



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 04:12 PM BST

PDB ID : 2BXE
Title : Human serum albumin complexed with diflunisal
Authors : Ghuman, J.; Zunszain, P.A.; Petitpas, I.; Bhattacharya, A.A.; Curry, S.
Deposited on : 2005-07-26
Resolution : 2.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
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

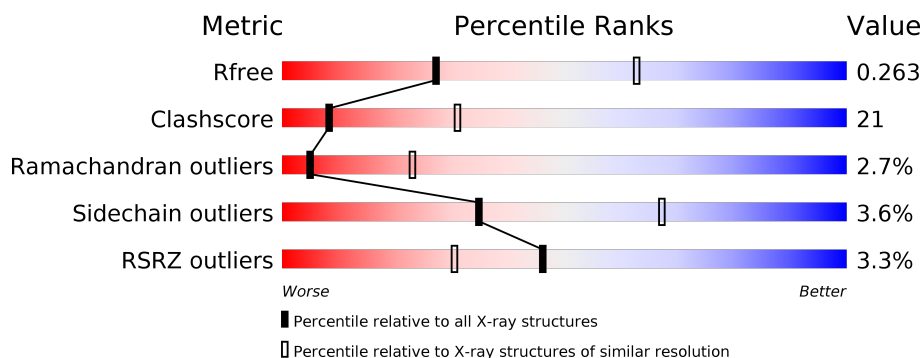
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 $\leq 5\%$. 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	585	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>33%</div> <div>• •</div> </div> </div>
1	B	585	<div> <div>4%</div> <div> <div></div> <div>58%</div> <div>35%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

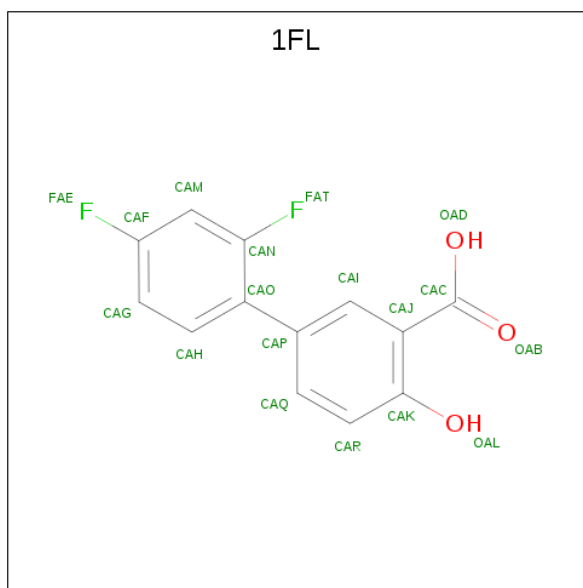
There are 2 unique types of molecules in this entry. The entry contains 8710 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERUM ALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	0	0
			4344	2743	722	839	40			
1	B	566	Total	C	N	O	S	0	0	0
			4258	2692	710	816	40			

- Molecule 2 is 5-(2,4-DIFLUOROPHENYL)-2-HYDROXY-BENZOIC ACID (three-letter code: 1FL) (formula: C₁₃H₈F₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	O	0	0
			18	13	2	3		
2	A	1	Total	C	F	O	0	0
			18	13	2	3		
2	A	1	Total	C	F	O	0	0
			18	13	2	3		
2	B	1	Total	C	F	O	0	0
			18	13	2	3		

Continued on next page...

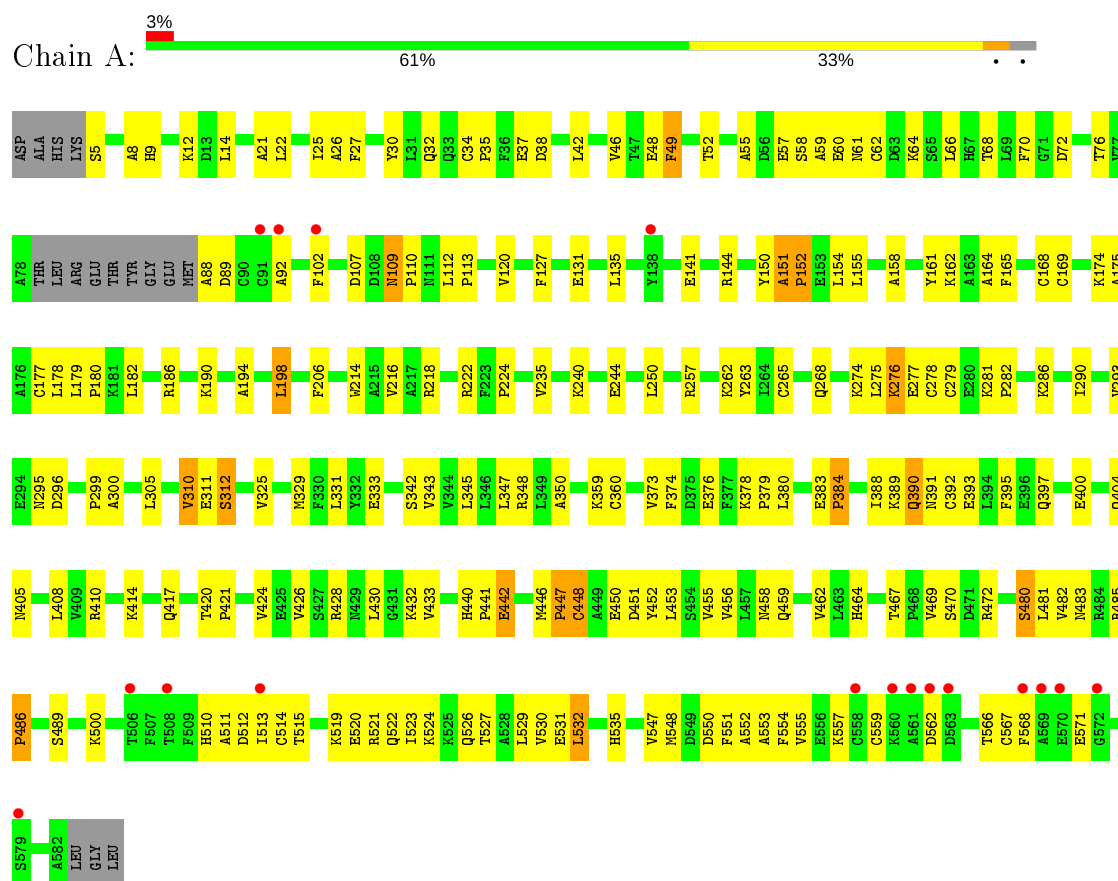
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	F	O	0	0
			18	13	2	3		
2	B	1	Total	C	F	O	0	0
			18	13	2	3		

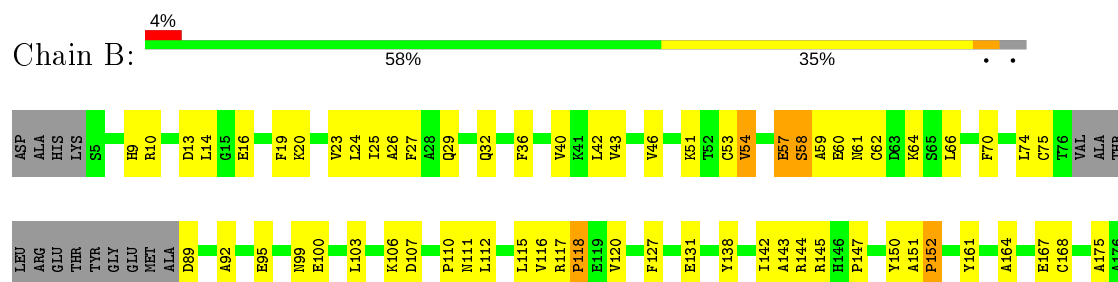
3 Residue-property plots [i](#)

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

• Molecule 1: SERUM ALBUMIN



• Molecule 1: SERUM ALBUMIN



P568	K574	K575	L576	A577	A578	S579	A582	LEU	GLY	LEU	P499	F502	N503	A504	F507	T508	F509	H510	A511	D512	L513	G514	T515	L516	S517	E518	R521	Q522	T523	K524	K525	Q526	V530	E531	L532	V533	K534	H535	K536	P537	T540	K541	E542	Q543	L544	K545	A546	V547	M548	A552	V555	E556	K557	C558	G559	K560	A561	D562	D563	K564	E565	T566	C567	C177	L178	L179	P180	K181	L182	A194	K195	Q196	F206	R209	W214	R222	P223	P224	D237	L238	C245	L250	L260	Y263	L264	C265	Q268	S272	S273	K274	L275	K276	K281	E285	K286	C289	L290	A291	E292	V293	E294	N295	D296	A300	L305	S312	V315	L331	Y332	E333	R337	S342	V343	V344	L345	R348	L349	A350	A363	A364	D365	P366	H367	E368	G369	Y370	A371	K372	V373	F374	D375	E376	F377	K378	P379	L380	E383	P384	L387	I388	F395	E396	Q397	L398	G399	E400	Y401	K402	F403	Q404	N405	L408	V409	R410	Y411	T412	K413	K414	V415	P416	V418	S419	T420	L423	V424	R428	M429	K432	V433	G434	C438	K439	H440	P441	E442	A443	R444	M446	P447	C448	A449	E450	D451	Y452	L453	S454	V455	V456	Q459	V462	L463	V469	S470	S480	L481	V482	N483	R484	R485	P486	C487	F488	S489	V498
------	------	------	------	------	------	------	------	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.41Å 55.53Å 120.52Å 81.54° 90.09° 65.93°	Depositor
Resolution (Å)	38.22 – 2.95 38.22 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.4 (38.22-2.95) 98.4 (38.22-2.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.270 0.222 , 0.263	Depositor DCC
R_{free} test set	1296 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8710	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1FL

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	0.45	0/4428	0.66	0/6011
1	B	0.45	0/4339	0.65	0/5895
All	All	0.45	0/8767	0.65	0/11906

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

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	4344	0	4056	159	0
1	B	4258	0	3962	193	0
2	A	54	0	18	3	0
2	B	54	0	18	7	0
All	All	8710	0	8054	352	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 21.

