Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2020 – 02:08 PM JST

PDB ID	:	7CTU
Title	:	Diabody H6 in complex with Leptin Receptor
Deposited on	:	2020-08-20
Resolution	:	3.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (i) symbol.

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

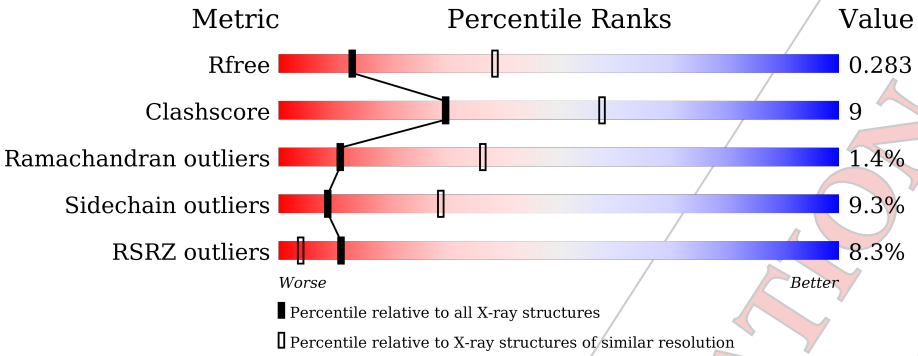
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	122	74% 22% • •
1	D	122	76% 19% • •
2	B	116	?% 55% 29% 7% 9%
2	E	116	66% 23% • 8%
3	C	206	16% 67% 21% • 10%
3	F	206	17% 71% 17% • 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6414 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 H6 scFv Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	120	Total	C	N	O	S	0	0	0
			922	582	159	177	4			
1	D	117	Total	C	N	O	S	0	0	0
			910	576	156	174	4			

- Molecule 2 is a protein called H6 scFv Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	106	Total	C	N	O	S	0	0	0
			792	499	132	159	2			
2	E	107	Total	C	N	O	S	0	0	0
			808	509	136	161	2			

- Molecule 3 is a protein called Leptin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	186	Total	C	N	O	S	0	0	0
			1491	962	244	276	9			
3	F	185	Total	C	N	O	S	0	0	0
			1486	960	240	277	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	604	SER	CYS	engineered mutation	UNP P48357
C	613	SER	CYS	engineered mutation	UNP P48357
F	604	SER	CYS	engineered mutation	UNP P48357
F	613	SER	CYS	engineered mutation	UNP P48357

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by author).

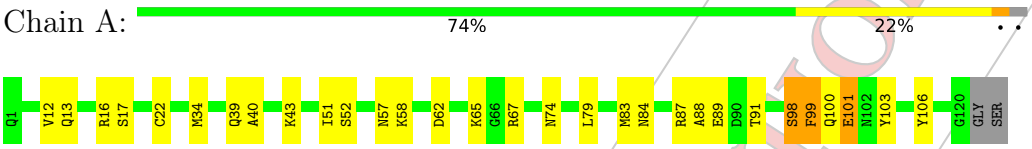
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0
4	D	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0

3 Residue-property plots

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

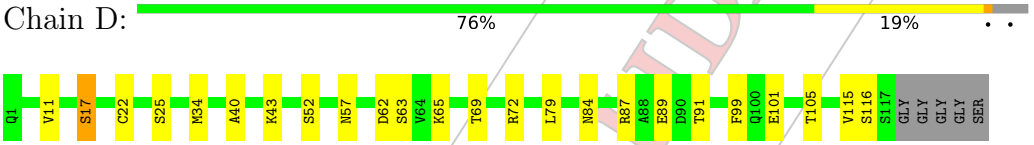
• Molecule 1: H6 scFv Heavy Chain

Chain A:



• Molecule 1: H6 scFv Heavy Chain

Chain D:

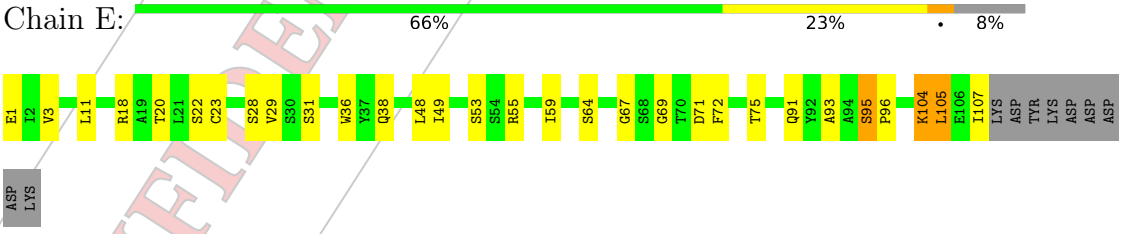


• Molecule 2: H6 scFv Light Chain

Chain B:

