



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:03 AM UTC

PDB ID : 1XV9 / pdb_00001xv9
Title : crystal structure of CAR/RXR heterodimer bound with SRC1 peptide, fatty acid, and 5b-pregnane-3,20-dione.
Authors : Xu, R.X.; Lambert, M.H.; Wisely, B.B.; Warren, E.N.; Weinert, E.E.; Waitt, G.M.; Williams, J.D.; Moore, L.B.; Willson, T.M.; Moore, J.T.
Deposited on : 2004-10-27
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

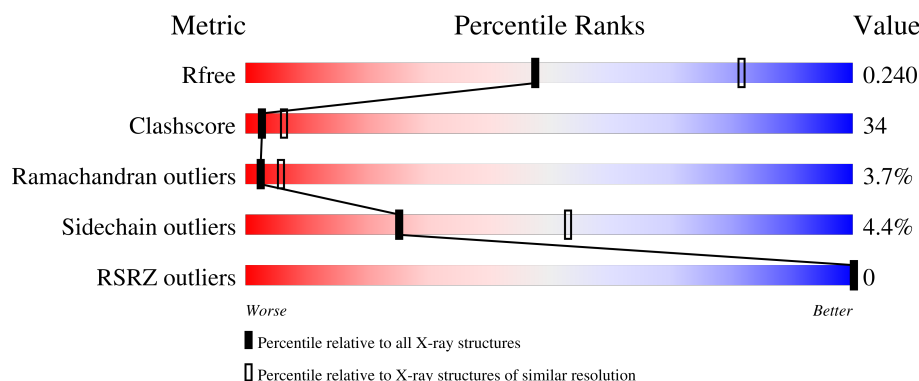
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	236	
1	C	236	
2	B	246	
2	D	246	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	13	31%38%8%23%
3	F	13	23%62%8%8%
3	G	13	23%62%8%8%
3	H	13	38%54%8%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8296 atoms, of which 122 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 Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1824	1166	311	336	11			
1	C	232	Total	C	N	O	S	0	0	0
			1824	1166	311	336	11			

- Molecule 2 is a protein called Orphan nuclear receptor NR1I3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	246	Total	C	N	O	S	0	0	0
			1990	1287	341	351	11			
2	D	246	Total	C	N	O	S	0	0	0
			1990	1287	341	351	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	VAL	deletion	UNP Q14994
B	?	-	SER	deletion	UNP Q14994
B	?	-	PRO	deletion	UNP Q14994
B	?	-	THR	deletion	UNP Q14994
D	?	-	VAL	deletion	UNP Q14994
D	?	-	SER	deletion	UNP Q14994
D	?	-	PRO	deletion	UNP Q14994
D	?	-	THR	deletion	UNP Q14994

- Molecule 3 is a protein called nuclear receptor coactivator 1 isoform 1.

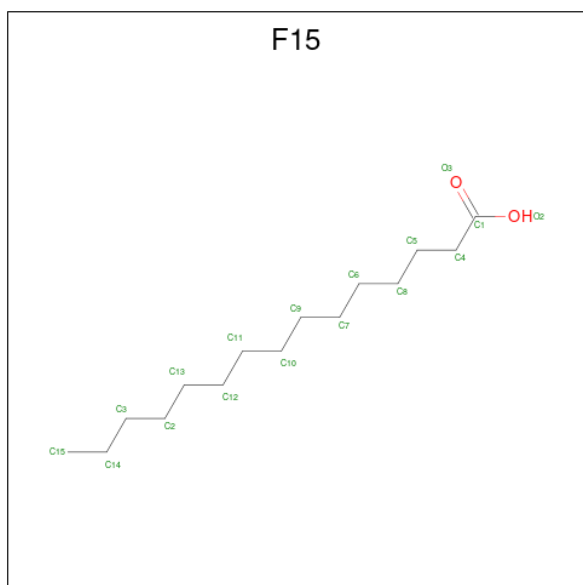
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	10	Total	C	N	O	0	0	0
			86	55	18	13			
3	F	12	Total	C	N	O	0	0	0
			102	63	23	16			

Continued on next page...

