Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:14 am BST

PDB ID	:	5H35
Title	:	Crystal structures of the TRIC trimeric intracellular cation channel orthologue from Sulfolobus solfataricus
Authors	:	Kasuya, G.; Hiraizumi, M.; Hattori, M.; Nureki, O.
Deposited on	:	2016-10-20
Resolution	:	2.64 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

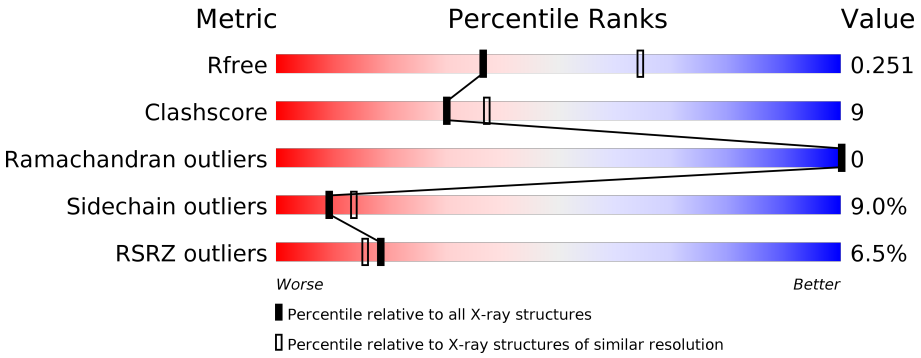
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.64 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	236	5% 71% 20% • 7%
1	F	236	3% 72% 16% 6% 7%
1	H	236	10% 71% 18% • 7%
2	B	219	11% 78% 20% ••
2	G	219	% 82% 16% ••
2	I	219	14% 74% 25% ••

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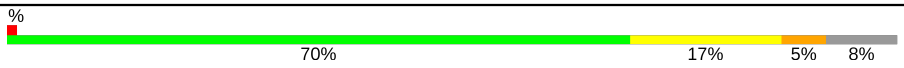
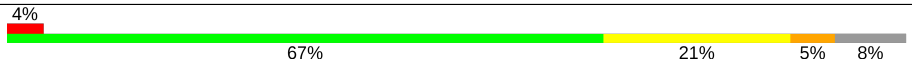
Mol	Chain	Length	Quality of chain
3	C	212	
3	D	212	
3	E	212	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14636 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 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1633	1041	262	321	9			
1	F	220	Total	C	N	O	S	0	0	0
			1653	1052	270	322	9			
1	H	220	Total	C	N	O	S	0	0	0
			1653	1052	270	322	9			

- Molecule 2 is a protein called Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1683	1056	284	337	6			
2	G	217	Total	C	N	O	S	0	0	0
			1687	1059	285	337	6			
2	I	217	Total	C	N	O	S	0	0	0
			1683	1056	284	337	6			

- Molecule 3 is a protein called Membrane protein TRIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	195	Total	C	N	O	S	0	0	0
			1483	1000	220	259	4			
3	D	195	Total	C	N	O	S	0	0	0
			1483	998	221	260	4			
3	E	195	Total	C	N	O	S	0	0	0
			1480	997	220	259	4			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	199	LEU	-	expression tag	UNP A0A0E3MGX1
C	200	GLU	-	expression tag	UNP A0A0E3MGX1

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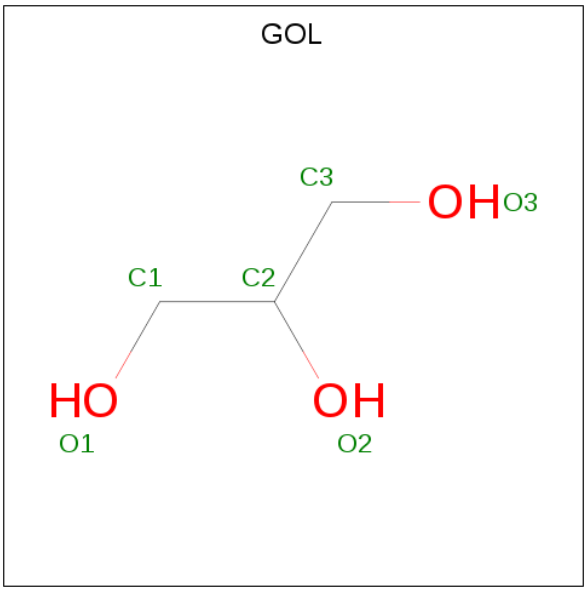
Chain	Residue	Modelled	Actual	Comment	Reference
C	201	SER	-	expression tag	UNP A0A0E3MGX1
C	202	LEU	-	expression tag	UNP A0A0E3MGX1
C	203	GLU	-	expression tag	UNP A0A0E3MGX1
C	204	SER	-	expression tag	UNP A0A0E3MGX1
C	205	SER	-	expression tag	UNP A0A0E3MGX1
C	206	GLY	-	expression tag	UNP A0A0E3MGX1
C	207	GLU	-	expression tag	UNP A0A0E3MGX1
C	208	ASN	-	expression tag	UNP A0A0E3MGX1
C	209	LEU	-	expression tag	UNP A0A0E3MGX1
C	210	TYR	-	expression tag	UNP A0A0E3MGX1
C	211	PHE	-	expression tag	UNP A0A0E3MGX1
C	212	GLN	-	expression tag	UNP A0A0E3MGX1
D	199	LEU	-	expression tag	UNP A0A0E3MGX1
D	200	GLU	-	expression tag	UNP A0A0E3MGX1
D	201	SER	-	expression tag	UNP A0A0E3MGX1
D	202	LEU	-	expression tag	UNP A0A0E3MGX1
D	203	GLU	-	expression tag	UNP A0A0E3MGX1
D	204	SER	-	expression tag	UNP A0A0E3MGX1
D	205	SER	-	expression tag	UNP A0A0E3MGX1
D	206	GLY	-	expression tag	UNP A0A0E3MGX1
D	207	GLU	-	expression tag	UNP A0A0E3MGX1
D	208	ASN	-	expression tag	UNP A0A0E3MGX1
D	209	LEU	-	expression tag	UNP A0A0E3MGX1
D	210	TYR	-	expression tag	UNP A0A0E3MGX1
D	211	PHE	-	expression tag	UNP A0A0E3MGX1
D	212	GLN	-	expression tag	UNP A0A0E3MGX1
E	199	LEU	-	expression tag	UNP A0A0E3MGX1
E	200	GLU	-	expression tag	UNP A0A0E3MGX1
E	201	SER	-	expression tag	UNP A0A0E3MGX1
E	202	LEU	-	expression tag	UNP A0A0E3MGX1
E	203	GLU	-	expression tag	UNP A0A0E3MGX1
E	204	SER	-	expression tag	UNP A0A0E3MGX1
E	205	SER	-	expression tag	UNP A0A0E3MGX1
E	206	GLY	-	expression tag	UNP A0A0E3MGX1
E	207	GLU	-	expression tag	UNP A0A0E3MGX1
E	208	ASN	-	expression tag	UNP A0A0E3MGX1
E	209	LEU	-	expression tag	UNP A0A0E3MGX1
E	210	TYR	-	expression tag	UNP A0A0E3MGX1
E	211	PHE	-	expression tag	UNP A0A0E3MGX1
E	212	GLN	-	expression tag	UNP A0A0E3MGX1

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

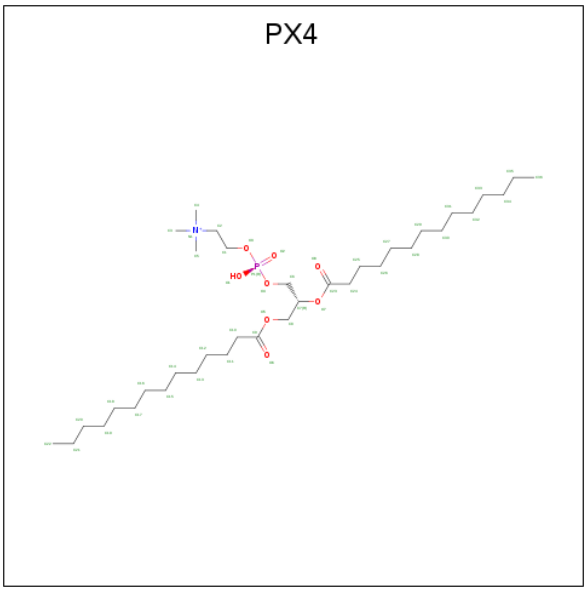


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Na 1 1	0	0

- Molecule 6 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: $C_{36}H_{73}NO_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C 14 14	0	0
6	E	1	Total C 14 14	0	0
6	E	1	Total C 14 14	0	0

- Molecule 7 is water.