All (352) 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:433:VAL:HG22	1:A:452:TYR:HD2	1.06	1.10
1:A:433:VAL:HG22	1:A:452:TYR:CD2	1.91	1.05
1:B:433:VAL:HG22	1:B:452:TYR:HD2	1.30	0.95
1:B:433:VAL:HG22	1:B:452:TYR:CD2	2.02	0.93
1:B:222:ARG:HD3	2:B:2003:1FL:FAE	1.59	0.91
1:B:120:VAL:HG21	1:B:175:ALA:HA	1.53	0.88
1:A:222:ARG:HD3	2:A:2003:1FL:FAE	1.63	0.88
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.55	0.87
1:B:364:ALA:O	1:B:366:PRO:HD3	1.75	0.87
1:B:95:GLU:OE1	1:B:99:ASN:HB2	1.74	0.85
1:B:57:GLU:HG3	1:B:58:SER:H	1.42	0.85
1:B:567:CYS:SG	1:B:571:GLU:HB2	2.16	0.85
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.56	0.85
1:A:276:LYS:HD2	1:A:277:GLU:H	1.42	0.83
1:A:222:ARG:HG3	1:A:295:ASN:OD1	1.79	0.82
1:B:540:THR:HG23	1:B:543:GLN:H	1.42	0.81
1:A:120:VAL:HG11	1:A:174:LYS:HB2	1.61	0.81
1:B:222:ARG:HG3	1:B:295:ASN:OD1	1.79	0.81
1:A:417:GLN:OE1	1:A:417:GLN:N	2.13	0.80
1:A:424:VAL:O	1:A:428:ARG:HG3	1.82	0.80
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.60	0.80
1:A:135:LEU:HD11	1:A:162:LYS:HG3	1.64	0.79
1:A:390:GLN:O	1:A:393:GLU:N	2.13	0.79
1:B:281:LYS:HD2	1:B:285:GLU:HG2	1.65	0.79
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.66	0.78
1:A:550:ASP:O	1:A:554:PHE:HD1	1.66	0.78
1:A:182:LEU:O	1:A:186:ARG:HG2	1.84	0.78
1:A:547:VAL:HG12	1:A:551:PHE:HE1	1.46	0.77
1:A:61:ASN:HD22	1:A:64:LYS:HE3	1.50	0.77
1:B:345:LEU:HD22	1:B:446:MET:CE	2.15	0.77
1:B:446:MET:HB3	1:B:447:PRO:HD3	1.69	0.75
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.27	0.74
1:A:107:ASP:OD2	1:A:110:PRO:HA	1.87	0.74
1:B:265:CYS:O	1:B:268:GLN:HG3	1.88	0.74
1:A:547:VAL:CG1	1:A:551:PHE:HE1	2.00	0.74
1:B:110:PRO:HB2	1:B:112:LEU:CD2	2.17	0.74
1:A:169:CYS:HA	1:A:174:LYS:HD3	1.71	0.73
1:A:414:LYS:O	1:A:472:ARG:NH1	2.23	0.72
1:B:127:PHE:O	1:B:131:GLU:HB3	1.91	0.71
1:B:106:LYS:HD3	1:B:147:PRO:HB2	1.71	0.71
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.73	0.70
1:A:376:GLU:O	1:A:379:PRO:HD2	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.55	0.70
1:B:499:PRO:HB3	1:B:535:HIS:O	1.89	0.70
1:A:400:GLU:O	1:A:404:GLN:HG3	1.91	0.70
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.75	0.69
1:B:194:ALA:HB1	1:B:455:VAL:CG1	2.22	0.69
1:B:214:TRP:CD1	1:B:343:VAL:HG11	2.27	0.69
1:B:285:GLU:O	1:B:289:CYS:HB2	1.93	0.69
1:B:561:ALA:HB3	1:B:563:ASP:OD1	1.93	0.69
1:B:483:ASN:O	1:B:486:PRO:HD2	1.92	0.68
1:B:206:PHE:CD2	1:B:481:LEU:HD22	2.29	0.68
1:A:276:LYS:CD	1:A:277:GLU:H	2.06	0.68
1:B:510:HIS:HA	1:B:568:PHE:CD2	2.28	0.68
1:A:151:ALA:HB3	1:A:152:PRO:CD	2.24	0.68
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.76	0.68
1:A:281:LYS:HB2	1:A:282:PRO:CD	2.25	0.67
1:B:32:GLN:NE2	1:B:110:PRO:HG2	2.10	0.67
1:B:260:LEU:O	1:B:260:LEU:HD23	1.94	0.67
1:A:35:PRO:HD2	1:A:38:ASP:OD2	1.95	0.67
1:A:305:LEU:HD21	1:A:333:GLU:HB3	1.77	0.66
1:B:110:PRO:HB2	1:B:112:LEU:HD22	1.76	0.66
1:B:10:ARG:O	1:B:14:LEU:HD23	1.95	0.66
1:B:344:VAL:HG22	1:B:451:ASP:OD1	1.96	0.65
1:A:66:LEU:O	1:A:70:PHE:HD1	1.78	0.65
1:B:565:GLU:O	1:B:568:PHE:HB3	1.96	0.65
1:B:290:ILE:O	1:B:293:VAL:HG12	1.98	0.64
1:A:483:ASN:O	1:A:486:PRO:HD2	1.98	0.64
1:A:276:LYS:HD3	1:A:277:GLU:HG2	1.81	0.63
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.33	0.63
1:A:529:LEU:HD22	1:A:548:MET:CE	2.28	0.63
1:B:66:LEU:O	1:B:70:PHE:HD1	1.82	0.63
1:B:400:GLU:O	1:B:404:GLN:HG3	1.97	0.62
1:B:441:PRO:O	1:B:443:ALA:N	2.31	0.62
1:B:151:ALA:HB3	1:B:152:PRO:CD	2.28	0.62
1:A:198:LEU:HD22	1:A:455:VAL:HA	1.82	0.61
1:B:558:CYS:SG	1:B:571:GLU:HB3	2.40	0.61
1:A:240:LYS:O	1:A:244:GLU:HG3	2.01	0.61
1:A:281:LYS:HB2	1:A:282:PRO:HD2	1.82	0.61
1:B:9:HIS:CD2	1:B:13:ASP:OD2	2.54	0.60
1:B:116:VAL:O	1:B:118:PRO:HD3	2.01	0.60
1:A:408:LEU:HD11	1:A:526:GLN:HB3	1.83	0.60
1:A:224:PRO:HB2	1:A:299:PRO:HD3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:LYS:O	1:A:523:ILE:HG13	2.02	0.60
1:B:42:LEU:O	1:B:46:VAL:HG23	2.02	0.59
1:A:150:TYR:OH	2:A:2003:1FL:OAD	2.19	0.59
1:B:263:TYR:C	1:B:263:TYR:CD2	2.75	0.59
1:A:426:VAL:O	1:A:430:LEU:HG	2.03	0.59
1:B:441:PRO:C	1:B:443:ALA:H	2.04	0.59
1:B:179:LEU:HB2	1:B:180:PRO:HD3	1.85	0.59
1:B:32:GLN:HE22	1:B:110:PRO:CG	2.16	0.59
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.38	0.58
1:B:29:GLN:HG2	1:B:143:ALA:O	2.03	0.58
1:B:510:HIS:HA	1:B:568:PHE:HD2	1.66	0.58
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.86	0.58
1:B:120:VAL:HG21	1:B:175:ALA:CA	2.31	0.58
1:B:57:GLU:OE1	1:B:57:GLU:HA	2.03	0.58
1:A:450:GLU:HG3	1:A:450:GLU:O	2.03	0.57
1:B:513:ILE:HD12	1:B:555:VAL:HG23	1.85	0.57
1:B:417:GLN:H	1:B:417:GLN:CD	2.07	0.57
1:B:424:VAL:O	1:B:428:ARG:HG3	2.04	0.57
1:B:518:GLU:O	1:B:522:GLN:HG3	2.04	0.57
1:B:420:THR:HG23	1:B:530:VAL:HG11	1.87	0.57
1:A:510:HIS:HA	1:A:568:PHE:CB	2.35	0.57
1:B:532:LEU:HD21	1:B:547:VAL:HG11	1.87	0.57
1:B:27:PHE:CD2	1:B:74:LEU:HD21	2.40	0.56
1:B:117:ARG:NH2	1:B:182:LEU:HB3	2.19	0.56
1:B:32:GLN:NE2	1:B:110:PRO:CG	2.67	0.56
1:B:424:VAL:HG23	1:B:530:VAL:HG21	1.86	0.56
1:A:194:ALA:HB1	1:A:455:VAL:CG1	2.36	0.56
1:A:345:LEU:HD23	1:A:446:MET:CE	2.35	0.56
1:B:405:ASN:O	1:B:409:VAL:HG23	2.04	0.56
1:B:348:ARG:NH2	1:B:450:GLU:OE2	2.30	0.56
1:A:5:SER:HA	1:A:62:CYS:O	2.05	0.56
1:B:502:PHE:HE2	1:B:507:PHE:HB2	1.70	0.56
1:B:376:GLU:O	1:B:379:PRO:HD2	2.06	0.56