Continued from previous page...

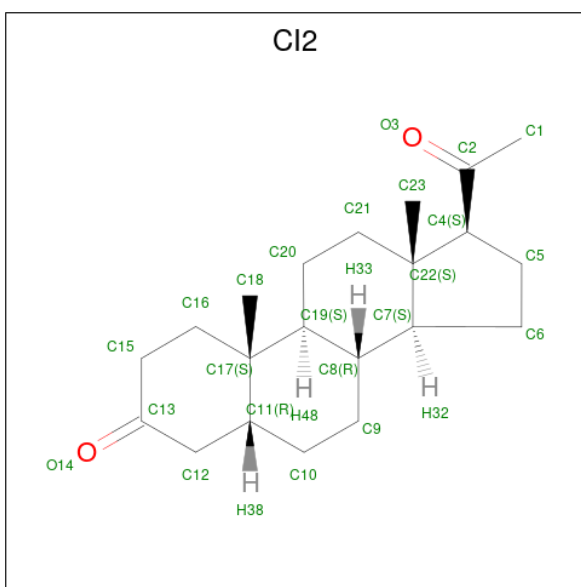
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	12	Total	C	N	O	0	0	0
			106	66	23	17			
3	H	12	Total	C	N	O	0	0	0
			106	66	23	17			

- Molecule 4 is PENTADECANOIC ACID (CCD ID: F15) (formula: C₁₅H₃₀O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			46	15	29	2		
4	C	1	Total	C	H	O	0	0
			46	15	29	2		

- Molecule 5 is (5BETA)-PREGNANE-3,20-DIONE (CCD ID: CI2) (formula: C₂₁H₃₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	H	O	0	1
			110	42	64	4		

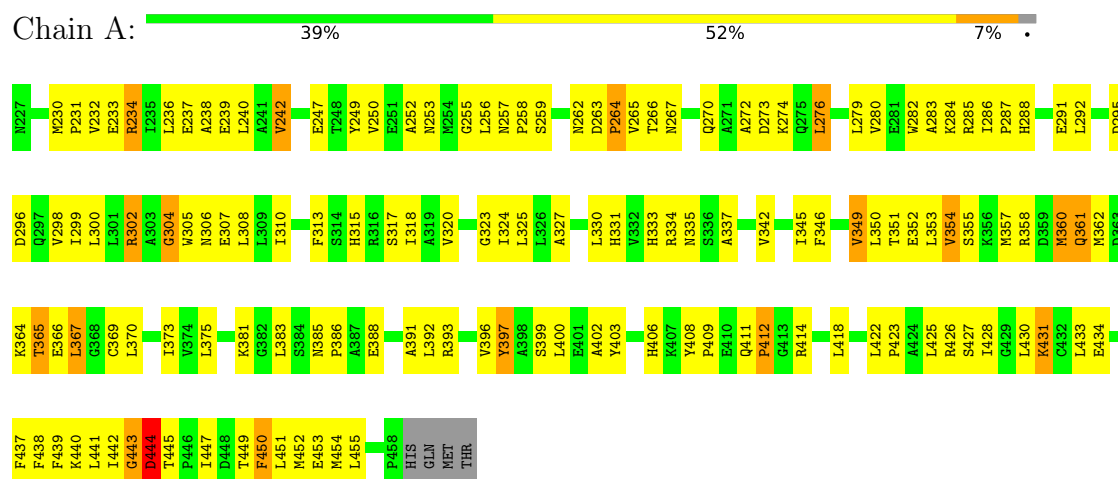
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	15	Total O 15 15	0	0
6	B	13	Total O 13 13	0	0
6	C	15	Total O 15 15	0	0
6	D	21	Total O 21 21	0	0
6	E	1	Total O 1 1	0	0
6	H	1	Total O 1 1	0	0