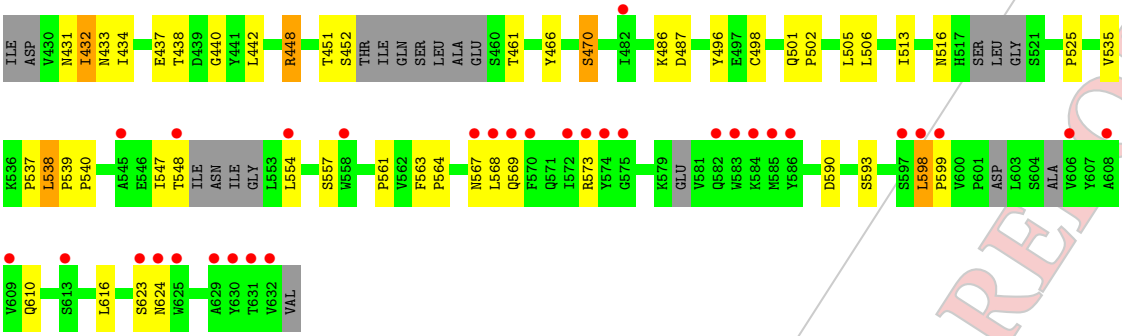
• Molecule 2: H6 scFv Light Chain

Chain E:

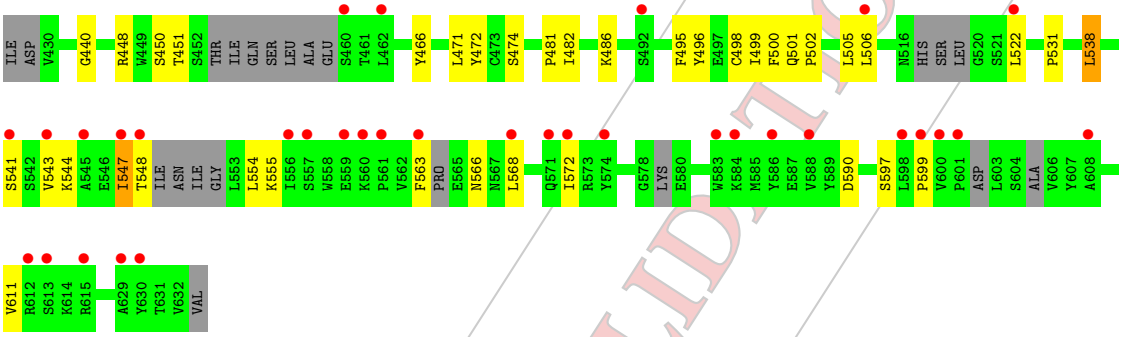


• Molecule 3: Leptin receptor

Chain C:



• Molecule 3: Leptin receptor



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	43.59Å 109.84Å 189.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.05 – 3.05 47.52 – 3.05	Depositor EDS
% Data completeness (in resolution range)	88.5 (95.05-3.05) 88.5 (47.52-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.238 , 0.274 0.243 , 0.283	Depositor DCC
R_{free} test set	841 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å^2)	66.4	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	6414	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: CL

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	0.55	0/944	0.72	0/1277
1	D	0.56	0/932	0.72	0/1262
2	B	0.49	0/811	0.75	0/1104
2	E	0.60	0/827	0.77	0/1125
3	C	0.44	0/1529	0.65	1/2077 (0.0%)
3	F	0.46	0/1523	0.66	0/2067
All	All	0.51	0/6566	0.70	1/8912 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	564	PRO	N-CA-CB	5.06	109.37	103.30