1:B:543:GLN:O	1:B:546:ALA:HB3	2.06	0.55
1:B:513:ILE:CD1	1:B:555:VAL:HG23	2.36	0.55
1:B:107:ASP:HB3	1:B:110:PRO:HG3	1.87	0.55
1:B:260:LEU:HD22	2:B:2003:1FL:HAR	1.87	0.55
1:B:441:PRO:C	1:B:443:ALA:N	2.58	0.55
1:B:408:LEU:HD11	1:B:526:GLN:HB3	1.89	0.55
1:B:151:ALA:CB	1:B:152:PRO:HD3	2.35	0.55
1:B:168:CYS:SG	1:B:177:CYS:C	2.84	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:MET:CB	1:B:447:PRO:HD3	2.37	0.55
1:A:325:VAL:O	1:A:329:MET:HG3	2.07	0.55
1:A:8:ALA:O	1:A:12:LYS:HG2	2.07	0.54
1:A:550:ASP:O	1:A:554:PHE:CD1	2.55	0.54
1:B:558:CYS:SG	1:B:571:GLU:CB	2.95	0.54
1:B:502:PHE:CE2	1:B:507:PHE:HB2	2.42	0.54
1:A:14:LEU:HD13	1:A:22:LEU:HD12	1.90	0.54
1:B:305:LEU:HD21	1:B:333:GLU:HB3	1.90	0.54
1:B:57:GLU:O	1:B:58:SER:C	2.46	0.54
1:A:380:LEU:O	1:A:384:PRO:HD2	2.08	0.53
1:A:222:ARG:C	1:A:224:PRO:HD3	2.29	0.53
1:A:547:VAL:CG1	1:A:551:PHE:CE1	2.88	0.53
1:B:117:ARG:HH22	1:B:182:LEU:HB3	1.73	0.53
1:A:276:LYS:CD	1:A:277:GLU:HG2	2.38	0.53
1:A:89:ASP:O	1:A:92:ALA:HB3	2.09	0.53
1:B:345:LEU:HD22	1:B:446:MET:HE1	1.89	0.53
1:A:331:LEU:HD13	1:A:350:ALA:HB2	1.90	0.53
1:B:331:LEU:HD13	1:B:350:ALA:HB2	1.91	0.53
1:A:522:GLN:O	1:A:526:GLN:HG3	2.09	0.53
1:B:567:CYS:SG	1:B:571:GLU:CB	2.95	0.53
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.90	0.52
1:B:115:LEU:HG	1:B:145:ARG:CZ	2.39	0.52
1:B:516:LEU:HD12	1:B:516:LEU:H	1.74	0.52
1:B:32:GLN:HE22	1:B:110:PRO:HG3	1.74	0.52
1:B:440:HIS:HB3	1:B:441:PRO:CD	2.39	0.52
1:B:480:SER:OG	1:B:483:ASN:HB2	2.09	0.52
1:A:279:CYS:HA	1:A:286:LYS:CD	2.40	0.52
1:A:49:PHE:O	1:A:49:PHE:HD2	1.93	0.52
1:A:464:HIS:HE1	1:A:470:SER:H	1.58	0.52
1:B:540:THR:HG22	1:B:543:GLN:HB2	1.91	0.52
1:A:151:ALA:CB	1:A:152:PRO:HD3	2.36	0.51
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.92	0.51
1:A:480:SER:OG	1:A:483:ASN:HB2	2.10	0.51
1:A:342:SER:HB2	1:A:451:ASP:OD2	2.10	0.51
1:B:25:ILE:O	1:B:29:GLN:HG3	2.10	0.51
1:A:161:TYR:O	1:A:164:ALA:HB3	2.11	0.51
1:B:26:ALA:HB2	1:B:250:LEU:HD12	1.92	0.51
1:A:9:HIS:C	1:A:9:HIS:HD1	2.14	0.51
1:B:432:LYS:O	1:B:433:VAL:C	2.47	0.51
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.40	0.51
1:B:237:ASP:CB	1:B:260:LEU:HD12	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:VAL:CG1	1:B:423:LEU:HG	2.41	0.50
1:B:51:LYS:HA	1:B:54:VAL:HG23	1.92	0.50
1:B:408:LEU:O	1:B:412:THR:OG1	2.20	0.50
1:A:531:GLU:HA	1:A:531:GLU:OE1	2.12	0.50
1:A:464:HIS:CE1	1:A:469:VAL:H	2.30	0.50
1:A:343:VAL:O	1:A:347:LEU:HG	2.12	0.50
1:B:456:VAL:O	1:B:459:GLN:N	2.42	0.50
1:B:36:PHE:O	1:B:40:VAL:HG23	2.11	0.50
1:B:535:HIS:O	1:B:537:PRO:HD3	2.11	0.50
1:A:420:THR:O	1:A:424:VAL:HG23	2.11	0.50
1:B:409:VAL:O	1:B:413:LYS:HG3	2.12	0.49
1:A:345:LEU:HD23	1:A:446:MET:HE1	1.94	0.49
1:B:150:TYR:HB2	1:B:196:GLN:HG2	1.94	0.49
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.95	0.49
1:A:186:ARG:O	1:A:190:LYS:HG3	2.12	0.49
1:B:535:HIS:C	1:B:537:PRO:HD3	2.31	0.49
1:A:447:PRO:O	1:A:448:CYS:C	2.50	0.49
1:B:384:PRO:O	1:B:388:ILE:HG12	2.13	0.49
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.76	0.49
1:A:42:LEU:O	1:A:46:VAL:HG23	2.12	0.49
1:B:100:GLU:HG2	1:B:103:LEU:HD12	1.93	0.49
1:A:417:GLN:CD	1:A:417:GLN:H	2.08	0.49
1:A:49:PHE:CD2	1:A:49:PHE:O	2.66	0.49
1:B:222:ARG:HA	1:B:295:ASN:OD1	2.13	0.49
1:B:552:ALA:O	1:B:555:VAL:HG12	2.13	0.49
1:A:551:PHE:O	1:A:552:ALA:C	2.50	0.48
1:A:512:ASP:O	1:A:515:THR:HG22	2.14	0.48
1:B:408:LEU:HD22	1:B:530:VAL:HG22	1.95	0.48
1:A:155:LEU:O	1:A:158:ALA:HB3	2.13	0.48
1:B:417:GLN:N	1:B:417:GLN:CD	2.66	0.48
1:B:576:VAL:HA	1:B:579:SER:HB2	1.94	0.48
1:A:279:CYS:HA	1:A:286:LYS:HD2	1.96	0.48
1:A:342:SER:HB3	1:A:447:PRO:HA	1.94	0.48
1:B:66:LEU:O	1:B:70:PHE:CD1	2.64	0.48
1:A:165:PHE:CE1	1:A:178:LEU:HD21	2.48	0.48
1:B:481:LEU:N	2:B:2002:1FL:OAB	2.42	0.48
1:B:498:VAL:O	1:B:498:VAL:HG23	2.14	0.48
1:A:388:ILE:O	1:A:389:LYS:C	2.52	0.48
1:B:453:LEU:HD22	2:B:2001:1FL:HAQ	1.96	0.48
1:A:27:PHE:CE2	1:A:70:PHE:HD2	2.32	0.47
1:B:237:ASP:HB3	1:B:260:LEU:HD12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:SER:HB3	1:B:447:PRO:HA	1.95	0.47
1:B:483:ASN:O	1:B:486:PRO:CD	2.62	0.47
1:A:26:ALA:HB2	1:A:250:LEU:HD12	1.96	0.47
1:A:275:LEU:HD23	1:A:293:VAL:HG11	1.96	0.47
1:B:274:LYS:CE	1:B:296:ASP:HA	2.44	0.47
1:A:141:GLU:OE1	1:A:144:ARG:HD3	2.14	0.47
1:A:168:CYS:SG	1:A:177:CYS:C	2.93	0.47
1:A:66:LEU:O	1:A:70:PHE:CD1	2.65	0.47
1:A:218:ARG:HD3	1:A:343:VAL:HG21	1.97	0.47
1:B:542:GLU:OE1	1:B:542:GLU:HA	2.14	0.47
1:B:453:LEU:CD2	2:B:2001:1FL:HAQ	2.44	0.47
1:A:550:ASP:O	1:A:553:ALA:HB3	2.15	0.47
1:B:260:LEU:C	1:B:260:LEU:HD23	2.35	0.47
1:B:9:HIS:HD2	1:B:13:ASP:OD2	1.96	0.47
1:B:540:THR:HG22	1:B:543:GLN:CG	2.45	0.47
1:A:32:GLN:HG2	1:A:144:ARG:O	2.15	0.47
1:A:532:LEU:O	1:A:535:HIS:HB3	2.15	0.47
1:B:521:ARG:O	1:B:525:LYS:HG3	2.15	0.46
1:A:348:ARG:HG3	1:A:482:VAL:HG12	1.96	0.46
1:A:88:ALA:O	1:A:89:ASP:C	2.53	0.46
1:B:384:PRO:HB2	1:B:446:MET:SD	2.55	0.46
1:B:151:ALA:CB	1:B:152:PRO:CD	2.93	0.46
1:B:398:LEU:HB3	1:B:402:LYS:HB2	1.96	0.46
1:B:138:TYR:O	1:B:142:ILE:HG12	2.14	0.46
1:A:390:GLN:O	1:A:392:CYS:N	2.49	0.46
1:A:206:PHE:CZ	1:A:481:LEU:HB2	2.51	0.46
1:A:420:THR:HB	1:A:421:PRO:HD3	1.97	0.46
1:B:312:SER:O	1:B:315:VAL:HG23	2.16	0.46
1:A:127:PHE:CE1	1:A:131:GLU:HG3	2.51	0.45