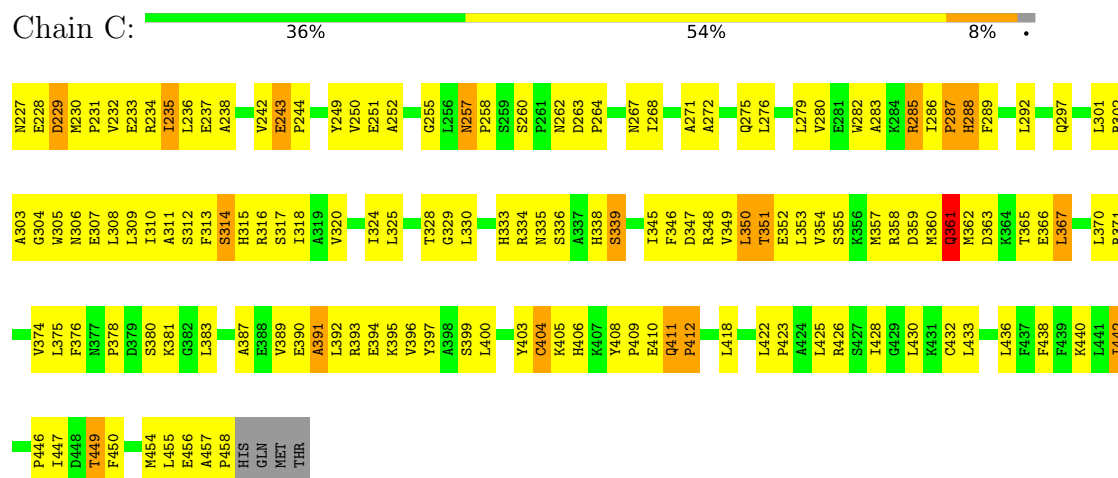
3 Residue-property plots

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: Retinoic acid receptor RXR-alpha