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	922	0	873	22	0
1	D	910	0	864	13	0
2	B	792	0	762	32	0
2	E	808	0	788	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1491	0	1461	30	0
3	F	1486	0	1455	22	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
All	All	6414	0	6203	118	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 (118) 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)
3:C:540:PRO:HA	3:C:561:PRO:HG3	1.52	0.89
3:F:501:GLN:HB3	3:F:502:PRO:HD3	1.53	0.88
2:B:6:GLN:NE2	2:B:89:CYS:SG	2.60	0.74
2:B:29:VAL:HG21	2:B:72:PHE:HZ	1.54	0.72
3:C:540:PRO:HA	3:C:561:PRO:CG	2.21	0.71
1:A:51:ILE:HD12	1:A:58:LYS:HG2	1.76	0.67
2:B:29:VAL:HG23	2:B:29:VAL:O	1.97	0.64
3:F:501:GLN:CB	3:F:502:PRO:HD3	2.24	0.64
1:A:100:GLN:HA	1:A:100:GLN:OE1	1.98	0.63
3:F:547:ILE:HD11	3:F:554:LEU:HD12	1.81	0.63
2:B:29:VAL:HG21	2:B:72:PHE:CZ	2.33	0.61
1:A:89:GLU:HG2	1:D:89:GLU:CD	2.20	0.61
3:F:547:ILE:O	3:F:548:THR:HG22	2.01	0.60
2:B:7:SER:CB	2:B:8:PRO:HD2	2.32	0.60
1:D:99:PHE:HB3	1:D:105:THR:HB	1.85	0.58
2:E:95:SER:O	3:F:472:TYR:OH	2.22	0.57
1:A:34:MET:SD	1:A:98:SER:OG	2.57	0.57
3:F:486:LYS:NZ	3:F:499:ILE:O	2.32	0.57
3:C:567:ASN:O	3:C:616:LEU:CB	2.52	0.57
3:C:432:ILE:HD13	3:C:513:ILE:HG12	1.86	0.56
2:B:91:GLN:OE1	2:B:94:ALA:N	2.31	0.56
1:A:101:GLU:HB2	3:C:470:SER:OG	2.05	0.55
2:B:7:SER:HB2	2:B:8:PRO:HD2	1.89	0.55
2:B:8:PRO:O	2:B:103:THR:HG23	2.07	0.54
3:C:461:THR:HG23	3:C:516:ASN:HB2	1.89	0.54
3:C:432:ILE:HD11	3:C:434:ILE:HD11	1.88	0.54
1:A:99:PHE:HB2	1:A:106:TYR:CD2	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:440:GLY:HA3	3:F:538:LEU:HD13	1.91	0.53
3:F:471:LEU:O	3:F:506:LEU:O	2.26	0.53
2:E:95:SER:CB	2:E:96:PRO:HD3	2.39	0.52
2:B:84:PHE:HA	2:B:105:LEU:HD21	1.90	0.52
3:C:548:THR:O	3:C:548:THR:HG23	2.10	0.52
3:F:486:LYS:HG3	3:F:500:PHE:CZ	2.44	0.52
3:C:501:GLN:HB3	3:C:502:PRO:HD3	1.91	0.52
2:B:95:SER:HB3	3:C:506:LEU:HD12	1.92	0.52
3:C:567:ASN:O	3:C:616:LEU:HB3	2.10	0.52
