (93%)	172 (98%)	3 (2%)	53	73
2	F	168/189 (89%)	161 (96%)	7 (4%)	26	43
2	H	180/189 (95%)	177 (98%)	3 (2%)	53	73
3	E	180/187 (96%)	177 (98%)	3 (2%)	53	73
3	G	175/187 (94%)	170 (97%)	5 (3%)	37	57
3	L	183/187 (98%)	179 (98%)	4 (2%)	45	66
All	All	1458/1749 (83%)	1428 (98%)	30 (2%)	47	67

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LEU
1	A	115	ILE
1	B	132	SER
1	B	247	GLU
1	C	185	GLU
2	H	133	SER
2	H	177	SER
2	H	196	THR
3	L	28	SER
3	L	106	VAL
3	L	111	THR
3	L	165	VAL
2	D	56	SER
2	D	153	GLU
2	D	201	CYS
3	E	22	SER
3	E	182	THR
3	E	183	LEU
2	F	14	VAL
2	F	87	SER
2	F	118	SER
2	F	125	SER
2	F	143	LEU

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Mol	Chain	Res	Type
2	F	164	LEU
2	F	188	THR
3	G	22	SER
3	G	26	SER
3	G	135	VAL
3	G	138	LEU
3	G	182	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	B	85	GLN
1	B	250	HIS
1	C	186	HIS
1	C	250	HIS
2	H	176	GLN
3	L	43	GLN
2	D	41	GLN
3	E	39	GLN
3	E	43	GLN
2	F	169	HIS
2	F	197	GLN
3	G	38	GLN
3	G	140	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

11 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	$\# Z > 2$
4	EDO	D	302	-	3,3,3	0.55	0	2,2,2	0.36	0
6	SO4	C	301	-	4,4,4	0.24	0	6,6,6	0.43	0
4	EDO	B	301	-	3,3,3	0.48	0	2,2,2	0.28	0
7	P33	L	301	-	21,21,21	0.54	0	20,20,20	0.63	1 (5%)
8	MPD	L	302	-	7,7,7	0.88	0	9,10,10	0.97	1 (11%)
9	P6G	G	301	-	18,18,18	0.56	0	17,17,17	0.37	0
4	EDO	D	301	-	3,3,3	0.52	0	2,2,2	0.22	0
4	EDO	A	301	-	3,3,3	0.48	0	2,2,2	0.44	0
4	EDO	F	301	-	3,3,3	0.45	0	2,2,2	0.29	0
4	EDO	E	301	-	3,3,3	0.46	0	2,2,2	0.22	0
5	IMD	B	302	-	5,5,5	0.87	0	5,5,5	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	302	-	-	1/1/1/1	-
7	P33	L	301	-	-	10/19/19/19	-
4	EDO	B	301	-	-	1/1/1/1	-
8	MPD	L	302	-	-	3/5/5/5	-
9	P6G	G	301	-	-	9/16/16/16	-
4	EDO	D	301	-	-	1/1/1/1	-
4	EDO	A	301	-	-	1/1/1/1	-
4	EDO	F	301	-	-	1/1/1/1	-
4	EDO	E	301	-	-	0/1/1/1	-
5	IMD	B	302	-	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	302	MPD	CM-C2-C1	-2.48	105.08	110.63
7	L	301	P33	O10-C9-C8	-2.03	101.11	110.35

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	301	P33	O16-C17-C18-O19
9	G	301	P6G	O7-C8-C9-O10
7	L	301	P33	O1-C2-C3-O4
4	A	301	EDO	O1-C1-C2-O2
9	G	301	P6G	O10-C11-C12-O13
7	L	301	P33	O4-C5-C6-O7
4	D	302	EDO	O1-C1-C2-O2
4	D	301	EDO	O1-C1-C2-O2
7	L	301	P33	O13-C14-C15-O16
7	L	301	P33	C2-C3-O4-C5
7	L	301	P33	C9-C8-O7-C6
8	L	302	MPD	C2-C3-C4-O4
8	L	302	MPD	CM-C2-C3-C4
9	G	301	P6G	O1-C2-C3-O4
7	L	301	P33	O10-C11-C12-O13
9	G	301	P6G	C5-C6-O7-C8
4	B	301	EDO	O1-C1-C2-O2
9	G	301	P6G	O16-C17-C18-O19
9	G	301	P6G	C8-C9-O10-C11
7	L	301	P33	C5-C6-O7-C8
9	G	301	P6G	O4-C5-C6-O7
9	G	301	P6G	C9-C8-O7-C6
7	L	301	P33	O7-C8-C9-O10
7	L	301	P33	C6-C5-O4-C3
8	L	302	MPD	C1-C2-C3-C4
9	G	301	P6G	O13-C14-C15-O16
4	F	301	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 28 short contacts:

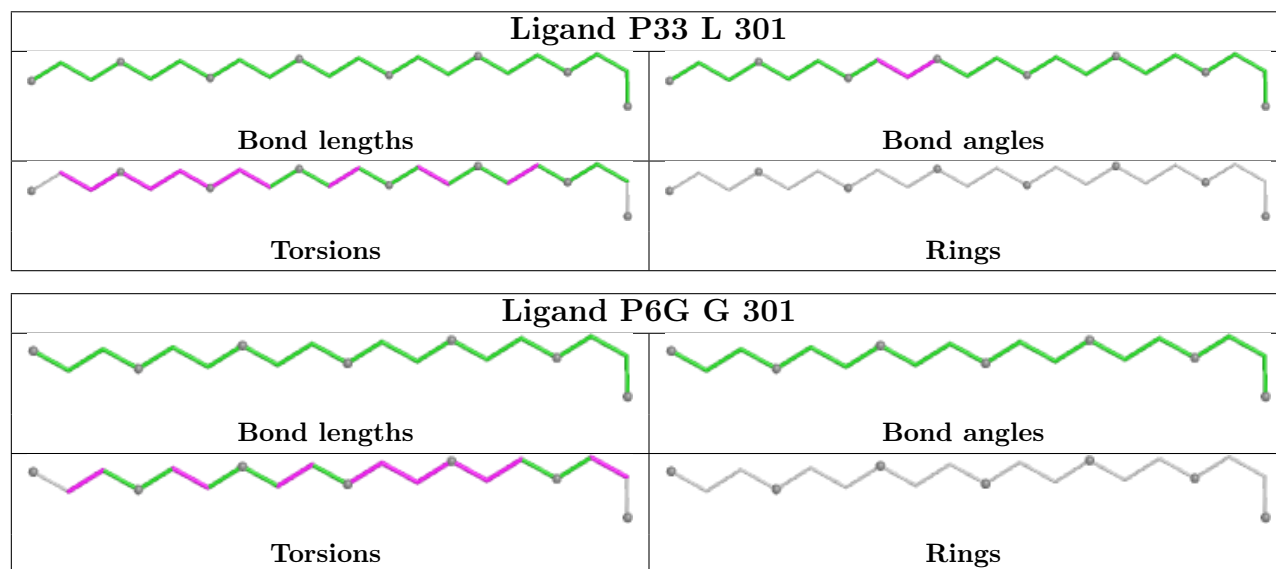
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	302	EDO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	EDO	5	0
7	L	301	P33	3	0
8	L	302	MPD	8	0
9	G	301	P6G	3	0
4	D	301	EDO	1	0
4	A	301	EDO	1	0
4	F	301	EDO	2	0
5	B	302	IMD	2	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	176/260 (67%)	0.04	0	100	100	40, 62, 86, 101	4 (2%)
1	B	176/260 (67%)	0.08	0	100	100	42, 61, 82, 95	3 (1%)
1	C	173/260 (66%)	0.29	5 (2%)	53	50	48, 67, 88, 103	5 (2%)
2	D	213/226 (94%)	0.09	3 (1%)	73	70	41, 60, 80, 96	3 (1%)
2	F	210/226 (92%)	0.75	14 (6%)	24	20	47, 78, 111, 118	5 (2%)
2	H	216/226 (95%)	-0.07	3 (1%)	73	70	39, 54, 74, 92	2 (0%)
3	E	214/216 (99%)	0.26	4 (1%)	66	63	42, 62, 98, 108	1 (0%)
3	G	206/216 (95%)	0.57	11 (5%)	32	28	50, 69, 106, 113	5 (2%)
3	L	214/216 (99%)	-0.06	0	100	100	38, 57, 79, 90	2 (0%)
All	All	1798/2106 (85%)	0.22	40 (2%)	62	59	38, 63, 100, 118	30 (1%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	80	PHE	3.4
2	F	126	VAL	3.2
3	G	127	LEU	3.1
2	F	187	VAL	3.1
3	G	118	PHE	3.0
1	C	86	ILE	2.9
3	E	193	VAL	2.8
2	F	146	LEU	2.7
3	G	198	VAL	2.7
2	F	131	PRO	2.6
1	C	87	GLU	2.6
2	F	164	LEU	2.5
2	F	212	VAL	2.5
3	G	210	SER	2.5
2	F	155	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	203	VAL	2.5
3	G	123	SER	2.4
2	D	56	SER	2.3
2	D	138	GLY	2.3
2	F	129	LEU	2.3
3	E	149	GLN	2.3
1	C	88	VAL	2.3
3	G	194	TYR	2.3
2	H	136	THR	2.3
2	F	157	VAL	2.3
2	F	143	LEU	2.2
3	G	206	PRO	2.2
2	F	210	THR	2.2
3	E	156	LEU	2.2
2	D	195	GLY	2.2
2	H	133	SER	2.2
3	G	186	ALA	2.1
3	G	197	GLU	2.1
3	G	211	PHE	2.1
3	E	137	LEU	2.1
1	C	219	SER	2.1
2	H	137	SER	2.1
2	F	204	ASN	2.1
3	G	137	LEU	2.1
2	F	147	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