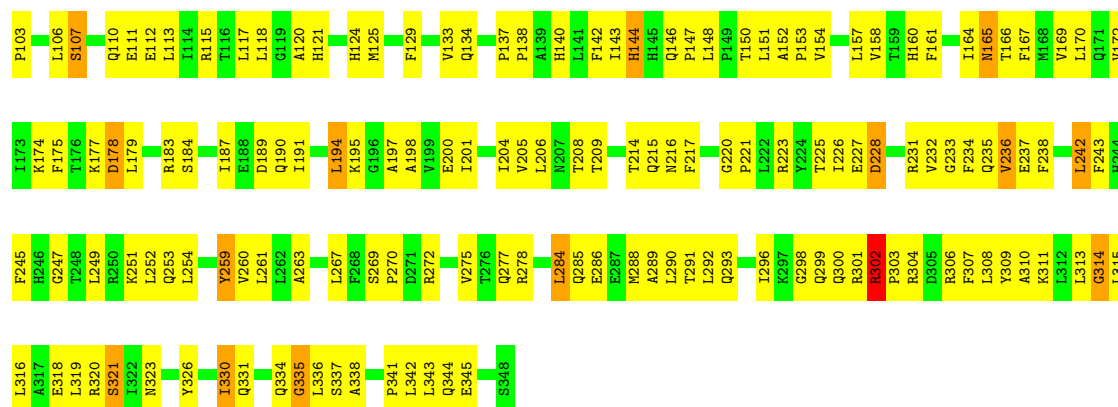


• Molecule 1: Retinoic acid receptor RXR-alpha



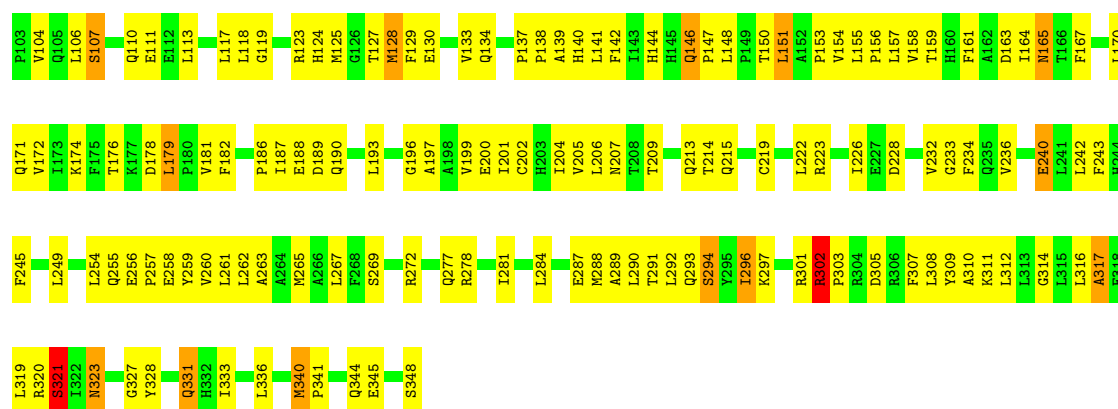
• Molecule 2: Orphan nuclear receptor NR1I3





• Molecule 2: Orphan nuclear receptor NR1I3

Chain D: 43% 51% 5%



• Molecule 3: nuclear receptor coactivator 1 isoform 1

Chain E: 31% 38% 8% 23%



• Molecule 3: nuclear receptor coactivator 1 isoform 1

Chain F: 23% 62% 8% 8%



• Molecule 3: nuclear receptor coactivator 1 isoform 1

Chain G: 23% 62% 8% 8%



- Molecule 3: nuclear receptor coactivator 1 isoform 1

Chain H:  38% 54% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.44Å 128.44Å 214.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	86.4 (50.00-2.70) 89.7 (50.00-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.181 , 0.239 0.187 , 0.240	Depositor DCC
R_{free} test set	3005 reflections (5.61%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtriage
Anisotropy	0.781	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 84.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.477 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8296	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: CI2, F15