2:B:46:ARG:HH11	2:B:46:ARG:HB2	1.75	0.51
1:D:91:THR:HG22	1:D:115:VAL:H	1.74	0.51
1:D:34:MET:HB3	1:D:79:LEU:HD22	1.91	0.51
2:B:91:GLN:NE2	2:B:98:THR:OG1	2.44	0.51
2:B:67:GLY:HA3	2:B:72:PHE:HA	1.92	0.51
1:D:40:ALA:HB3	1:D:43:LYS:HB2	1.93	0.51
1:A:34:MET:HB3	1:A:79:LEU:HD22	1.91	0.51
3:F:481:PRO:HG2	3:F:482:ILE:HD12	1.93	0.50
3:F:544:LYS:HE2	3:F:544:LYS:HA	1.93	0.50
2:B:46:ARG:NH1	2:B:46:ARG:HB2	2.26	0.50
2:B:95:SER:HB2	2:B:96:PRO:HD3	1.93	0.50
2:E:11:LEU:HB3	2:E:105:LEU:HD12	1.94	0.50
1:A:62:ASP:HA	1:A:65:LYS:HG3	1.92	0.50
3:F:448:ARG:HA	3:F:496:TYR:O	2.11	0.50
3:C:590:ASP:HB3	3:C:593:SER:HB2	1.94	0.49
1:D:17:SER:OG	1:D:84:ASN:ND2	2.42	0.49
1:A:87:ARG:NH2	1:D:87:ARG:HD2	2.26	0.49
1:A:87:ARG:CZ	1:D:87:ARG:HD2	2.43	0.49
3:C:431:ASN:ND2	3:C:452:SER:OG	2.43	0.49
3:C:440:GLY:HA3	3:C:538:LEU:HD13	1.95	0.48
1:D:91:THR:HG22	1:D:115:VAL:N	2.28	0.48
1:A:40:ALA:HB3	1:A:43:LYS:HB2	1.95	0.48
3:F:547:ILE:HD11	3:F:554:LEU:CD1	2.43	0.48
2:E:67:GLY:HA3	2:E:72:PHE:HA	1.96	0.48
3:C:569:GLN:HG2	3:C:616:LEU:HA	1.97	0.47
1:A:52:SER:HB2	1:A:57:ASN:HB2	1.97	0.47
1:D:34:MET:HG2	1:D:72:ARG:NH2	2.30	0.47
1:A:67:ARG:HB3	1:A:84:ASN:O	2.15	0.47
1:A:17:SER:HA	1:A:83:MET:O	2.14	0.46
3:C:537:PRO:HD2	3:C:623:SER:HB2	1.96	0.46
3:C:442:LEU:HD13	3:C:505:LEU:HD11	1.98	0.46
2:E:38:GLN:HB2	2:E:48:LEU:HD11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:572:ILE:HG12	3:F:611:VAL:HG13	1.96	0.46
1:A:101:GLU:HB2	3:C:470:SER:CB	2.46	0.46
2:B:17:GLU:OE2	2:B:18:ARG:N	2.49	0.46
2:B:39:GLN:HG3	2:B:45:PRO:HG3	1.98	0.46
1:A:101:GLU:CB	3:C:470:SER:OG	2.64	0.46
1:D:52:SER:HB2	1:D:57:ASN:HB2	1.98	0.45
2:B:49:ILE:HD13	2:B:55:ARG:HB3	1.98	0.45
3:C:573:ARG:NH2	3:C:610:GLN:OE1	2.50	0.45
3:C:432:ILE:HD12	3:C:432:ILE:HA	1.85	0.45
3:F:505:LEU:HD23	3:F:531:PRO:HB2	1.99	0.45
3:C:539:PRO:HB3	3:C:624:ASN:O	2.16	0.44
1:A:12:VAL:HG22	1:A:16:ARG:HB2	1.98	0.44
2:B:21:LEU:HD23	2:B:103:THR:HG21	1.99	0.44