1:A:265:CYS:O	1:A:268:GLN:HG3	2.15	0.45
1:B:223:PHE:CD1	1:B:272:SER:HB2	2.51	0.45
1:A:555:VAL:O	1:A:559:CYS:HB2	2.16	0.45
1:B:522:GLN:HA	1:B:525:LYS:HD3	1.98	0.45
1:B:462:VAL:HG23	1:B:463:LEU:N	2.32	0.45
1:A:206:PHE:CE2	1:A:481:LEU:HB2	2.50	0.45
1:B:292:GLU:HG2	1:B:292:GLU:O	2.17	0.45
1:A:61:ASN:ND2	1:A:64:LYS:HE3	2.27	0.45
1:B:521:ARG:O	1:B:524:LYS:HB2	2.16	0.45
1:A:456:VAL:O	1:A:459:GLN:N	2.50	0.45
1:A:420:THR:CG2	1:A:527:THR:HG23	2.47	0.45
1:A:21:ALA:HB1	1:A:155:LEU:HD21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:CD2	1:A:333:GLU:HB3	2.46	0.45
1:B:429:ASN:O	1:B:432:LYS:HB2	2.17	0.45
1:A:513:ILE:HD11	1:A:555:VAL:HG13	1.99	0.45
1:A:66:LEU:HD22	1:A:70:PHE:HE1	1.82	0.45
1:B:485:ARG:HE	1:B:485:ARG:HB3	1.63	0.45
1:A:520:GLU:O	1:A:524:LYS:HG3	2.17	0.45
1:B:19:PHE:O	1:B:23:VAL:HG23	2.17	0.45
1:A:49:PHE:CD2	1:A:49:PHE:C	2.88	0.44
1:A:500:LYS:O	1:A:535:HIS:ND1	2.47	0.44
1:A:532:LEU:HD11	1:A:547:VAL:HG11	1.99	0.44
1:B:150:TYR:OH	2:B:2003:1FL:OAB	2.22	0.44
1:A:290:ILE:HA	1:A:293:VAL:HG13	1.99	0.44
1:A:511:ALA:O	1:A:514:CYS:SG	2.76	0.44
1:A:405:ASN:O	1:A:408:LEU:HB2	2.17	0.44
1:B:274:LYS:HE2	1:B:296:ASP:HA	1.98	0.44
1:B:533:VAL:CG2	1:B:544:LEU:HD21	2.48	0.44
1:B:16:GLU:O	1:B:20:LYS:HG3	2.18	0.44
1:B:558:CYS:C	1:B:560:LYS:H	2.20	0.44
1:A:521:ARG:O	1:A:524:LYS:N	2.48	0.44
1:A:30:TYR:CD1	1:A:102:PHE:HB3	2.53	0.44
1:A:441:PRO:O	1:A:442:GLU:C	2.56	0.44
1:B:274:LYS:HD2	1:B:294:GLU:OE2	2.18	0.44
1:B:14:LEU:N	1:B:14:LEU:HD22	2.33	0.44
1:A:216:VAL:HG22	1:A:235:VAL:HG21	2.00	0.44
1:B:286:LYS:O	1:B:289:CYS:HB3	2.18	0.44
1:A:278:CYS:O	1:A:281:LYS:HG2	2.18	0.43
1:A:34:CYS:HA	1:A:35:PRO:HD3	1.88	0.43
1:A:567:CYS:O	1:A:571:GLU:N	2.46	0.43
1:B:383:GLU:HB3	1:B:384:PRO:CD	2.41	0.43
1:B:502:PHE:CZ	1:B:504:ALA:HA	2.54	0.43
1:A:141:GLU:OE1	1:A:141:GLU:HA	2.17	0.43
1:A:257:ARG:HG2	1:A:257:ARG:O	2.18	0.43
1:A:458:ASN:O	1:A:462:VAL:HG22	2.18	0.43
1:B:161:TYR:O	1:B:164:ALA:HB3	2.17	0.43
1:B:483:ASN:C	1:B:486:PRO:HD2	2.38	0.43
1:A:120:VAL:HG21	1:A:175:ALA:CA	2.45	0.43
1:B:533:VAL:HG22	1:B:544:LEU:HD21	2.01	0.43
1:B:567:CYS:O	1:B:571:GLU:N	2.50	0.43
1:A:68:THR:O	1:A:72:ASP:OD2	2.37	0.43
1:B:110:PRO:HB2	1:B:112:LEU:HD21	1.97	0.43
1:B:414:LYS:HE3	1:B:488:PHE:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:CYS:C	1:B:560:LYS:N	2.71	0.43
1:B:557:LYS:HB3	1:B:571:GLU:OE2	2.18	0.43
1:A:112:LEU:HA	1:A:113:PRO:HD3	1.91	0.43
1:A:206:PHE:CE2	1:A:481:LEU:HD13	2.54	0.43
1:B:433:VAL:O	1:B:434:GLY:C	2.54	0.43
1:B:194:ALA:HB1	1:B:455:VAL:HG13	2.01	0.42
1:B:209:ARG:HH21	2:B:2002:1FL:HAH	1.84	0.42
1:B:410:ARG:O	1:B:414:LYS:HG3	2.20	0.42
1:B:447:PRO:O	1:B:448:CYS:C	2.57	0.42
1:B:333:GLU:O	1:B:337:ARG:HG3	2.19	0.42
1:B:417:GLN:OE1	1:B:417:GLN:N	2.35	0.42
1:B:272:SER:HB3	1:B:275:LEU:HG	2.01	0.42
1:B:531:GLU:OE1	1:B:531:GLU:HA	2.19	0.42
1:B:51:LYS:C	1:B:53:CYS:H	2.23	0.42
1:A:483:ASN:O	1:A:486:PRO:CD	2.64	0.42
1:A:432:LYS:O	1:A:433:VAL:C	2.56	0.42
1:B:89:ASP:O	1:B:92:ALA:HB3	2.18	0.42
1:A:345:LEU:HD23	1:A:446:MET:HE3	2.02	0.42
1:B:434:GLY:HA2	1:B:438:CYS:SG	2.60	0.42
1:A:25:ILE:HD13	1:A:154:LEU:HD23	2.01	0.42
1:A:48:GLU:O	1:A:52:THR:HG23	2.20	0.42
1:A:464:HIS:CE1	1:A:470:SER:H	2.36	0.41
1:B:107:ASP:O	1:B:110:PRO:HG3	2.20	0.41
1:B:367:HIS:O	1:B:371:ALA:HB2	2.19	0.41
1:B:563:ASP:OD2	1:B:567:CYS:N	2.50	0.41
1:A:109:ASN:HA	1:A:109:ASN:HD22	1.62	0.41
1:A:384:PRO:HB2	1:A:446:MET:SD	2.60	0.41
1:B:293:VAL:HG22	1:B:294:GLU:N	2.34	0.41
1:B:512:ASP:O	1:B:515:THR:HG22	2.21	0.41
1:B:540:THR:CG2	1:B:543:GLN:HB2	2.50	0.41
1:B:117:ARG:HG3	1:B:117:ARG:O	2.21	0.41
1:B:545:LYS:HA	1:B:548:MET:HB2	2.01	0.41
1:A:120:VAL:CG1	1:A:174:LYS:HB2	2.41	0.41
1:A:290:ILE:O	1:A:293:VAL:HG22	2.21	0.41
1:A:373:VAL:O	1:A:376:GLU:HB2	2.21	0.41
1:B:540:THR:CG2	1:B:543:GLN:HG3	2.51	0.41
1:B:107:ASP:OD2	1:B:110:PRO:HA	2.20	0.41
1:B:349:LEU:HD22	1:B:377:PHE:CG	2.55	0.41
1:B:417:GLN:HB2	1:B:470:SER:HB2	2.03	0.41
1:B:24:LEU:HD13	1:B:43:VAL:HG21	2.01	0.41
1:A:395:PHE:O	1:A:397:GLN:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ALA:O	1:A:161:TYR:HB3	2.21	0.41
1:A:453:LEU:CD2	2:A:2001:1FL:HAQ	2.51	0.41
1:A:262:LYS:O	1:A:263:TYR:C	2.59	0.41
1:A:274:LYS:HA	1:A:276:LYS:HE3	2.02	0.41
1:B:32:GLN:NE2	1:B:144:ARG:O	2.45	0.41
1:B:238:LEU:HA	1:B:238:LEU:HD12	1.87	0.41
1:B:237:ASP:HB2	1:B:260:LEU:HD12	2.02	0.41
1:B:395:PHE:C	1:B:397:GLN:N	2.74	0.41
1:B:412:THR:O	1:B:416:PRO:HG3	2.21	0.41
1:B:459:GLN:O	1:B:462:VAL:HG22	2.21	0.41
1:A:310:VAL:HG11	1:A:374:PHE:CE1	2.56	0.40
1:B:370:TYR:C	1:B:370:TYR:CD1	2.95	0.40
1:B:408:LEU:HD22	1:B:530:VAL:CG2	2.51	0.40
1:B:441:PRO:O	1:B:445:ARG:HG3	2.21	0.40
1:A:311:GLU:O	1:A:312:SER:C	2.59	0.40
1:A:359:LYS:HG3	1:A:360:CYS:N	2.36	0.40
1:A:410:ARG:O	1:A:414:LYS:HG3	2.22	0.40
1:A:72:ASP:O	1:A:76:THR:HG23	2.20	0.40
1:B:380:LEU:O	1:B:384:PRO:CD	2.68	0.40
1:B:61:ASN:HD22	1:B:64:LYS:CD	2.35	0.40
1:A:408:LEU:HD22	1:A:530:VAL:HG22	2.03	0.40
1:A:566:THR:C	1:A:568:PHE:N	2.73	0.40
1:B:446:MET:CB	1:B:447:PRO:CD	2.99	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	565/585 (97%)	486 (86%)	65 (12%)	14 (2%)	5	25
1	B	562/585 (96%)	478 (85%)	68 (12%)	16 (3%)	5	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1127/1170 (96%)	964 (86%)	133 (12%)	30 (3%)	5	23