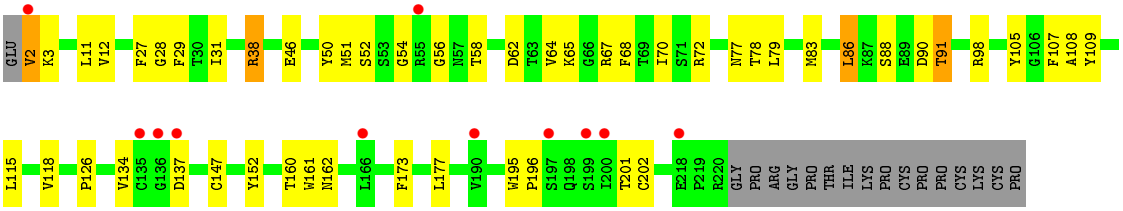
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	28	Total O 28 28	0	0
7	B	25	Total O 25 25	0	0
7	C	12	Total O 12 12	0	0
7	D	4	Total O 4 4	0	0
7	E	11	Total O 11 11	0	0
7	F	25	Total O 25 25	0	0
7	G	13	Total O 13 13	0	0
7	H	14	Total O 14 14	0	0
7	I	11	Total O 11 11	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

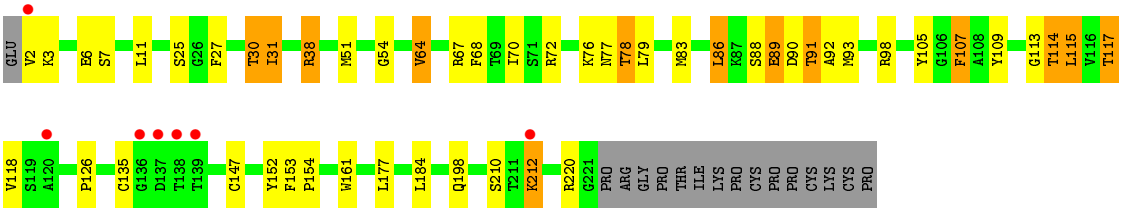
- Molecule 1: Fab Heavy Chain

Chain A:



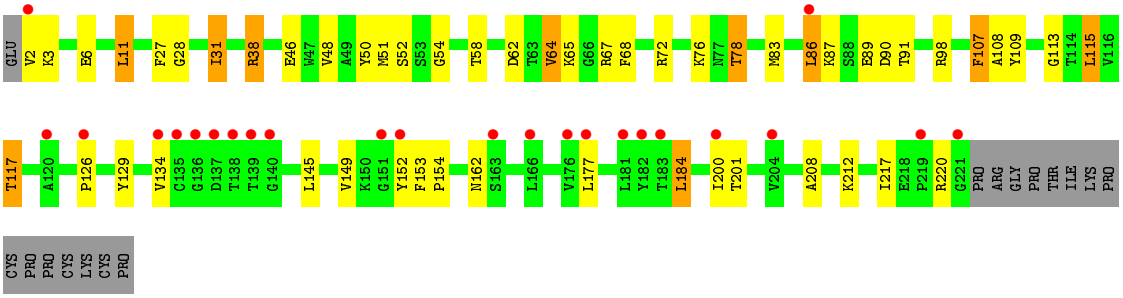
- Molecule 1: Fab Heavy Chain

Chain F:



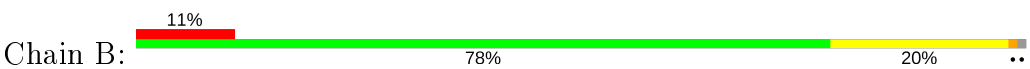
- Molecule 1: Fab Heavy Chain

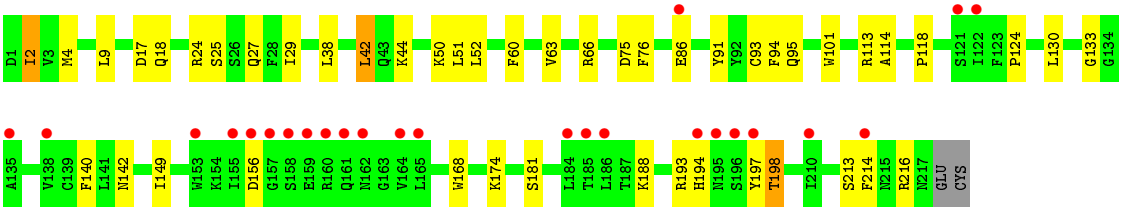
Chain H:



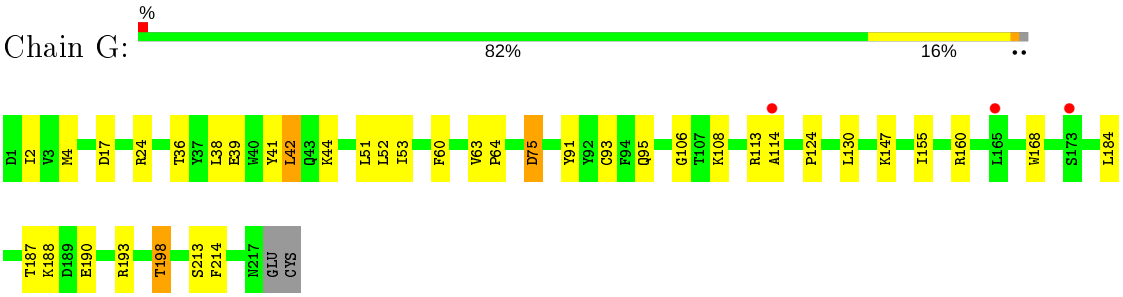
- Molecule 2: Fab Light Chain

Chain B:

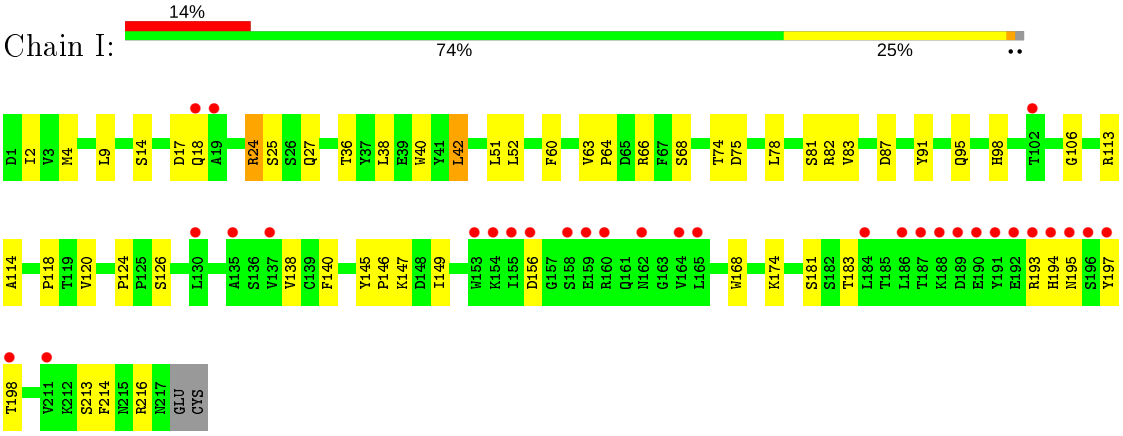




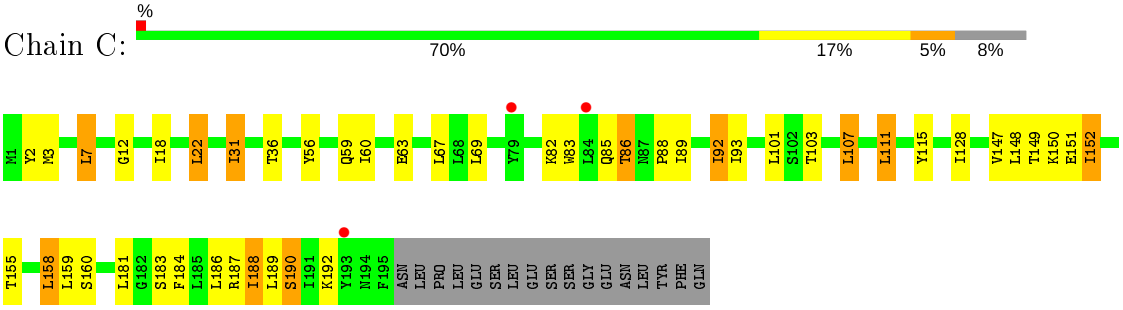
• Molecule 2: Fab Light Chain



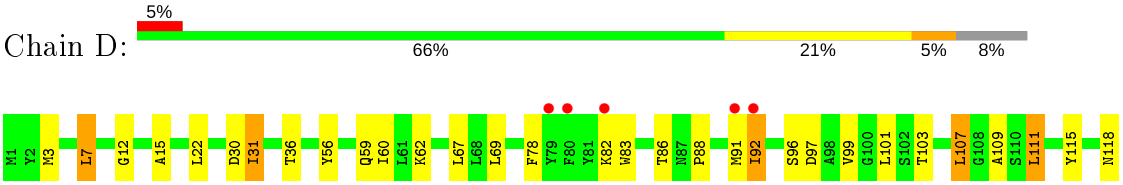
• Molecule 2: Fab Light Chain



• Molecule 3: Membrane protein TRIC

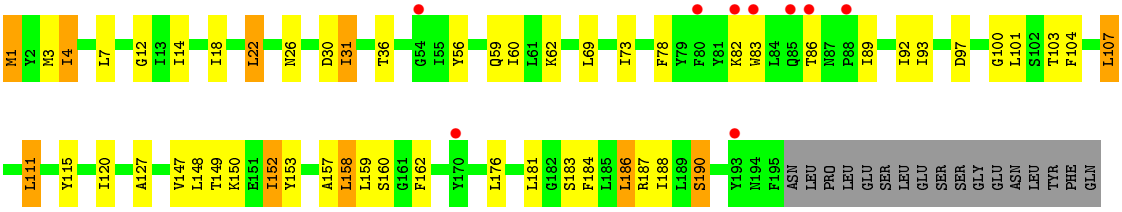


• Molecule 3: Membrane protein TRIC



- Molecule 3: Membrane protein TRIC

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.73Å 171.39Å 103.27Å 90.00° 117.94° 90.00°	Depositor
Resolution (Å)	49.40 – 2.64 49.40 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.40-2.64) 91.0 (49.40-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.211 , 0.252 0.214 , 0.251	Depositor DCC
R_{free} test set	4573 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	57.0	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.009 for -h-l,k,h 0.009 for l,k,-h-l 0.024 for h,-k,-h-l 0.027 for -h-l,-k,l 0.022 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14636	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PX4, NA

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	0.54	1/1677 (0.1%)	0.68	0/2291
1	F	0.57	0/1697	0.73	1/2314 (0.0%)
1	H	0.44	0/1697	0.62	1/2314 (0.0%)
2	B	0.52	1/1724 (0.1%)	0.63	0/2343
2	G	0.57	1/1728 (0.1%)	0.68	0/2347
2	I	0.41	0/1724	0.61	0/2343
3	C	0.57	0/1516	0.68	0/2066
3	D	0.49	0/1516	0.63	0/2066
3	E	0.53	0/1513	0.65	0/2062
All	All	0.52	3/14792 (0.0%)	0.66	2/20146 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	93	CYS	CB-SG	-9.56	1.66	1.82
2	G	93	CYS	CB-SG	-9.25	1.66	1.82
1	A	2	VAL	CB-CG1	-5.86	1.40	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	115	LEU	CA-CB-CG	5.29	127.47	115.30
1	F	115	LEU	CB-CG-CD1	-5.26	102.05	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1633	0	1568	36	0
1	F	1653	0	1604	37	0
1	H	1653	0	1604	44	0
2	B	1683	0	1608	28	0
2	G	1687	0	1619	21	0
2	I	1683	0	1608	38	0
3	C	1483	0	1559	31	0
3	D	1483	0	1554	32	0
3	E	1480	0	1550	34	0
4	A	6	0	8	0	0
4	C	6	0	8	0	0
5	C	1	0	0	0	0
6	C	14	0	27	2	0
6	E	28	0	54	0	0
7	A	28	0	0	2	0
7	B	25	0	0	3	0
7	C	12	0	0	0	0
7	D	4	0	0	0	0
7	E	11	0	0	0	0
7	F	25	0	0	2	0
7	G	13	0	0	2	0
7	H	14	0	0	1	0
7	I	11	0	0	1	0
All	All	14636	0	14371	267	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 9.