2:B:7:SER:OG	2:B:8:PRO:HD2	2.17	0.44
1:A:100:GLN:HB3	1:A:103:TYR:CZ	2.53	0.43
1:A:88:ALA:O	1:A:91:THR:HG23	2.18	0.43
3:C:466:TYR:CD1	3:C:486:LYS:HG2	2.53	0.43
3:C:599:PRO:HD2	3:F:599:PRO:CG	2.48	0.43
2:B:80:GLU:HB3	2:B:81:PRO:HD2	2.00	0.43
3:C:554:LEU:O	3:C:598:LEU:N	2.49	0.43
3:F:466:TYR:CD1	3:F:486:LYS:HG2	2.53	0.43
2:E:11:LEU:N	2:E:104:LYS:O	2.51	0.43
1:A:39:GLN:NE2	2:B:39:GLN:OE1	2.46	0.43
3:F:466:TYR:CE1	3:F:486:LYS:HG2	2.53	0.43
2:B:8:PRO:HB3	2:B:11:LEU:HD23	2.01	0.43
3:C:623:SER:OG	3:C:624:ASN:N	2.51	0.43
2:E:23:CYS:HB2	2:E:36:TRP:CH2	2.54	0.43
2:B:96:PRO:O	2:B:98:THR:HG23	2.18	0.42
1:A:99:PHE:CE2	1:A:100:GLN:HG2	2.54	0.42
2:B:38:GLN:HB2	2:B:48:LEU:HD11	2.01	0.42
1:A:99:PHE:CZ	1:A:100:GLN:HG2	2.54	0.42
2:B:87:TYR:CE1	2:B:105:LEU:HD22	2.55	0.42
2:B:11:LEU:HA	2:B:11:LEU:HD22	1.93	0.42
3:C:438:THR:HB	3:C:535:VAL:HG22	2.01	0.42
1:D:91:THR:CG2	1:D:115:VAL:H	2.33	0.42
1:D:62:ASP:OD1	1:D:65:LYS:NZ	2.52	0.42
2:B:80:GLU:HB3	2:B:81:PRO:CD	2.50	0.41
3:F:450:SER:HB2	3:F:495:PHE:CD1	2.54	0.41
2:B:21:LEU:CD2	2:B:103:THR:HG21	2.50	0.41
3:C:599:PRO:HD2	3:F:599:PRO:HG2	2.02	0.41
2:B:7:SER:HB2	2:B:8:PRO:CD	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:55:ARG:HD3	2:E:59:ILE:HG22	2.02	0.41
2:B:7:SER:CB	2:B:8:PRO:CD	2.99	0.41
2:E:36:TRP:HB2	2:E:49:ILE:HB	2.01	0.41
2:B:55:ARG:NH1	2:B:61:ASP:HA	2.35	0.41
3:F:555:LYS:HA	3:F:597:SER:HA	2.03	0.41
3:C:432:ILE:HG21	3:C:525:PRO:O	2.21	0.41
2:E:29:VAL:HG13	2:E:93:ALA:HB2	2.03	0.40
3:F:501:GLN:CB	3:F:502:PRO:CD	2.98	0.40
3:C:448:ARG:HA	3:C:496:TYR:O	2.22	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	118/122 (97%)	111 (94%)	6 (5%)	1 (1%)	19	50
1	D	115/122 (94%)	109 (95%)	5 (4%)	1 (1%)	17	47
2	B	104/116 (90%)	92 (88%)	7 (7%)	5 (5%)	2	11
2	E	105/116 (90%)	97 (92%)	7 (7%)	1 (1%)	15	45
3	C	172/206 (84%)	161 (94%)	9 (5%)	2 (1%)	13	40
3	F	169/206 (82%)	161 (95%)	7 (4%)	1 (1%)	25	55
All	All	783/888 (88%)	731 (93%)	41 (5%)	11 (1%)	11	36