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ALA
1	A	60	GLU
1	B	54	VAL
1	B	57	GLU
1	B	58	SER
1	B	300	ALA
1	B	565	GLU
1	A	390	GLN
1	A	391	ASN
1	A	562	ASP
1	B	442	GLU
1	A	58	SER
1	A	312	SER
1	A	447	PRO
1	A	557	LYS
1	B	315	VAL
1	B	363	ALA
1	A	300	ALA
1	A	448	CYS
1	B	447	PRO
1	A	57	GLU
1	B	276	LYS
1	A	55	ALA
1	B	60	GLU
1	B	75	CYS
1	B	281	LYS
1	B	448	CYS
1	B	118	PRO
1	B	469	VAL
1	A	151	ALA

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	447/511 (88%)	432 (97%)	15 (3%)	37	69
1	B	432/511 (84%)	415 (96%)	17 (4%)	32	65
All	All	879/1022 (86%)	847 (96%)	32 (4%)	35	67

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	49	PHE
1	A	109	ASN
1	A	152	PRO
1	A	198	LEU
1	A	276	LYS
1	A	310	VAL
1	A	384	PRO
1	A	440	HIS
1	A	442	GLU
1	A	467	THR
1	A	480	SER
1	A	486	PRO
1	A	489	SER
1	A	532	LEU
1	B	111	ASN
1	B	152	PRO
1	B	167	GLU
1	B	182	LEU
1	B	209	ARG
1	B	245	CYS
1	B	263	TYR
1	B	344	VAL
1	B	368	GLU
1	B	375	ASP
1	B	387	LEU
1	B	446	MET
1	B	480	SER
1	B	486	PRO
1	B	489	SER
1	B	516	LEU
1	B	548	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	61	ASN
1	A	99	ASN
1	A	109	ASN
1	A	318	ASN
1	A	338	HIS
1	A	429	ASN
1	A	459	GLN
1	A	464	HIS
1	A	483	ASN
1	A	543	GLN
1	B	9	HIS
1	B	111	ASN
1	B	338	HIS
1	B	464	HIS
1	B	483	ASN

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](#)

6 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	$\# Z > 2$
2	1FL	A	2003	-	17,19,19	0.56	0	22,27,27	0.93	0
2	1FL	B	2003	-	17,19,19	1.42	3 (17%)	22,27,27	1.34	3 (13%)
2	1FL	A	2002	-	17,19,19	1.28	1 (5%)	22,27,27	1.17	2 (9%)
2	1FL	B	2001	-	17,19,19	1.31	1 (5%)	22,27,27	1.04	1 (4%)
2	1FL	A	2001	-	17,19,19	1.31	2 (11%)	22,27,27	1.05	1 (4%)
2	1FL	B	2002	-	17,19,19	1.31	1 (5%)	22,27,27	1.17	2 (9%)

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
2	1FL	A	2003	-	-	0/4/8/8	0/2/2/2
2	1FL	B	2003	-	-	0/4/8/8	0/2/2/2
2	1FL	A	2002	-	-	0/4/8/8	0/2/2/2
2	1FL	B	2001	-	-	0/4/8/8	0/2/2/2
2	1FL	A	2001	-	-	0/4/8/8	0/2/2/2
2	1FL	B	2002	-	-	0/4/8/8	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	1FL	CAO-CAN	3.36	1.43	1.39
2	B	2003	1FL	CAH-CAO	3.36	1.45	1.40
2	A	2002	1FL	CAO-CAN	3.28	1.43	1.39
2	A	2001	1FL	CAO-CAN	3.24	1.43	1.39
2	B	2002	1FL	CAO-CAN	3.23	1.43	1.39
2	B	2003	1FL	CAH-CAG	2.27	1.42	1.38
2	A	2001	1FL	CAM-CAN	2.16	1.41	1.37
2	B	2003	1FL	CAJ-CAC	2.10	1.49	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2002	1FL	FAT-CAN-CAO	2.92	123.28	118.89
2	B	2002	1FL	FAT-CAN-CAO	2.89	123.24	118.89
2	B	2003	1FL	CAN-CAM-CAF	2.87	119.64	116.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2003	1FL	CAH-CAG-CAF	-2.40	115.88	118.36
2	B	2001	1FL	FAT-CAN-CAO	2.22	122.23	118.89
2	B	2002	1FL	CAN-CAM-CAF	2.15	118.87	116.62
2	A	2001	1FL	FAT-CAN-CAO	2.14	122.12	118.89
2	B	2003	1FL	OAL-CAK-CAJ	2.02	125.70	120.23
2	A	2002	1FL	CAN-CAM-CAF	2.02	118.74	116.62

There are no chirality outliers.