All (267) 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:F:2:VAL:HG21	1:F:109:TYR:HB3	1.41	0.98
1:A:2:VAL:HB	1:A:98:ARG:HH21	1.30	0.96
1:H:2:VAL:HG12	1:H:98:ARG:HH21	1.35	0.90
1:H:2:VAL:HG21	1:H:109:TYR:HB3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:MET:HE1	1:F:72:ARG:HB2	1.55	0.87
1:A:31:ILE:HG23	3:C:111:LEU:HD13	1.58	0.86
1:H:51:MET:HE1	1:H:72:ARG:HB2	1.60	0.83
1:F:67:ARG:NH2	1:F:90:ASP:OD2	2.18	0.76
1:F:126:PRO:HB3	1:F:152:TYR:HB3	1.68	0.75
2:B:75:ASP:OD2	7:B:301:HOH:O	2.04	0.74
2:G:113:ARG:NH1	2:G:114:ALA:O	2.21	0.72
3:D:82:LYS:HG3	3:D:83:TRP:HD1	1.56	0.71
1:F:88:SER:O	1:F:91:THR:HG23	1.91	0.71
1:H:28:GLY:O	1:H:31:ILE:HG12	1.90	0.71
3:E:62:LYS:NZ	1:F:77:ASN:OD1	2.16	0.71
1:F:64:VAL:HG13	1:F:68:PHE:HB2	1.75	0.69
1:H:126:PRO:HB3	1:H:152:TYR:HB3	1.72	0.69
3:D:101:LEU:HD11	3:D:157:ALA:HB2	1.76	0.68
2:B:194:HIS:O	2:B:216:ARG:NE	2.24	0.68
1:A:67:ARG:NH2	1:A:90:ASP:OD2	2.27	0.67
2:B:24:ARG:NH2	7:B:302:HOH:O	2.24	0.67
1:A:51:MET:HE1	1:A:72:ARG:HB2	1.76	0.67
3:D:59:GLN:HA	3:D:62:LYS:HE3	1.75	0.67
3:D:88:PRO:O	3:D:92:ILE:HG22	1.95	0.67
3:C:160:SER:HB2	3:C:183:SER:HB2	1.78	0.65
3:E:127:ALA:HB2	3:E:158:LEU:HD13	1.79	0.65
1:A:2:VAL:HG12	3:C:2:TYR:CG	2.32	0.65
3:C:152:ILE:HG13	3:C:190:SER:CB	2.26	0.64
2:B:50:LYS:NZ	7:B:304:HOH:O	2.30	0.64
3:C:149:THR:HG22	3:C:150:LYS:HD3	1.80	0.64
1:A:88:SER:O	1:A:91:THR:HG23	1.97	0.63
3:E:111:LEU:HD13	1:F:31:ILE:HG12	1.79	0.63
1:A:28:GLY:O	1:A:31:ILE:HG13	1.99	0.62
3:D:149:THR:HG22	3:D:150:LYS:HD3	1.81	0.62
3:E:149:THR:HG22	3:E:150:LYS:HD3	1.82	0.62
1:H:2:VAL:HG21	1:H:109:TYR:CB	2.29	0.62
1:H:64:VAL:HG13	1:H:68:PHE:HB2	1.80	0.61
3:C:158:LEU:HD21	6:C:303:PX4:H52	1.82	0.61
1:A:126:PRO:HB3	1:A:152:TYR:HB3	1.81	0.60
1:F:83:MET:HB3	1:F:86:LEU:HD11	1.82	0.60
1:F:2:VAL:HG21	1:F:109:TYR:CB	2.24	0.60
2:B:2:ILE:HD11	2:B:25:SER:HB2	1.84	0.60
1:F:91:THR:HB	1:F:117:THR:HA	1.85	0.59
2:G:124:PRO:HB3	2:G:214:PHE:CE2	2.37	0.59
3:D:152:ILE:HG13	3:D:190:SER:CB	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:MET:HB3	1:A:86:LEU:HD11	1.85	0.59
1:H:67:ARG:NH2	1:H:90:ASP:OD2	2.33	0.58
1:H:220:ARG:CZ	2:I:124:PRO:HG2	2.34	0.58
2:I:194:HIS:O	2:I:216:ARG:NE	2.36	0.58
2:G:42:LEU:HB2	2:G:52:LEU:HD11	1.86	0.57
1:A:64:VAL:HG13	1:A:68:PHE:HB2	1.86	0.57
2:I:42:LEU:HB2	2:I:52:LEU:HD11	1.85	0.57
3:E:82:LYS:HG3	3:E:83:TRP:HD1	1.69	0.57
3:D:111:LEU:HD13	1:H:31:ILE:HG23	1.85	0.56
2:I:195:ASN:HA	2:I:216:ARG:HE	1.70	0.56
3:C:82:LYS:HG3	3:C:83:TRP:HD1	1.70	0.56
1:F:2:VAL:HG12	1:F:98:ARG:HH21	1.70	0.56
2:I:4:MET:HE3	2:I:95:GLN:HG2	1.87	0.56
3:D:12:GLY:CA	3:D:103:THR:HG21	2.36	0.56
2:I:113:ARG:NH1	2:I:114:ALA:O	2.38	0.56
1:H:162:ASN:OD1	1:H:201:THR:N	2.38	0.55
1:H:62:ASP:OD1	1:H:65:LYS:NZ	2.24	0.55
2:I:124:PRO:HB3	2:I:214:PHE:CE1	2.42	0.55
2:I:118:PRO:HG3	2:I:149:ILE:HD11	1.88	0.55
1:A:70:ILE:HD11	1:A:79:LEU:HD11	1.89	0.55
3:D:168:THR:HG23	3:D:169:PRO:HD3	1.88	0.55
2:G:124:PRO:HB3	2:G:214:PHE:CZ	2.41	0.55
3:D:101:LEU:HD23	3:D:187:ARG:HG3	1.89	0.55
3:E:12:GLY:CA	3:E:103:THR:HG21	2.36	0.55
3:E:101:LEU:HD11	3:E:157:ALA:HB2	1.89	0.55
2:B:130:LEU:O	2:B:188:LYS:HE2	2.06	0.55
1:A:2:VAL:HG21	1:A:98:ARG:HE	1.72	0.54
3:C:12:GLY:CA	3:C:103:THR:HG21	2.38	0.54
2:I:82:ARG:NH1	7:I:303:HOH:O	2.40	0.54
2:B:42:LEU:HB2	2:B:52:LEU:HD11	1.90	0.54
3:C:36:THR:HG21	3:E:147:VAL:HG12	1.90	0.54
3:C:86:THR:O	3:C:89:ILE:HB	2.07	0.54
3:E:152:ILE:HG13	3:E:190:SER:CB	2.38	0.54
3:D:147:VAL:HG12	3:E:36:THR:HG21	1.89	0.54
2:I:18:GLN:HG2	2:I:81:SER:HA	1.90	0.54
3:D:118:ASN:ND2	3:E:62:LYS:O	2.41	0.54
2:G:2:ILE:H	2:G:2:ILE:HD12	1.73	0.54
2:I:138:VAL:HG22	2:I:183:THR:HG23	1.90	0.54
7:A:413:HOH:O	2:B:50:LYS:HD3	2.08	0.54
3:D:164:TYR:O	3:D:168:THR:HG22	2.09	0.53
3:C:128:ILE:HG12	6:C:303:PX4:H62	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:184:PHE:CZ	3:C:188:ILE:HD12	2.44	0.53
1:A:162:ASN:OD1	1:A:201:THR:N	2.38	0.53
1:A:134:VAL:HG21	2:B:214:PHE:HB2	1.90	0.53
1:H:38:ARG:HD3	1:H:46:GLU:HB2	1.90	0.53
2:I:147:LYS:O	2:I:168:TRP:HZ3	1.91	0.52
3:D:160:SER:HB2	3:D:183:SER:HB2	1.91	0.52
3:E:120:ILE:HD12	3:E:120:ILE:H	1.75	0.52
1:H:87:LYS:HB2	1:H:89:GLU:HG2	1.92	0.52
1:H:83:MET:HB3	1:H:86:LEU:HD11	1.91	0.52
1:H:98:ARG:HD2	7:H:310:HOH:O	2.09	0.52
3:E:184:PHE:CZ	3:E:188:ILE:HD12	2.45	0.52
1:F:3:LYS:HB2	1:F:25:SER:OG	2.10	0.51
2:I:124:PRO:HB3	2:I:214:PHE:CZ	2.46	0.51
3:C:151:GLU:CD	3:D:30:ASP:HB3	2.31	0.51
3:E:160:SER:HB2	3:E:183:SER:HB2	1.93	0.51
1:F:220:ARG:CZ	2:G:124:PRO:HG2	2.41	0.51
2:B:118:PRO:HG3	2:B:149:ILE:HD11	1.93	0.50
3:D:31:ILE:HG23	3:D:78:PHE:CD2	2.46	0.50
3:E:115:TYR:OH	1:F:30:THR:HG21	2.12	0.50
1:H:2:VAL:HG12	1:H:98:ARG:NH2	2.17	0.50
3:C:147:VAL:HG12	3:D:36:THR:HG21	1.93	0.50
2:G:198:THR:HG22	2:G:213:SER:OG	2.11	0.50
3:D:107:LEU:HG	1:H:27:PHE:CZ	2.46	0.50
2:I:60:PHE:O	2:I:63:VAL:HG13	2.11	0.50
2:G:155:ILE:HD11	2:G:184:LEU:HD21	1.94	0.50
2:B:149:ILE:HG22	2:B:168:TRP:CH2	2.47	0.49
1:H:162:ASN:HD21	1:H:200:ILE:HA	1.75	0.49
1:H:91:THR:HG23	1:H:117:THR:HA	1.93	0.49
1:A:51:MET:CE	1:A:72:ARG:HB2	2.42	0.49
1:F:76:LYS:HB2	1:F:78:THR:HG23	1.93	0.49
1:H:2:VAL:HG21	1:H:109:TYR:CG	2.47	0.49
1:F:89:GLU:OE2	1:F:89:GLU:N	2.40	0.49
3:E:97:ASP:OD1	3:E:153:TYR:OH	2.22	0.49
2:I:149:ILE:HG22	2:I:168:TRP:CH2	2.48	0.49
1:A:2:VAL:HG12	3:C:2:TYR:CB	2.42	0.49
1:A:2:VAL:HG13	1:A:109:TYR:CD1	2.48	0.48
3:E:152:ILE:HG13	3:E:190:SER:HB2	1.95	0.48
2:G:60:PHE:O	2:G:63:VAL:HG13	2.13	0.48
3:D:120:ILE:H	3:D:120:ILE:HD12	1.79	0.48
2:G:4:MET:HE3	2:G:95:GLN:HG2	1.96	0.48
1:A:105:TYR:CD1	1:A:108:ALA:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:134:VAL:HG21	2:I:214:PHE:HB2	1.96	0.48
1:H:76:LYS:HB2	1:H:78:THR:HG23	1.96	0.48
2:I:17:ASP:O	2:I:83:VAL:HG13	2.13	0.48
2:G:187:THR:OG1	2:G:190:GLU:HB2	2.13	0.47
1:A:52:SER:O	1:A:56:GLY:HA2	2.14	0.47
1:H:134:VAL:HG21	2:I:214:PHE:CB	2.44	0.47
3:D:115:TYR:CZ	1:H:54:GLY:HA2	2.49	0.47
2:G:91:TYR:O	2:G:106:GLY:HA2	2.14	0.47
2:I:2:ILE:HD11	2:I:98:HIS:HB2	1.97	0.47
1:A:134:VAL:HG22	2:B:124:PRO:HG3	1.96	0.47
2:B:2:ILE:HD11	2:B:4:MET:HE2	1.96	0.47
3:C:86:THR:HA	3:C:89:ILE:HD12	1.96	0.47
1:F:198:GLN:HB3	7:F:312:HOH:O	2.15	0.47
2:I:113:ARG:HG3	2:I:114:ALA:O	2.15	0.47
1:A:50:TYR:O	1:A:58:THR:HA	2.14	0.47
3:E:26:ASN:OD1	3:E:89:ILE:HG21	2.15	0.47