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	8	PRO
2	B	53	SER
2	B	83	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	101	GLU
3	C	563	PHE
3	F	590	ASP
2	B	7	SER
2	B	52	ALA
2	E	69	GLY
1	A	99	PHE
3	C	432	ILE

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	96/98 (98%)	91 (95%)	5 (5%)	23 52
1	D	96/98 (98%)	89 (93%)	7 (7%)	14 40
2	B	85/97 (88%)	70 (82%)	15 (18%)	2 7
2	E	88/97 (91%)	72 (82%)	16 (18%)	1 6
3	C	173/191 (91%)	161 (93%)	12 (7%)	15 42
3	F	173/191 (91%)	162 (94%)	11 (6%)	17 44
All	All	711/772 (92%)	645 (91%)	66 (9%)	9 29

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	22	CYS
1	A	74	ASN
1	A	98	SER
1	A	101	GLU
2	B	1	GLU
2	B	4	LEU
2	B	5	THR
2	B	11	LEU
2	B	12	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	13	LEU
2	B	17	GLU
2	B	28	SER
2	B	39	GLN
2	B	55	ARG
2	B	57	THR
2	B	73	THR
2	B	75	THR
2	B	91	GLN
2	B	105	LEU
3	C	433	ASN
3	C	437	GLU
3	C	448	ARG
3	C	451	THR
3	C	470	SER
3	C	487	ASP
3	C	498	CYS
3	C	538	LEU
3	C	547	ILE
3	C	557	SER
3	C	568	LEU
3	C	598	LEU
1	D	11	VAL
1	D	17	SER
1	D	22	CYS
1	D	25	SER
1	D	63	SER
1	D	69	THR
1	D	116	SER
2	E	1	GLU
2	E	3	VAL
2	E	18	ARG
2	E	20	THR
2	E	22	SER
2	E	28	SER
2	E	31	SER
2	E	53	SER
2	E	64	SER
2	E	71	ASP
2	E	75	THR
2	E	91	GLN
2	E	95	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	104	LYS
2	E	105	LEU
2	E	107	ILE
3	F	451	THR
3	F	474	SER
3	F	498	CYS
3	F	522	LEU
3	F	538	LEU
3	F	541	SER
3	F	543	VAL
3	F	547	ILE
3	F	563	PHE
3	F	566	ASN
3	F	568	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	120/122 (98%)	-0.17	0 100 100	38, 51, 70, 87	0
1	D	117/122 (95%)	-0.36	0 100 100	34, 44, 59, 69	0
2	B	106/116 (91%)	0.14	2 (1%) 66 43	54, 83, 133, 159	0
2	E	107/116 (92%)	-0.16	0 100 100	34, 53, 77, 85	0
3	C	186/206 (90%)	0.87	32 (17%) 1 0	58, 94, 175, 205	0
3	F	185/206 (89%)	0.88	34 (18%) 1 0	47, 96, 151, 177	0
All	All	821/888 (92%)	0.32	68 (8%) 11 4	34, 67, 152, 205	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	547	ILE	9.1
3	C	584	LYS	7.8
3	C	575	GLY	6.9
3	C	599	PRO	6.8
3	C	632	VAL	6.5
3	F	572	ILE	5.7
3	C	613	SER	5.7
3	C	585	MET	5.6
3	F	557	SER	5.3
3	C	598	LEU	5.0
3	F	629	ALA	4.8
3	C	567	ASN	4.6
3	F	586	TYR	4.6
3	F	599	PRO	4.6
3	C	624	ASN	4.5
3	C	625	TRP	4.4
3	C	608	ALA	4.2
3	F	584	LYS	4.1
3	C	583	TRP	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	630	TYR	4.1
3	F	460	SER	3.9
3	C	569	GLN	3.8
2	B	77	SER	3.8
3	F	561	PRO	3.8
3	C	548	THR	3.6
3	C	606	VAL	3.5
3	F	559	GLU	3.5
3	C	573	ARG	3.5
3	F	522	LEU	3.4
3	C	609	VAL	3.3
3	F	545	ALA	3.2
3	C	597	SER	3.2
3	C	582	GLN	3.2
3	C	630	TYR	3.2
3	F	571	GLN	3.1
3	F	615	ARG	3.1
3	C	629	ALA	3.1
3	F	563	PHE	3.1
3	F	600	VAL	3.0
3	C	631	THR	3.0
3	F	556	ILE	3.0
3	F	543	VAL	3.0
2	B	13	LEU	3.0
3	F	608	ALA	3.0
3	C	586	TYR	3.0
3	F	560	LYS	2.9
3	F	548	THR	2.7
3	C	545	ALA	2.7
3	F	598	LEU	2.6
3	F	601	PRO	2.6
3	C	570	PHE	2.6
3	C	574	TYR	2.6
3	F	541	SER	2.5
3	C	568	LEU	2.5
3	F	568	LEU	2.4
3	F	492	SER	2.4
3	F	612	ARG	2.4
3	C	554	LEU	2.4
3	C	482	ILE	2.4
3	C	623	SER	2.4
3	F	583	TRP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	574	TYR	2.2
3	C	558	TRP	2.1
3	F	588	VAL	2.1
3	F	462	LEU	2.1
3	F	613	SER	2.1
3	F	506	LEU	2.0
3	C	572	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

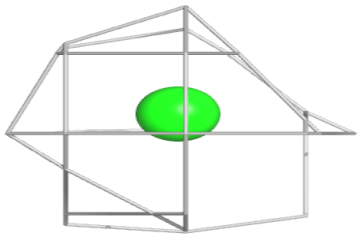
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

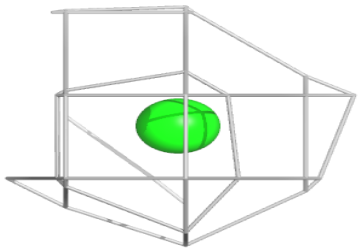
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	A	201	1/1	0.82	0.18	79,79,79,79	0
4	CL	C	701	1/1	0.92	0.19	75,75,75,75	0
4	CL	D	201	1/1	0.93	0.11	66,66,66,66	0
4	CL	A	202	1/1	0.96	0.37	67,67,67,67	0
4	CL	E	201	1/1	0.99	0.15	56,56,56,56	0