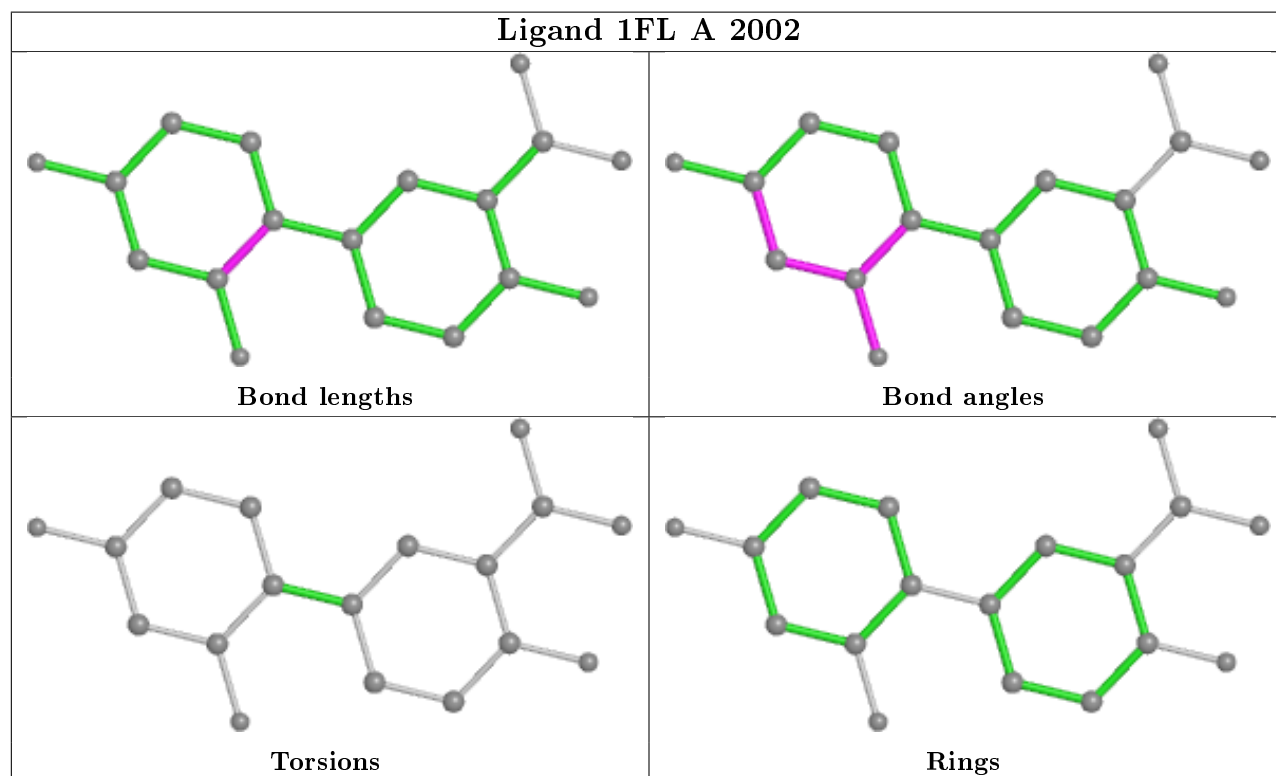
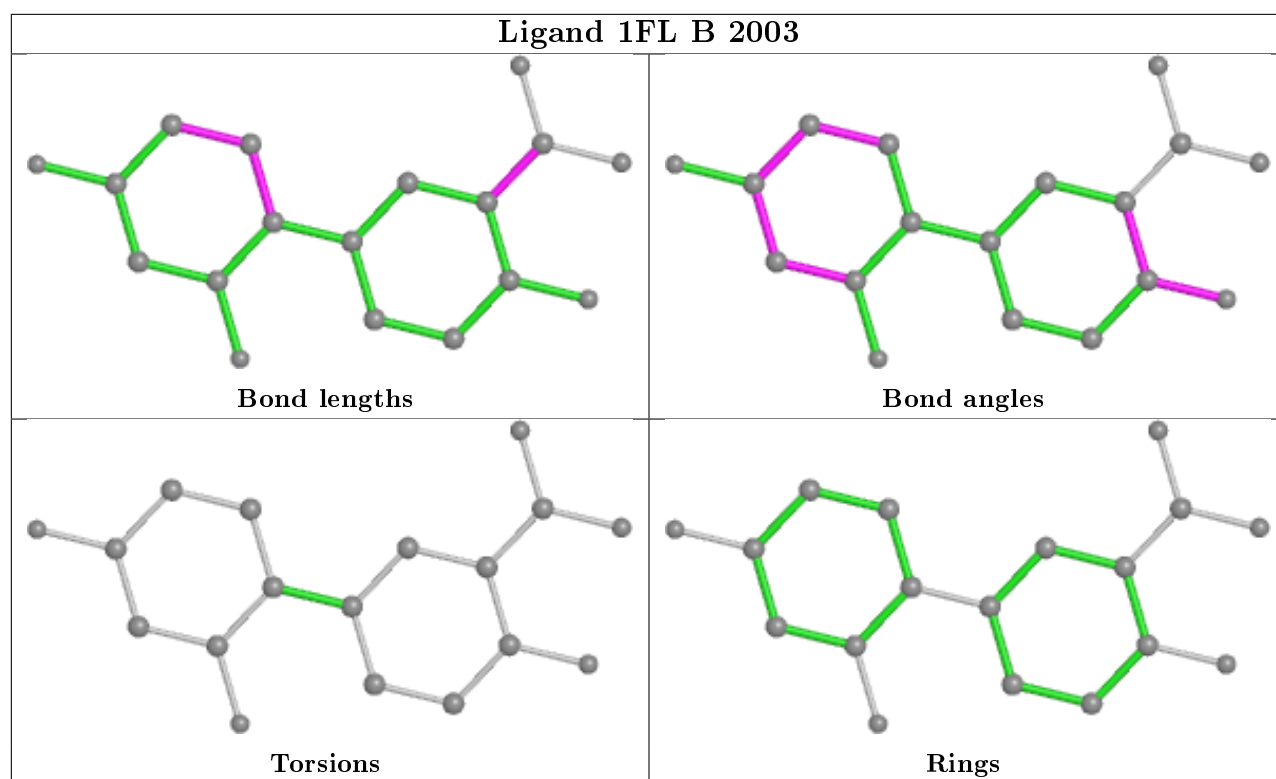
There are no torsion outliers.

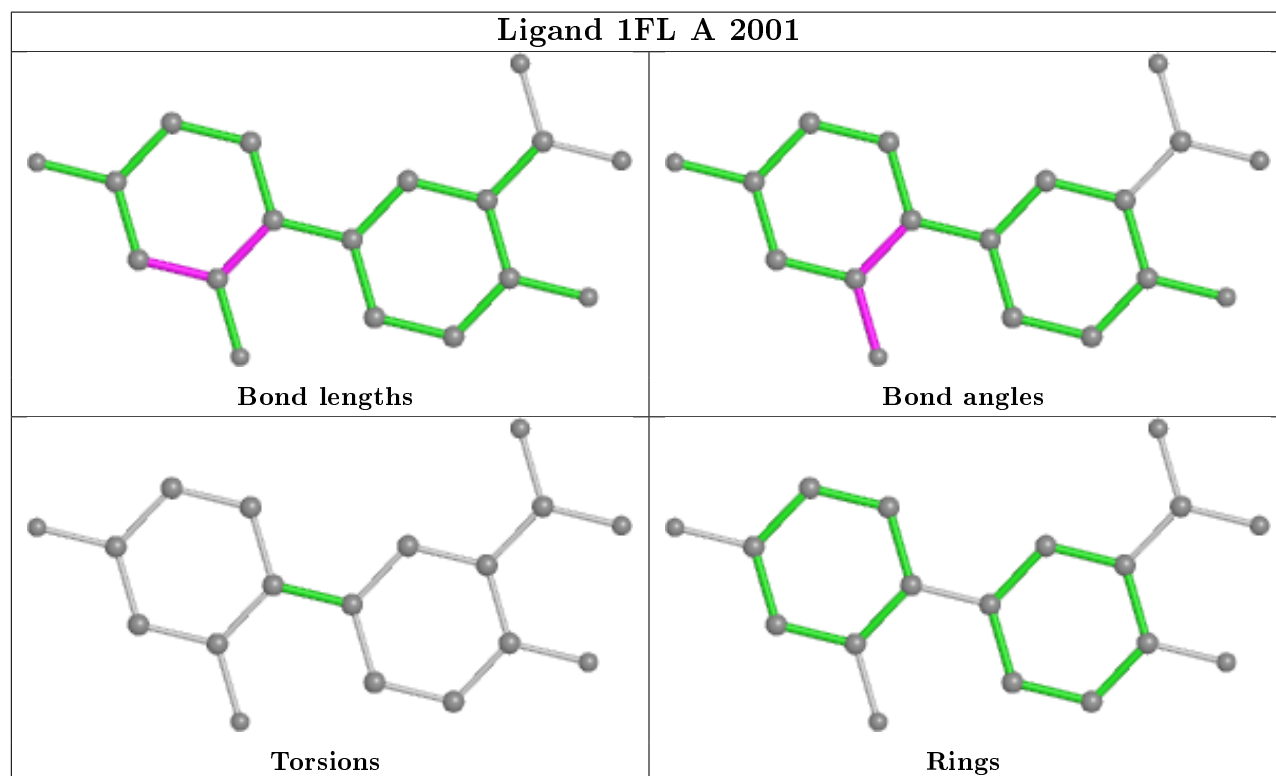
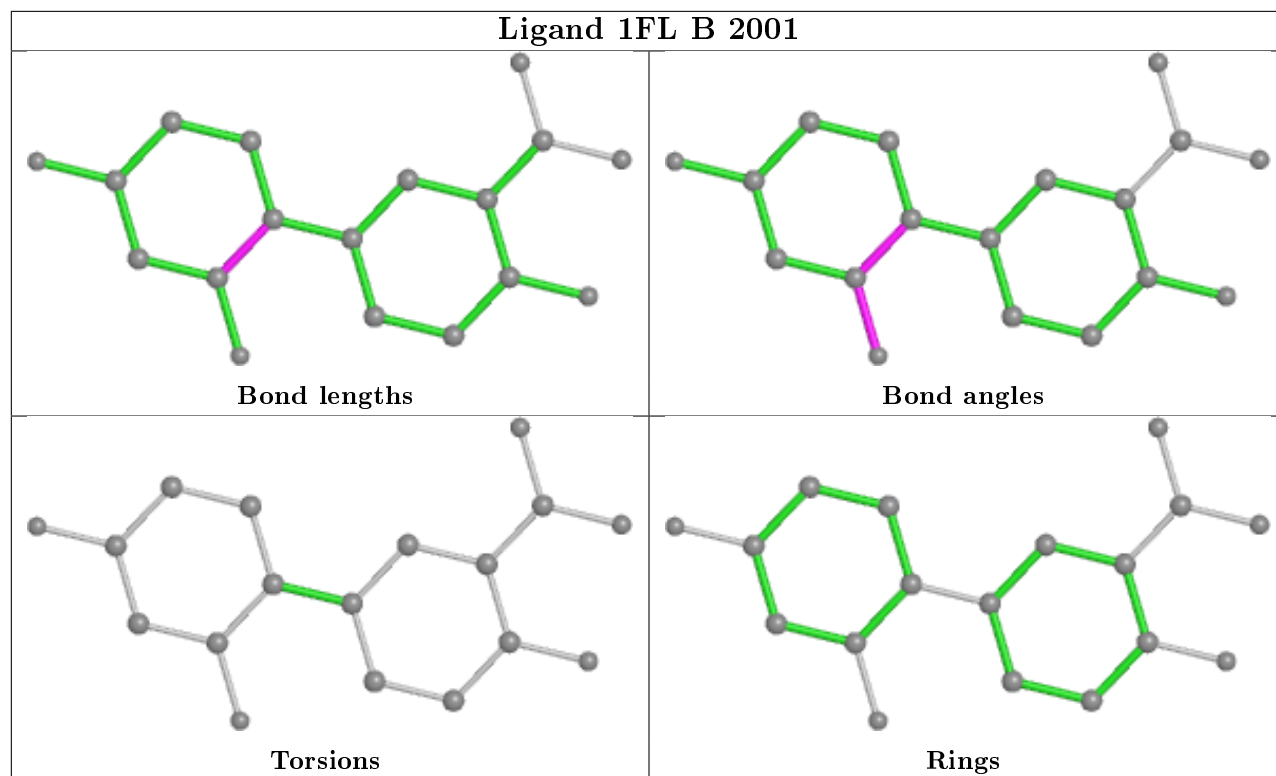
There are no ring outliers.