2:G:193:ARG:NH1	7:G:305:HOH:O	2.48	0.47
3:E:12:GLY:HA2	3:E:103:THR:HG21	1.96	0.46
1:F:76:LYS:HG2	7:F:311:HOH:O	2.15	0.46
1:H:154:PRO:HD2	1:H:208:ALA:CB	2.46	0.46
3:E:18:ILE:O	3:E:22:LEU:HB2	2.14	0.46
2:B:42:LEU:HD13	2:B:44:LYS:HG2	1.98	0.46
1:A:91:THR:HG22	1:A:118:VAL:H	1.81	0.46
3:C:7:LEU:HD12	3:C:7:LEU:HA	1.78	0.46
1:H:6:GLU:CD	1:H:113:GLY:H	2.19	0.46
2:I:68:SER:O	2:I:78:LEU:HD12	2.15	0.46
3:E:22:LEU:HD13	3:E:93:ILE:HG13	1.97	0.46
2:I:42:LEU:HG	2:I:91:TYR:CZ	2.51	0.46
3:E:31:ILE:HG23	3:E:78:PHE:CD2	2.51	0.46
1:H:149:VAL:HB	1:H:184:LEU:HD23	1.98	0.46
2:I:120:VAL:HA	2:I:140:PHE:O	2.16	0.46
3:C:31:ILE:HG13	3:C:31:ILE:H	1.51	0.45
3:D:82:LYS:HG3	3:D:83:TRP:CD1	2.45	0.45
2:B:4:MET:HE3	2:B:95:GLN:HG2	1.97	0.45
3:C:88:PRO:O	3:C:92:ILE:HG22	2.16	0.45
1:A:12:VAL:HG11	1:A:86:LEU:HD23	1.97	0.45
1:F:7:SER:HA	1:F:114:THR:HG21	1.98	0.45
3:C:18:ILE:O	3:C:22:LEU:HB2	2.16	0.45
2:G:63:VAL:HA	2:G:64:PRO:HD3	1.86	0.45
1:H:3:LYS:HD3	1:H:3:LYS:HA	1.73	0.45
1:H:52:SER:O	1:H:72:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:PHE:O	2:B:63:VAL:HG13	2.17	0.44
3:E:4:ILE:HD11	3:E:176:LEU:HB3	1.99	0.44
2:I:197:TYR:HB2	2:I:214:PHE:CE2	2.52	0.44
1:A:3:LYS:HA	1:A:3:LYS:HD3	1.76	0.44
1:H:134:VAL:HG22	2:I:124:PRO:HG3	2.00	0.44
3:C:22:LEU:HD13	3:C:93:ILE:HG13	1.98	0.44
3:D:127:ALA:HB2	3:D:158:LEU:HD22	1.97	0.44
1:F:107:PHE:HB2	2:G:41:TYR:OH	2.17	0.44
1:F:76:LYS:O	1:F:78:THR:HG22	2.17	0.44
1:H:2:VAL:HG23	1:H:2:VAL:O	2.16	0.44
2:I:40:TRP:CE2	2:I:78:LEU:HB2	2.53	0.44
1:A:38:ARG:HD3	1:A:46:GLU:OE1	2.17	0.44
1:F:51:MET:CE	1:F:72:ARG:HB2	2.36	0.44
2:G:168:TRP:CD1	2:G:168:TRP:N	2.85	0.44
3:E:115:TYR:CZ	1:F:54:GLY:HA2	2.53	0.44
2:G:198:THR:HG23	7:G:309:HOH:O	2.18	0.44
1:H:76:LYS:O	1:H:78:THR:HG22	2.18	0.44
1:A:62:ASP:OD1	1:A:65:LYS:NZ	2.35	0.44
1:A:161:TRP:CZ3	1:A:202:CYS:HB2	2.53	0.43
2:B:66:ARG:NH2	2:B:86:GLU:OE2	2.51	0.43
1:F:2:VAL:HG23	1:F:2:VAL:O	2.18	0.43
2:G:24:ARG:HD3	2:G:75:ASP:OD1	2.18	0.43
2:I:145:TYR:CD1	2:I:146:PRO:HA	2.53	0.43
2:I:25:SER:OG	2:I:74:THR:HA	2.19	0.43
2:B:94:PHE:CZ	2:B:101:TRP:HB3	2.53	0.43
1:F:147:CYS:HB2	1:F:161:TRP:CH2	2.53	0.43
2:B:29:ILE:HD11	2:B:76:PHE:CE1	2.53	0.43
3:D:99:VAL:O	3:D:103:THR:HG22	2.19	0.43
1:F:126:PRO:CB	1:F:152:TYR:HB3	2.45	0.43
2:B:113:ARG:HG3	2:B:114:ALA:O	2.19	0.43
2:B:113:ARG:NH1	2:B:114:ALA:O	2.51	0.43
2:B:133:GLY:HA2	2:B:188:LYS:HB2	2.01	0.43
1:F:6:GLU:CD	1:F:113:GLY:H	2.21	0.43
1:A:195:TRP:CG	1:A:196:PRO:HA	2.53	0.43
1:A:29:PHE:HB3	3:C:59:GLN:HE22	1.83	0.43
1:A:98:ARG:HD2	7:A:407:HOH:O	2.18	0.43
2:I:197:TYR:O	2:I:213:SER:HA	2.18	0.43
2:B:197:TYR:HB2	2:B:214:PHE:CE2	2.53	0.43
1:H:108:ALA:HB1	2:I:60:PHE:CZ	2.54	0.43
3:E:127:ALA:HA	3:E:157:ALA:CB	2.49	0.43
1:H:107:PHE:CD1	1:H:107:PHE:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:GLY:HA3	3:C:103:THR:HG21	2.00	0.42
3:E:59:GLN:HA	3:E:62:LYS:HD3	2.01	0.42
2:B:42:LEU:HG	2:B:91:TYR:CE2	2.54	0.42
1:A:31:ILE:CG2	3:C:111:LEU:HD13	2.41	0.42
1:F:3:LYS:HD3	1:F:3:LYS:HA	1.72	0.42
2:I:66:ARG:HH21	2:I:87:ASP:CG	2.21	0.42
3:C:158:LEU:HA	3:C:158:LEU:HD13	1.92	0.42
3:D:152:ILE:HG13	3:D:190:SER:HB2	2.00	0.42
1:H:38:ARG:HD2	1:H:48:VAL:CG2	2.49	0.42
3:D:7:LEU:HA	3:D:7:LEU:HD12	1.91	0.42
1:A:54:GLY:HA2	3:C:115:TYR:CZ	2.55	0.42
3:C:85:GLN:O	3:C:88:PRO:HG2	2.20	0.42
3:E:14:ILE:HG23	3:E:73:ILE:HD13	2.02	0.42
2:I:63:VAL:HA	2:I:64:PRO:HD3	1.85	0.42
1:H:28:GLY:HA3	1:H:31:ILE:CD1	2.50	0.42
3:D:97:ASP:CG	3:D:153:TYR:HH	2.23	0.42
3:E:103:THR:HG23	3:E:104:PHE:N	2.34	0.42
3:D:151:GLU:CD	3:E:30:ASP:HB3	2.41	0.41
2:G:130:LEU:O	2:G:188:LYS:HE2	2.21	0.41
2:G:42:LEU:HD13	2:G:44:LYS:HG2	2.02	0.41
3:D:12:GLY:HA2	3:D:103:THR:HG21	2.01	0.41
2:G:39:GLU:HA	2:G:53:ILE:O	2.19	0.41
3:D:159:LEU:HD22	3:D:159:LEU:HA	1.85	0.41
1:H:162:ASN:ND2	1:H:200:ILE:HA	2.36	0.41
2:B:140:PHE:HB3	2:B:142:ASN:OD1	2.21	0.41
1:F:91:THR:HG22	1:F:118:VAL:H	1.84	0.41
2:I:24:ARG:NE	2:I:75:ASP:OD2	2.54	0.41
3:D:109:ALA:HB2	3:D:126:ALA:HB2	2.02	0.41
3:E:186:LEU:HA	3:E:186:LEU:HD22	1.91	0.41
1:F:70:ILE:HD11	1:F:79:LEU:HD11	2.02	0.41
1:H:153:PHE:HA	1:H:154:PRO:HA	1.89	0.41
1:H:50:TYR:O	1:H:58:THR:HA	2.19	0.41
1:H:51:MET:CE	1:H:72:ARG:HB2	2.40	0.41
2:B:198:THR:HG22	2:B:213:SER:OG	2.21	0.41
1:H:11:LEU:HB2	1:H:154:PRO:HG3	2.03	0.41
1:H:129:TYR:HB3	2:I:126:SER:OG	2.21	0.41
1:A:27:PHE:CZ	3:C:107:LEU:HG	2.55	0.41
1:F:153:PHE:HA	1:F:154:PRO:HA	1.85	0.41
1:A:2:VAL:HG12	3:C:2:TYR:HB2	2.03	0.41
3:D:15:ALA:HB1	3:D:96:SER:O	2.21	0.41
3:E:100:GLY:HA2	3:E:103:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:156:ASP:OD2	2:I:194:HIS:HB3	2.20	0.41
1:F:91:THR:HG22	1:F:118:VAL:HB	2.02	0.41
1:A:147:CYS:HB2	1:A:161:TRP:CH2	2.56	0.40
1:A:173:PHE:CD2	2:B:181:SER:HB2	2.56	0.40
2:I:91:TYR:O	2:I:106:GLY:HA2	2.21	0.40
2:B:156:ASP:OD2	2:B:194:HIS:HB3	2.21	0.40
3:C:22:LEU:HA	3:C:22:LEU:HD23	1.86	0.40
3:E:107:LEU:HG	1:F:27:PHE:CZ	2.56	0.40
2:I:195:ASN:HA	2:I:216:ARG:NE	2.35	0.40
3:C:82:LYS:HG3	3:C:83:TRP:CD1	2.54	0.40
3:E:1:MET:CE	1:F:105:TYR:HE1	2.35	0.40
3:D:185:LEU:HA	3:D:185:LEU:HD23	1.85	0.40
1:F:38:ARG:HG3	1:F:92:ALA:HB3	2.02	0.40
1:H:145:LEU:HB3	1:H:217:ILE:HG21	2.03	0.40
2:I:2:ILE:HD12	2:I:2:ILE:N	2.37	0.40
3:E:22:LEU:HD12	3:E:92:ILE:HG22	2.02	0.40
1:F:212:LYS:HE2	1:F:212:LYS:HB3	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/236 (92%)	210 (97%)	7 (3%)	0	100	100
1	F	218/236 (92%)	212 (97%)	6 (3%)	0	100	100
1	H	218/236 (92%)	210 (96%)	8 (4%)	0	100	100
2	B	215/219 (98%)	210 (98%)	5 (2%)	0	100	100
2	G	215/219 (98%)	209 (97%)	6 (3%)	0	100	100
2	I	215/219 (98%)	211 (98%)	4 (2%)	0	100	100
3	C	193/212 (91%)	187 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	193/212 (91%)	186 (96%)	7 (4%)	0	100	100
3	E	193/212 (91%)	187 (97%)	6 (3%)	0	100	100
All	All	1877/2001 (94%)	1822 (97%)	55 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/199 (90%)	168 (94%)	11 (6%)	18	29
1	F	182/199 (92%)	163 (90%)	19 (10%)	7	9
1	H	182/199 (92%)	170 (93%)	12 (7%)	16	25
2	B	192/196 (98%)	181 (94%)	11 (6%)	20	31
2	G	193/196 (98%)	183 (95%)	10 (5%)	23	36
2	I	192/196 (98%)	180 (94%)	12 (6%)	18	27
3	C	158/177 (89%)	132 (84%)	26 (16%)	2	2
3	D	158/177 (89%)	136 (86%)	22 (14%)	3	3
3	E	157/177 (89%)	136 (87%)	21 (13%)	4	4
All	All	1593/1716 (93%)	1449 (91%)	144 (9%)	9	14