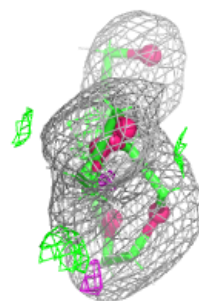
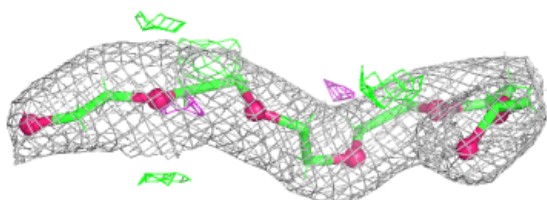
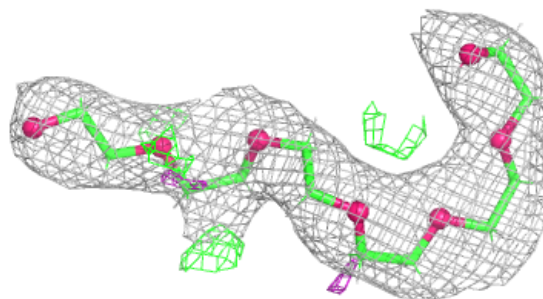
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	F	301	4/4	0.75	0.12	94,113,114,119	0
9	P6G	G	301	19/19	0.83	0.12	60,84,100,102	0
4	EDO	E	301	4/4	0.85	0.13	68,81,88,95	0
4	EDO	A	301	4/4	0.86	0.28	49,58,70,71	0
8	MPD	L	302	8/8	0.88	0.13	45,56,72,72	0
4	EDO	D	302	4/4	0.88	0.32	54,65,67,68	0
4	EDO	B	301	4/4	0.90	0.27	54,65,74,74	0
6	SO4	C	301	5/5	0.91	0.08	65,70,79,81	0
7	P33	L	301	22/22	0.91	0.10	47,63,82,85	0
5	IMD	B	302	5/5	0.92	0.10	51,60,69,72	0
4	EDO	D	301	4/4	0.95	0.21	50,60,65,66	0

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

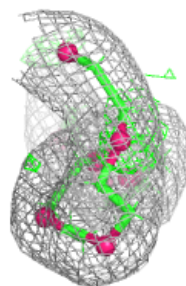
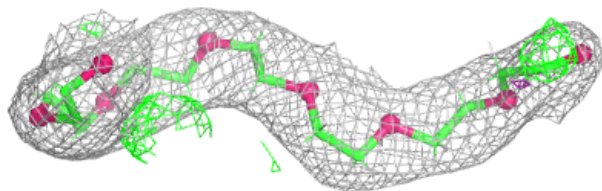
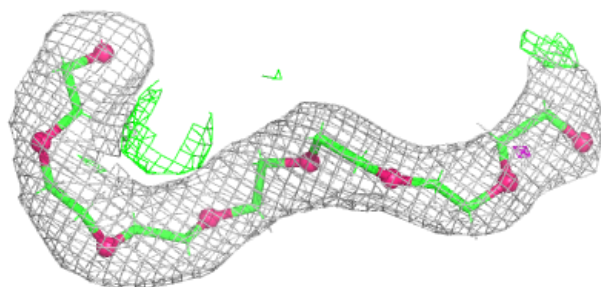
Electron density around P6G G 301:

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 P33 L 301:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.