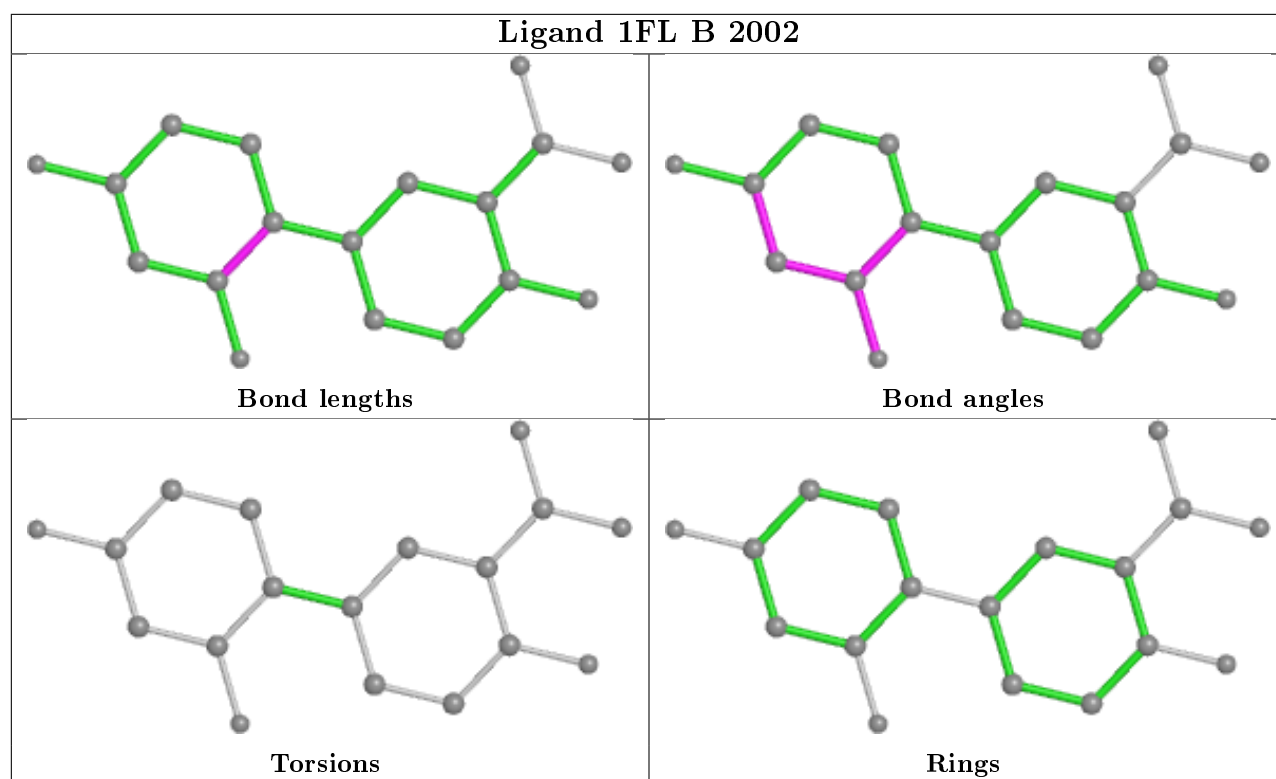
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2003	1FL	2	0
2	B	2003	1FL	3	0
2	B	2001	1FL	2	0
2	A	2001	1FL	1	0
2	B	2002	1FL	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	569/585 (97%)	-0.18	17 (2%)	50 34	35, 78, 156, 170	0
1	B	566/585 (96%)	-0.08	21 (3%)	41 27	35, 78, 148, 175	0
All	All	1135/1170 (97%)	-0.13	38 (3%)	46 30	35, 78, 150, 175	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	582	ALA	6.6
1	B	566	THR	6.3
1	B	562	ASP	5.6
1	B	579	SER	5.5
1	B	577	ALA	5.5
1	B	575	LEU	5.3
1	B	564	LYS	4.9
1	B	578	ALA	4.7
1	A	508	THR	4.6
1	B	508	THR	4.2
1	A	563	ASP	3.6
1	B	568	PHE	3.4
1	B	561	ALA	3.2
1	A	569	ALA	2.9
1	A	572	GLY	2.8
1	B	513	ILE	2.8
1	B	563	ASP	2.7
1	B	576	VAL	2.6
1	A	560	LYS	2.6
1	A	506	THR	2.6
1	B	507	PHE	2.6
1	A	579	SER	2.6
1	A	513	ILE	2.5
1	A	561	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	570	GLU	2.4
1	A	91	CYS	2.4
1	B	574	LYS	2.3
1	A	558	CYS	2.3
1	A	562	ASP	2.3
1	A	138	TYR	2.3
1	B	560	LYS	2.2
1	B	569	ALA	2.2
1	B	567	CYS	2.2
1	B	510	HIS	2.1
1	A	568	PHE	2.1
1	B	515	THR	2.1
1	A	92	ALA	2.0
1	A	102	PHE	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 monosaccharides 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.

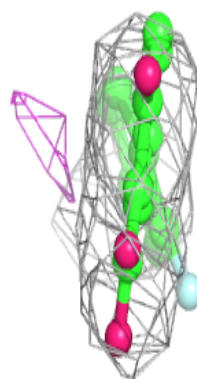
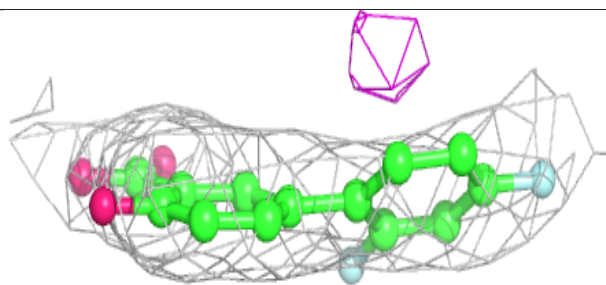
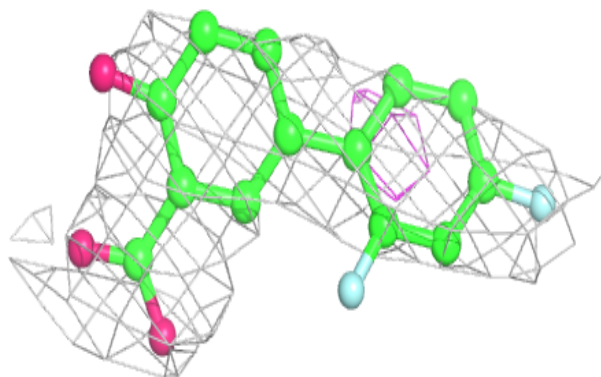
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	1FL	A	2003	18/18	0.83	0.28	109,109,111,111	0
2	1FL	B	2003	18/18	0.87	0.35	98,101,102,104	0
2	1FL	A	2002	18/18	0.91	0.25	77,82,91,92	0
2	1FL	B	2001	18/18	0.92	0.25	63,67,71,73	0
2	1FL	B	2002	18/18	0.92	0.31	91,94,99,100	0
2	1FL	A	2001	18/18	0.95	0.20	55,58,66,68	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

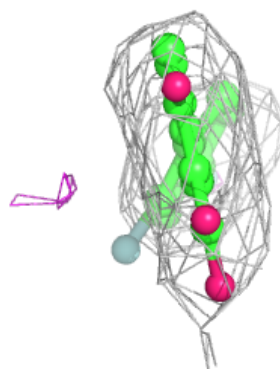
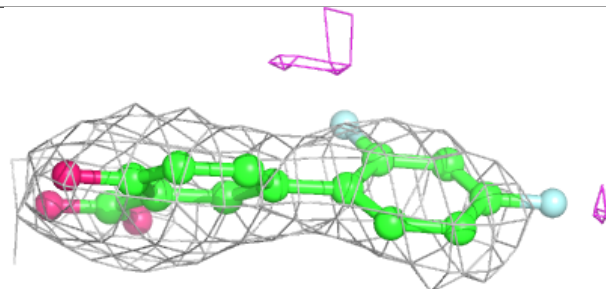
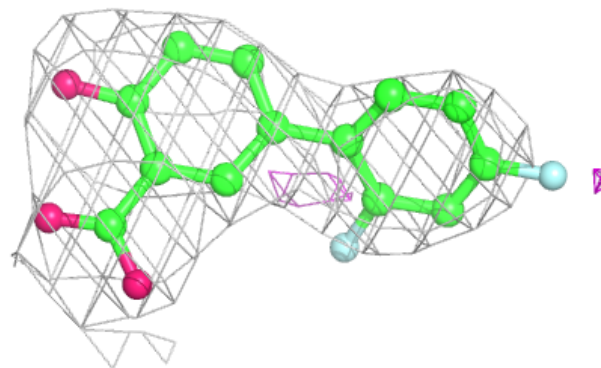
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 1FL B 2003:

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

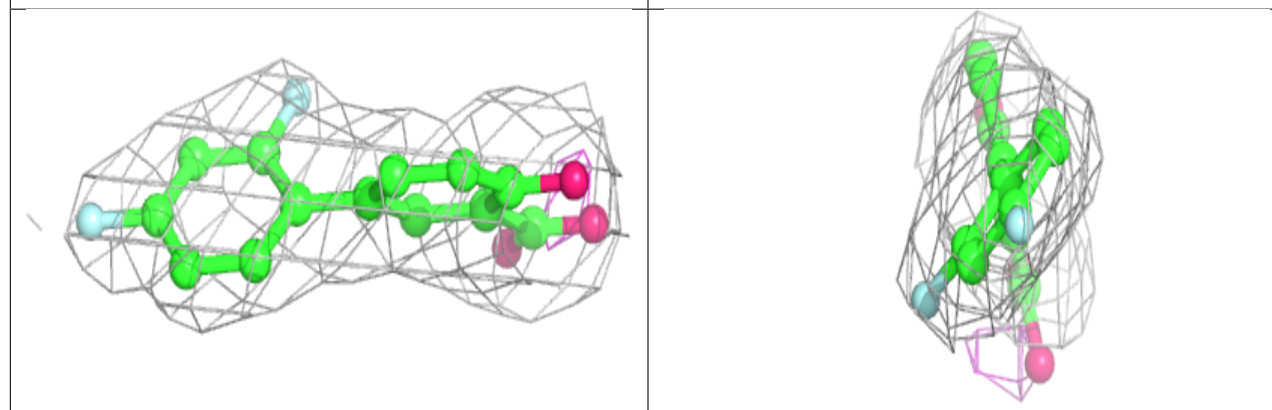
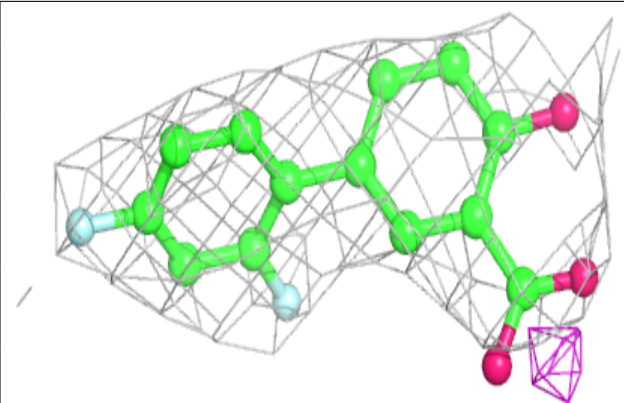
**Electron density around 1FL A 2002:**

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

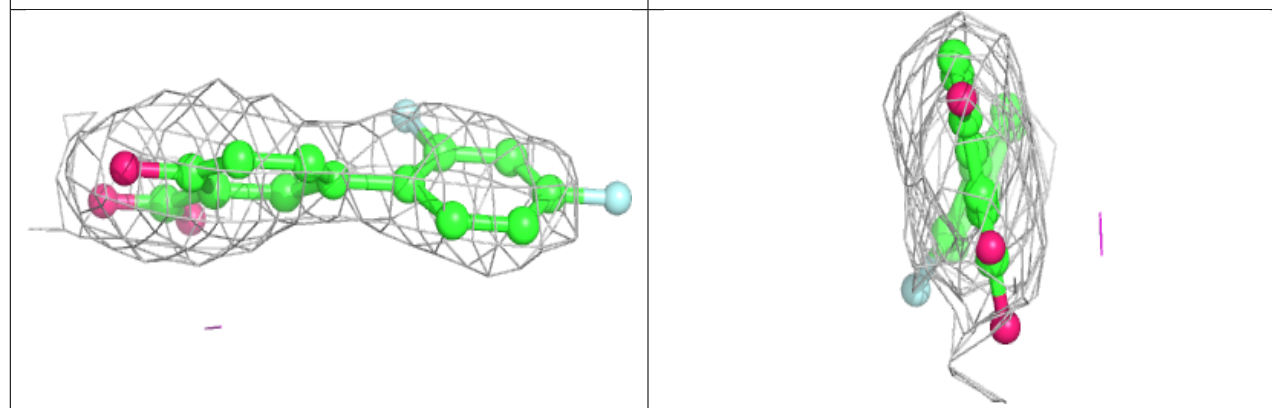
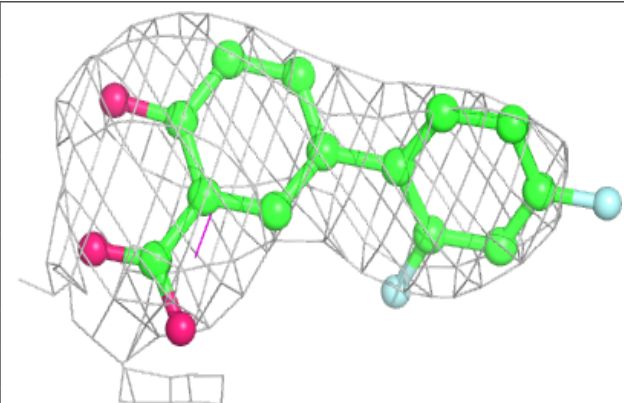


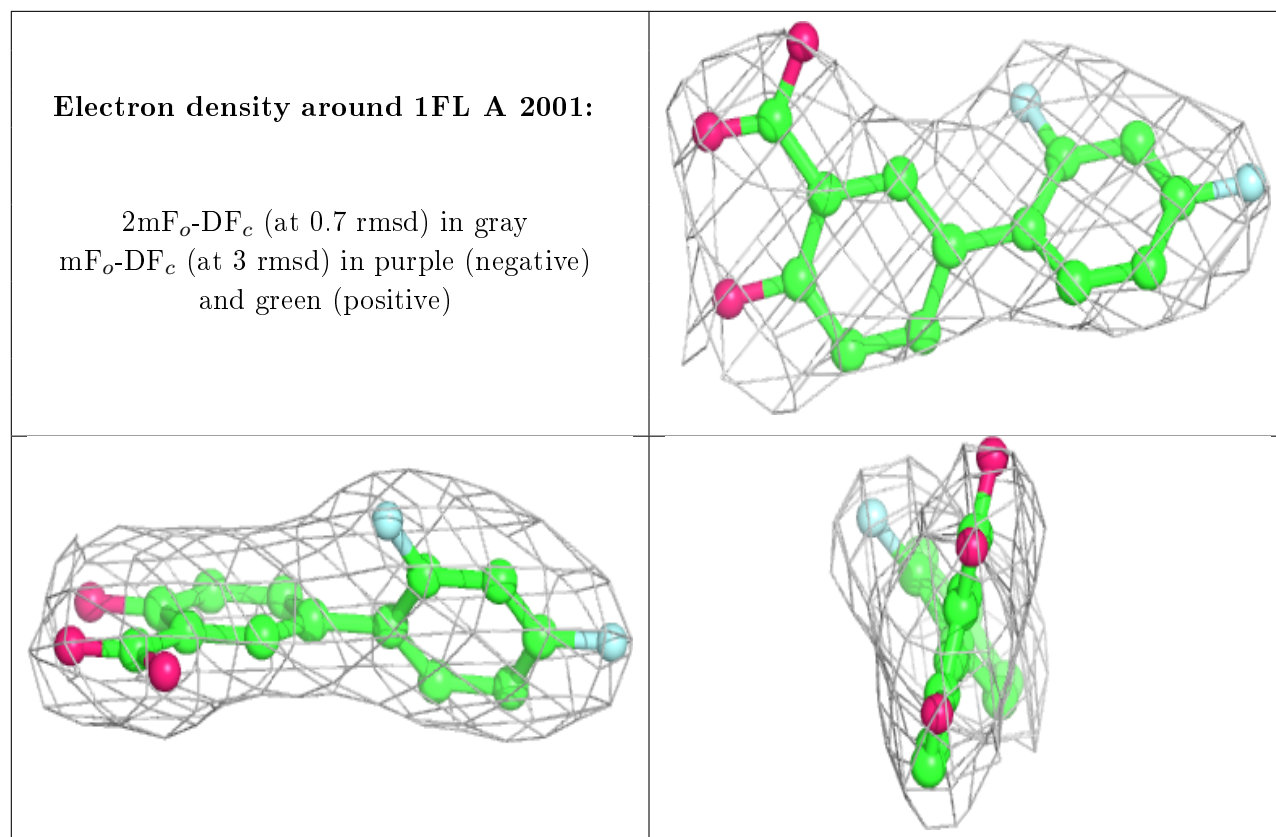
Electron density around 1FL B 2001:

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

**Electron density around 1FL B 2002:**

$2mF_o-DF_c$ (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.