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	38	ARG
1	A	77	ASN
1	A	78	THR
1	A	86	LEU
1	A	91	THR
1	A	107	PHE
1	A	115	LEU

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Mol	Chain	Res	Type
1	A	137	ASP
1	A	160	THR
1	A	177	LEU
2	B	2	ILE
2	B	9	LEU
2	B	17	ASP
2	B	18	GLN
2	B	27	GLN
2	B	38	LEU
2	B	42	LEU
2	B	51	LEU
2	B	174	LYS
2	B	193	ARG
2	B	198	THR
3	C	3	MET
3	C	7	LEU
3	C	22	LEU
3	C	31	ILE
3	C	56	TYR
3	C	60	ILE
3	C	63	GLU
3	C	67	LEU
3	C	69	LEU
3	C	86	THR
3	C	92	ILE
3	C	101	LEU
3	C	107	LEU
3	C	111	LEU
3	C	148	LEU
3	C	152	ILE
3	C	155	THR
3	C	158	LEU
3	C	159	LEU
3	C	181	LEU
3	C	186	LEU
3	C	187	ARG
3	C	188	ILE
3	C	189	LEU
3	C	190	SER
3	C	192	LYS
3	D	3	MET
3	D	7	LEU

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Mol	Chain	Res	Type
3	D	22	LEU
3	D	31	ILE
3	D	56	TYR
3	D	60	ILE
3	D	67	LEU
3	D	69	LEU
3	D	86	THR
3	D	91	MET
3	D	92	ILE
3	D	107	LEU
3	D	111	LEU
3	D	148	LEU
3	D	152	ILE
3	D	155	THR
3	D	158	LEU
3	D	159	LEU
3	D	181	LEU
3	D	186	LEU
3	D	187	ARG
3	D	190	SER
3	E	1	MET
3	E	3	MET
3	E	4	ILE
3	E	7	LEU
3	E	22	LEU
3	E	31	ILE
3	E	56	TYR
3	E	60	ILE
3	E	69	LEU
3	E	86	THR
3	E	107	LEU
3	E	111	LEU
3	E	148	LEU
3	E	152	ILE
3	E	158	LEU
3	E	159	LEU
3	E	162	PHE
3	E	181	LEU
3	E	186	LEU
3	E	187	ARG
3	E	190	SER
1	F	11	LEU

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Mol	Chain	Res	Type
1	F	30	THR
1	F	31	ILE
1	F	38	ARG
1	F	64	VAL
1	F	78	THR
1	F	86	LEU
1	F	89	GLU
1	F	91	THR
1	F	93	MET
1	F	107	PHE
1	F	114	THR
1	F	115	LEU
1	F	117	THR
1	F	135	CYS
1	F	177	LEU
1	F	184	LEU
1	F	210	SER
1	F	212	LYS
2	G	17	ASP
2	G	36	THR
2	G	38	LEU
2	G	42	LEU
2	G	51	LEU
2	G	75	ASP
2	G	108	LYS
2	G	147	LYS
2	G	160	ARG
2	G	198	THR
1	H	11	LEU
1	H	31	ILE
1	H	38	ARG
1	H	64	VAL
1	H	78	THR
1	H	86	LEU
1	H	107	PHE
1	H	115	LEU
1	H	117	THR
1	H	177	LEU
1	H	184	LEU
1	H	212	LYS
2	I	9	LEU
2	I	14	SER