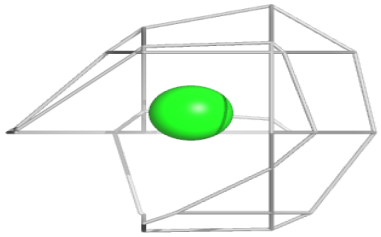
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CL A 201:

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

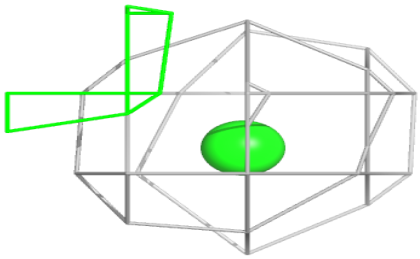


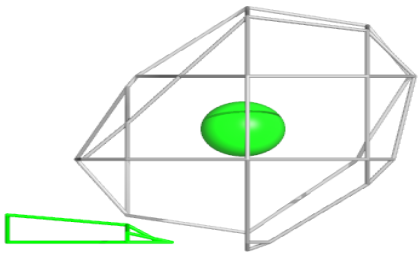


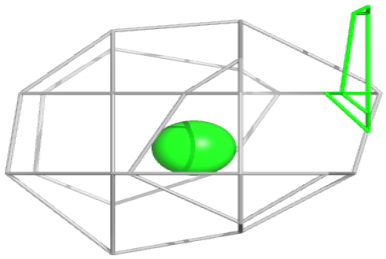


Electron density around CL C 701:

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

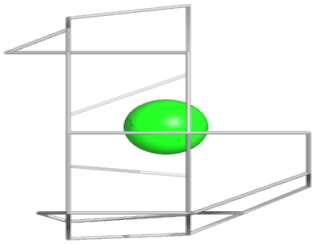


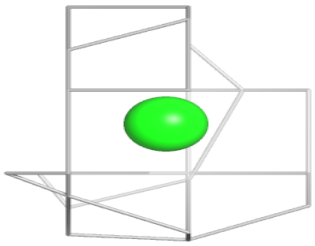


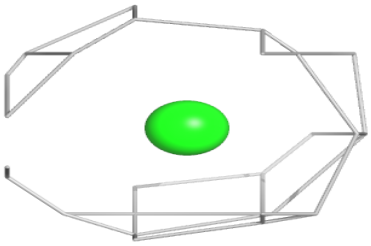


Electron density around CL D 201:

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

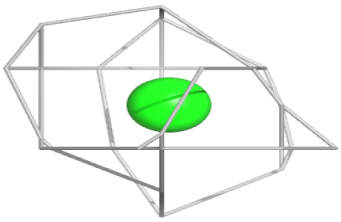


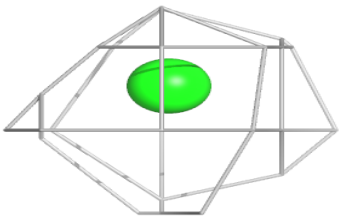


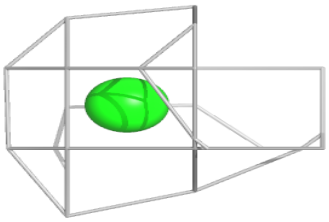


Electron density around CL A 202:

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

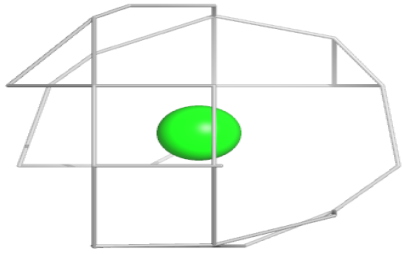


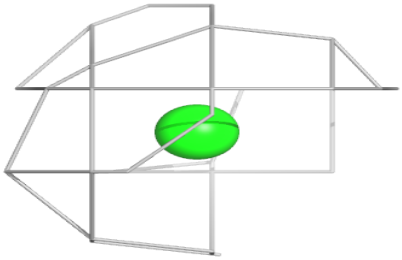


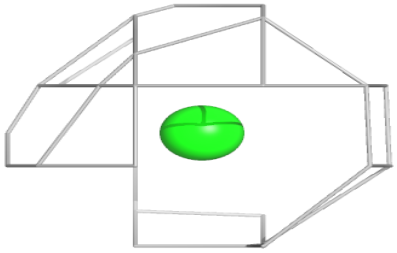


Electron density around CL E 201:

$2mF_o$-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.