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	0.49	0/1862	1.11	10/2523 (0.4%)
1	C	0.51	0/1862	1.13	11/2523 (0.4%)
2	B	0.50	0/2036	1.06	11/2758 (0.4%)
2	D	0.51	0/2036	1.11	19/2758 (0.7%)
3	E	0.45	0/87	1.13	1/116 (0.9%)
3	F	0.47	0/103	1.19	2/135 (1.5%)
3	G	0.41	0/107	1.00	1/142 (0.7%)
3	H	0.44	0/107	0.84	0/142
All	All	0.50	0/8200	1.10	55/11097 (0.5%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	179	LEU	CA-C-N	9.07	131.17	119.84
2	D	179	LEU	C-N-CA	9.07	131.17	119.84
1	C	411	GLN	CA-C-N	8.59	130.57	119.84
1	C	411	GLN	C-N-CA	8.59	130.57	119.84
1	A	385	ASN	CA-C-N	8.08	128.77	120.04
1	A	385	ASN	C-N-CA	8.08	128.77	120.04
2	D	278	ARG	N-CA-C	7.83	119.82	111.28
2	D	302	ARG	CA-C-N	-7.76	113.81	121.65
2	D	302	ARG	C-N-CA	-7.76	113.81	121.65
1	C	235	ILE	N-CA-C	-7.74	103.70	110.74
1	C	243	GLU	CA-C-N	7.62	127.63	119.78
1	C	243	GLU	C-N-CA	7.62	127.63	119.78
1	C	336	SER	N-CA-C	-7.35	103.77	112.89
3	F	691	HIS	N-CA-C	-7.11	102.35	111.02
1	A	444	ASP	N-CA-C	-7.06	103.93	112.54
3	E	632	ILE	N-CA-C	6.95	117.09	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	331	GLN	N-CA-C	-6.85	103.57	112.68
2	B	302	ARG	CA-C-N	-6.69	113.31	120.47
2	B	302	ARG	C-N-CA	-6.69	113.31	120.47
2	D	172	VAL	N-CA-C	-6.34	104.16	110.62
2	D	165	ASN	N-CA-C	-6.32	104.08	110.97
1	A	408	TYR	CA-C-N	6.26	126.00	119.05
1	A	408	TYR	C-N-CA	6.26	126.00	119.05
2	B	314	GLY	N-CA-C	-6.13	105.37	112.73
2	B	284	LEU	N-CA-C	-6.11	104.70	111.36
1	A	276	LEU	N-CA-C	-6.10	103.95	111.40
2	B	236	VAL	N-CA-C	6.10	116.22	110.30
2	D	340	MET	CA-C-N	6.09	125.98	119.28
2	D	340	MET	C-N-CA	6.09	125.98	119.28
1	A	273	ASP	N-CA-C	-5.97	104.46	110.97
2	D	321	SER	N-CA-C	-5.89	105.19	112.38
2	B	233	GLY	N-CA-C	5.88	121.78	114.37
2	B	331	GLN	N-CA-C	-5.78	105.49	113.18
1	C	391	ALA	N-CA-C	-5.75	104.93	111.14
2	D	178	ASP	N-CA-C	-5.56	104.69	112.25
2	D	317	ALA	N-CA-C	-5.52	104.90	111.69
2	D	146	GLN	CA-C-N	5.46	126.67	119.84
2	D	146	GLN	C-N-CA	5.46	126.67	119.84
2	D	314	GLY	N-CA-C	-5.38	105.79	113.86
2	B	220	GLY	CA-C-N	5.37	126.55	119.84
2	B	220	GLY	C-N-CA	5.37	126.55	119.84
1	C	257	ASN	CA-C-N	5.36	126.54	119.84
1	C	257	ASN	C-N-CA	5.36	126.54	119.84
2	D	151	LEU	N-CA-C	5.32	119.76	113.16
3	G	636	LEU	N-CA-C	5.31	116.88	111.14
1	A	367	LEU	N-CA-C	-5.27	105.23	110.97
2	B	178	ASP	N-CA-C	-5.18	105.67	112.72
2	B	228	ASP	N-CA-C	-5.14	105.59	111.14
1	C	249	TYR	N-CA-C	5.14	116.79	108.26
2	D	323	ASN	N-CA-C	-5.14	106.11	112.38
1	C	389	VAL	N-CA-C	5.10	115.53	110.23
1	A	247	GLU	N-CA-C	5.07	117.22	109.62
1	A	349	VAL	N-CA-C	-5.07	105.39	110.30
3	F	689	ILE	N-CA-C	5.04	116.37	110.62
2	D	188	GLU	N-CA-C	5.04	116.46	111.07

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	1824	0	1849	133	0
1	C	1824	0	1849	152	0
2	B	1990	0	2023	135	0
2	D	1990	0	2023	131	0
3	E	86	0	86	6	0
3	F	102	0	102	7	0
3	G	106	0	105	10	0
3	H	106	0	105	9	0
4	A	17	29	29	2	0
4	C	17	29	29	4	0
5	D	46	64	64	7	0
6	A	15	0	0	0	0
6	B	13	0	0	3	0
6	C	15	0	0	3	0
6	D	21	0	0	1	0
6	E	1	0	0	1	0
6	H	1	0	0	0	0
All	All	8174	122	8264	549	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 34.