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Mol	Chain	Res	Type
2	I	24	ARG
2	I	27	GLN
2	I	36	THR
2	I	38	LEU
2	I	42	LEU
2	I	51	LEU
2	I	174	LYS
2	I	181	SER
2	I	193	ARG
2	I	198	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
2	B	142	ASN
3	C	59	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\#\|Z\| > 2$
6	PX4	E	301	-	13,13,45	0.88	0	12,12,53	0.80	0
4	GOL	C	302	-	5,5,5	0.24	0	5,5,5	0.58	0
6	PX4	C	303	-	13,13,45	0.78	0	12,12,53	0.85	0
6	PX4	E	302	-	13,13,45	0.76	0	12,12,53	1.08	0
4	GOL	A	301	-	5,5,5	0.38	0	5,5,5	0.45	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
6	PX4	E	301	-	-	7/11/11/49	-
4	GOL	C	302	-	-	1/4/4/4	-
6	PX4	C	303	-	-	8/11/11/49	-
6	PX4	E	302	-	-	5/11/11/49	-
4	GOL	A	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	302	PX4	C27-C28-C29-C30
6	E	301	PX4	C27-C28-C29-C30
6	C	303	PX4	C27-C28-C29-C30
4	A	301	GOL	O1-C1-C2-C3
4	C	302	GOL	O1-C1-C2-C3
6	E	302	PX4	C32-C33-C34-C35
6	E	301	PX4	C31-C32-C33-C34
6	C	303	PX4	C23-C24-C25-C26
6	E	302	PX4	C25-C26-C27-C28
6	E	301	PX4	C24-C25-C26-C27
6	E	301	PX4	C29-C30-C31-C32
6	C	303	PX4	C28-C29-C30-C31
6	E	301	PX4	C28-C29-C30-C31

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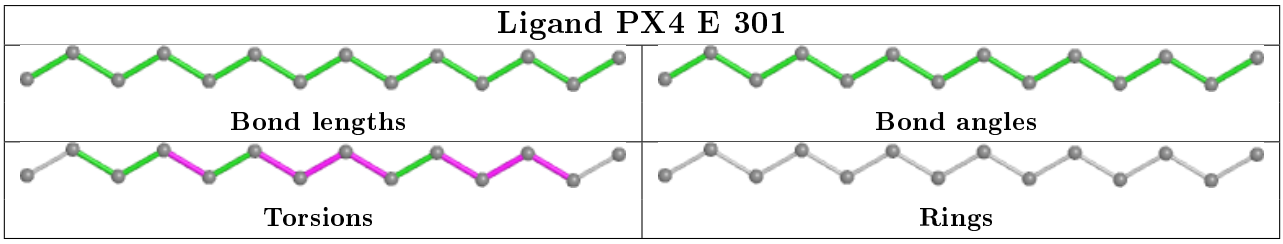
Mol	Chain	Res	Type	Atoms
4	A	301	GOL	O1-C1-C2-O2
6	C	303	PX4	C30-C31-C32-C33
6	E	301	PX4	C23-C24-C25-C26
6	C	303	PX4	C25-C26-C27-C28
6	E	301	PX4	C25-C26-C27-C28
6	E	302	PX4	C29-C30-C31-C32
6	C	303	PX4	C26-C27-C28-C29
6	E	302	PX4	C24-C25-C26-C27
6	C	303	PX4	C24-C25-C26-C27
6	C	303	PX4	C29-C30-C31-C32

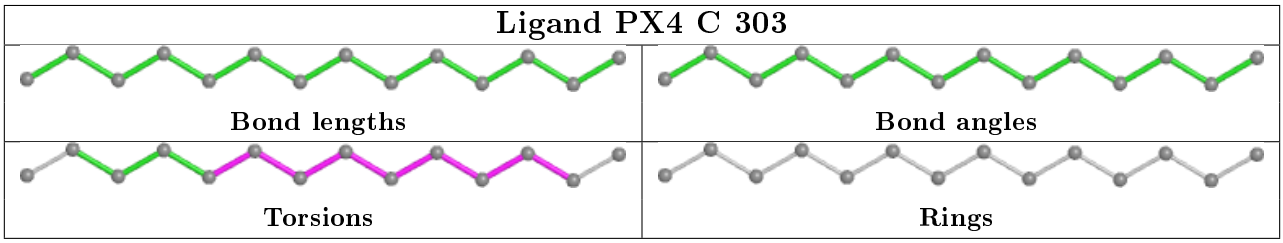
There are no ring outliers.

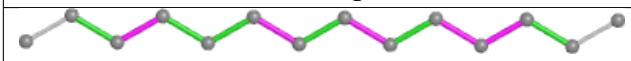
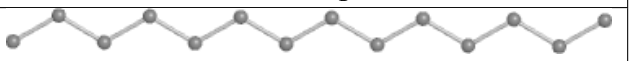
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	303	PX4	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





Ligand PX4 E 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	219/236 (92%)	0.29	11 (5%) 28 25	44, 64, 117, 155	0
1	F	220/236 (93%)	0.11	7 (3%) 47 44	46, 60, 87, 150	0
1	H	220/236 (93%)	0.68	24 (10%) 5 4	54, 80, 136, 186	0
2	B	217/219 (99%)	0.50	25 (11%) 4 3	42, 78, 137, 155	0
2	G	217/219 (99%)	0.08	3 (1%) 75 73	47, 63, 80, 99	0
2	I	217/219 (99%)	0.64	31 (14%) 2 1	60, 82, 144, 155	0
3	C	195/212 (91%)	0.17	3 (1%) 73 71	44, 53, 77, 112	0
3	D	195/212 (91%)	0.28	11 (5%) 24 21	50, 65, 100, 135	0
3	E	195/212 (91%)	0.29	9 (4%) 32 28	46, 58, 92, 122	0
All	All	1895/2001 (94%)	0.34	124 (6%) 18 16	42, 65, 127, 186	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	137	ASP	12.0
2	B	155	ILE	7.9
2	I	186	LEU	7.7
2	I	160	ARG	6.4
2	I	197	TYR	6.3
1	H	2	VAL	6.0
2	I	193	ARG	5.9
2	B	157	GLY	5.8
1	H	136	GLY	5.7
2	I	189	ASP	5.7
3	E	193	TYR	5.6
2	B	158	SER	5.5
2	B	186	LEU	5.5
1	H	139	THR	5.4
1	H	182	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
2	B	160	ARG	5.1
3	D	193	TYR	5.0
1	F	138	THR	4.9
2	I	155	ILE	4.8
3	C	193	TYR	4.6
2	B	159	GLU	4.5
2	B	197	TYR	4.4
2	B	156	ASP	4.4
1	A	136	GLY	4.4
1	H	140	GLY	4.2
2	I	153	TRP	4.2
3	D	192	LYS	4.2
2	I	191	TYR	4.2
2	I	164	VAL	4.1
2	B	184	LEU	4.1
1	H	177	LEU	4.1
2	I	192	GLU	3.9
2	I	137	VAL	3.9
3	D	80	PHE	3.9
1	H	221	GLY	3.8
1	A	2	VAL	3.8
1	H	138	THR	3.7
2	I	184	LEU	3.7
2	I	18	GLN	3.7
3	D	194	ASN	3.7
2	I	159	GLU	3.6
2	B	195	ASN	3.5
3	E	86	THR	3.4
2	B	153	TRP	3.4
2	I	194	HIS	3.4
1	F	136	GLY	3.4
2	B	161	GLN	3.4
2	I	165	LEU	3.4
2	I	188	LYS	3.4
2	I	135	ALA	3.3
1	H	181	LEU	3.3
2	G	173	SER	3.3
3	E	80	PHE	3.3
2	G	114	ALA	3.3
2	B	185	THR	3.2
1	H	86	LEU	3.2
1	H	135	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	I	195	ASN	3.2
1	A	166	LEU	3.2
2	I	196	SER	3.1
2	B	122	ILE	3.0
1	A	197	SER	3.0
1	F	2	VAL	3.0
1	A	137	ASP	2.9
2	B	164	VAL	2.9
3	D	177	PHE	2.9
2	I	19	ALA	2.9
3	D	79	TYR	2.9
2	B	214	PHE	2.8
2	B	162	ASN	2.8
3	E	88	PRO	2.8
2	I	187	THR	2.8
2	I	130	LEU	2.8
2	I	102	THR	2.8
2	B	194	HIS	2.8
3	E	83	TRP	2.7
2	B	165	LEU	2.7
2	B	86	GLU	2.7
1	H	204	VAL	2.7
1	H	166	LEU	2.7
2	I	162	ASN	2.7
2	I	156	ASP	2.7
3	D	82	LYS	2.6
1	A	200	ILE	2.6
3	D	189	LEU	2.6
1	F	139	THR	2.5
2	G	165	LEU	2.5
1	H	163	SER	2.5
2	I	190	GLU	2.5
1	H	120	ALA	2.5
1	A	190	VAL	2.5
1	A	135	CYS	2.5
1	A	218	GLU	2.5
3	D	92	ILE	2.5
2	B	196	SER	2.4
3	D	91	MET	2.4
1	F	120	ALA	2.4
1	F	137	ASP	2.4
1	H	200	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	121	SER	2.4
1	H	176	VAL	2.4
1	H	151	GLY	2.3
3	C	84	LEU	2.3
2	B	135	ALA	2.3
2	I	158	SER	2.3
1	A	199	SER	2.3
3	E	170	TYR	2.2
2	I	198	THR	2.2
3	E	82	LYS	2.2
3	D	191	ILE	2.2
1	F	212	LYS	2.2
1	A	55	ARG	2.2
2	B	138	VAL	2.1
3	C	79	TYR	2.1
2	B	210	ILE	2.1
1	H	126	PRO	2.1
1	H	152	TYR	2.1
1	H	183	THR	2.0
1	H	219	PRO	2.0
2	I	211	VAL	2.0
2	I	154	LYS	2.0
3	E	54	GLY	2.0
3	E	85	GLN	2.0
1	H	134	VAL	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 carbohydrates in this entry.

6.4 Ligands (i)

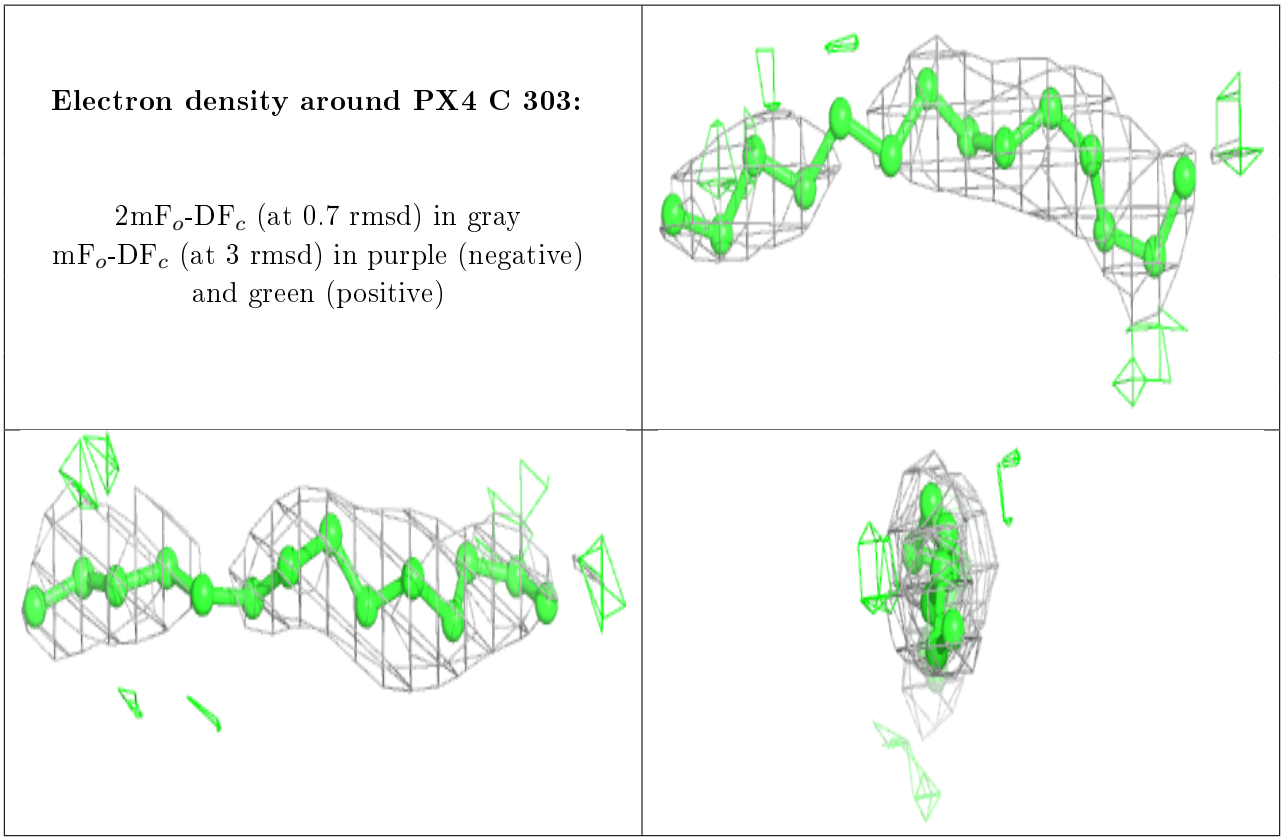
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PX4	C	303	14/46	0.86	0.29	55,62,67,68	0
4	GOL	C	302	6/6	0.88	0.19	65,67,74,77	0
6	PX4	E	301	14/46	0.89	0.31	54,64,70,71	0
6	PX4	E	302	14/46	0.90	0.34	66,73,79,79	0
5	NA	C	301	1/1	0.94	0.24	54,54,54,54	0
4	GOL	A	301	6/6	0.96	0.17	62,66,69,71	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.

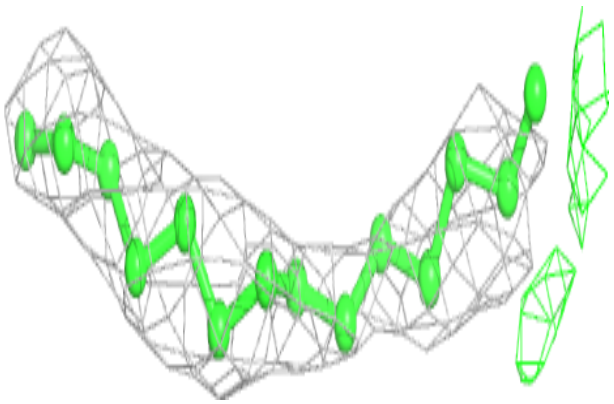
Electron density around PX4 C 303:

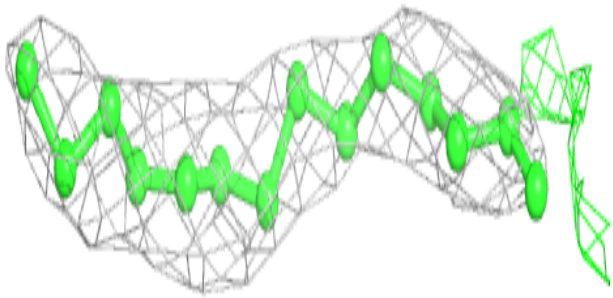
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

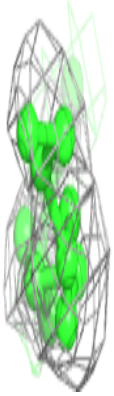


Electron density around PX4 E 301:

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

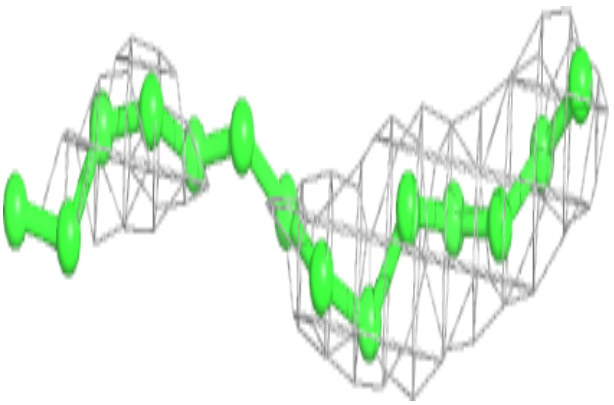


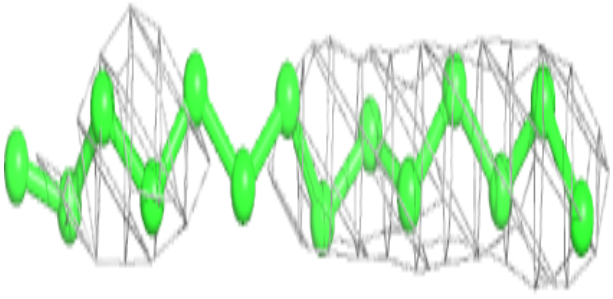


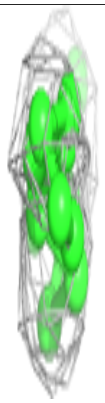


Electron density around PX4 E 302:

$2mF_o$-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.