All (549) 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:C:317:SER:HA	1:C:325:LEU:HD12	1.41	1.02
2:B:307:PHE:O	2:B:311:LYS:HG3	1.68	0.94
1:C:426:ARG:HG2	2:D:317:ALA:O	1.72	0.88
2:B:166:THR:O	2:B:170:LEU:HG	1.73	0.88
1:C:297:GLN:O	1:C:301:LEU:HG	1.73	0.88
2:B:167:PHE:HA	2:B:170:LEU:HD12	1.56	0.87
1:C:347:ASP:O	1:C:351:THR:HG22	1.75	0.86
2:D:118:LEU:HD11	2:D:257:PRO:HA	1.57	0.85
2:B:296:ILE:HD12	2:B:309:TYR:HB2	1.56	0.85
2:B:200:GLU:HG2	2:B:319:LEU:HB3	1.58	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:ILE:HD11	5:D:1001[A]:CI2:H42	1.57	0.84
2:D:104:VAL:HG22	2:D:297:LYS:HB2	1.59	0.84
2:D:113:LEU:HD23	2:D:291:THR:HG21	1.61	0.83
2:D:307:PHE:HB3	2:D:310:ALA:HB3	1.61	0.83
1:A:276:LEU:HB3	1:A:450:PHE:HD2	1.43	0.83
1:C:397:TYR:CE1	2:D:310:ALA:HB1	2.13	0.82
2:D:296:ILE:HD12	2:D:309:TYR:HB2	1.61	0.82
2:D:117:LEU:HD12	2:D:261:LEU:HD23	1.62	0.81
2:B:117:LEU:HB3	2:B:260:VAL:HG11	1.59	0.81
1:A:411:GLN:HG3	1:A:414:ARG:HB2	1.62	0.81
2:D:129:PHE:HE2	2:D:206:LEU:HD12	1.46	0.80
2:B:120:ALA:HB2	2:B:178:ASP:HB3	1.65	0.79
2:B:270:PRO:O	2:B:275:VAL:HG21	1.83	0.79
2:D:144:HIS:HB2	2:D:223:ARG:HD2	1.65	0.78
3:H:687:HIS:HB3	3:H:690:LEU:HD12	1.64	0.77
1:C:400:LEU:O	1:C:404:CYS:HB2	1.85	0.77
1:A:238:ALA:O	1:A:242:VAL:HG23	1.84	0.77
2:D:200:GLU:HG2	2:D:319:LEU:HB3	1.65	0.77
1:C:432:CYS:O	1:C:436:LEU:HG	1.84	0.77
2:B:107:SER:O	2:B:111:GLU:HG2	1.83	0.77
1:C:360:MET:HE1	1:C:418:LEU:HD12	1.65	0.77
1:C:233:GLU:O	1:C:237:GLU:HB2	1.85	0.76
2:D:117:LEU:HB3	2:D:260:VAL:CG1	2.15	0.76
2:D:170:LEU:O	2:D:174:LYS:HG3	1.85	0.76
2:B:206:LEU:HG	2:B:217:PHE:CE2	2.21	0.76
1:C:292:LEU:HD21	1:C:392:LEU:HD11	1.66	0.76
1:C:271:ALA:HB2	1:C:328:THR:HG23	1.68	0.76
2:B:143:ILE:O	2:B:143:ILE:HG22	1.86	0.75
1:A:279:LEU:HD11	1:A:308:LEU:HD13	1.68	0.75
2:D:110:GLN:HB3	2:D:291:THR:HG23	1.69	0.75
1:A:279:LEU:HD21	1:A:308:LEU:HD12	1.67	0.75
1:A:414:ARG:O	1:A:418:LEU:HD13	1.87	0.74
2:B:302:ARG:HD2	2:B:302:ARG:O	1.86	0.74
1:C:280:VAL:HG21	3:G:636:LEU:HD23	1.69	0.74
1:C:302:ARG:HD3	3:G:630:HIS:NE2	2.03	0.74
1:A:315:HIS:O	1:A:318:ILE:HG13	1.87	0.74
2:D:307:PHE:O	2:D:311:LYS:HG3	1.87	0.74
2:D:117:LEU:HB3	2:D:260:VAL:HG11	1.70	0.73
1:C:229:ASP:HB3	1:C:395:LYS:HD3	1.71	0.72
2:B:103:PRO:HA	2:B:298:GLY:HA2	1.72	0.72
2:D:345:GLU:OE2	3:H:689:ILE:HG22	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:PHE:O	1:A:441:LEU:HG	1.90	0.72
1:A:369:CYS:O	1:A:373:ILE:HG13	1.90	0.71
1:A:249:TYR:CE2	1:A:325:LEU:HB3	2.26	0.71
2:D:129:PHE:CE2	2:D:206:LEU:HA	2.26	0.70
1:C:376:PHE:O	1:C:393:ARG:HD2	1.91	0.70
2:D:104:VAL:HG21	2:D:294:SER:HA	1.73	0.70
2:D:262:LEU:O	2:D:262:LEU:HD12	1.92	0.70
2:B:113:LEU:HD23	2:B:291:THR:HG21	1.74	0.69
2:D:345:GLU:CD	3:H:689:ILE:HG22	2.18	0.69
1:A:318:ILE:HG23	1:A:358:ARG:HB2	1.75	0.69
2:D:255:GLN:HG3	2:D:258:GLU:OE1	1.93	0.69
1:A:362:MET:HE3	1:A:367:LEU:HB2	1.73	0.68
2:D:301:ARG:HB3	2:D:303:PRO:HD3	1.73	0.68
2:B:330:ILE:O	2:B:337:SER:HB2	1.93	0.68
2:D:129:PHE:CE2	2:D:206:LEU:HD12	2.29	0.68
2:B:200:GLU:O	2:B:204:ILE:HG13	1.92	0.68
2:D:124:HIS:CD2	2:D:174:LYS:HB3	2.29	0.68
1:A:438:PHE:CZ	1:A:442:ILE:HD12	2.29	0.68
1:A:440:LYS:HG3	1:A:452:MET:HE1	1.75	0.68
2:D:201:ILE:O	2:D:205:VAL:HG23	1.94	0.67
2:B:299:GLN:O	2:B:299:GLN:HG3	1.93	0.67
2:D:164:ILE:HD11	5:D:1001[B]:CI2:C15	2.25	0.67
2:B:124:HIS:CD2	2:B:174:LYS:HB3	2.29	0.67
1:C:302:ARG:HG2	1:C:454:MET:HE1	1.76	0.67
1:C:362:MET:HE1	1:C:367:LEU:HD13	1.76	0.67
2:D:182:PHE:CE1	2:D:267:LEU:HD11	2.30	0.67
2:B:269:SER:O	2:B:272:ARG:HG2	1.95	0.67
1:C:318:ILE:HG23	1:C:358:ARG:HB2	1.76	0.67
1:C:230:MET:HB3	1:C:399:SER:OG	1.95	0.66
2:D:107:SER:O	2:D:111:GLU:HG2	1.94	0.66
1:C:350:LEU:HA	1:C:354:VAL:HB	1.75	0.66
2:B:345:GLU:CD	3:F:689:ILE:HG22	2.20	0.66
1:A:259:SER:HA	3:H:685:GLU:HG2	1.78	0.66
1:C:279:LEU:HD21	1:C:308:LEU:HD12	1.77	0.66
2:B:345:GLU:OE2	3:F:690:LEU:HG	1.96	0.66
2:D:302:ARG:HD2	2:D:302:ARG:O	1.95	0.66
3:F:689:ILE:O	3:F:693:LEU:HG	1.95	0.66
1:A:292:LEU:HD21	1:A:392:LEU:HD11	1.78	0.66
1:C:378:PRO:HA	1:C:383:LEU:CD2	2.26	0.66
2:D:104:VAL:CG2	2:D:294:SER:HA	2.26	0.66
2:D:119:GLY:O	2:D:123:ARG:HG3	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:MET:HE1	1:C:367:LEU:CD1	2.26	0.65
2:B:228:ASP:O	2:B:232:VAL:HG23	1.97	0.65
1:A:250:VAL:HG23	1:A:330:LEU:HD12	1.78	0.65
1:C:405:LYS:O	1:C:409:PRO:HB3	1.97	0.65
2:D:296:ILE:HD13	2:D:308:LEU:HB3	1.79	0.65
1:A:383:LEU:HB3	1:A:386:PRO:HG3	1.77	0.65
2:D:254:LEU:HD13	2:D:258:GLU:HB3	1.78	0.65
1:A:302:ARG:HD3	3:E:630:HIS:NE2	2.11	0.64
1:C:433:LEU:HD23	1:C:436:LEU:HD12	1.78	0.64
1:C:455:LEU:O	1:C:456:GLU:HG3	1.97	0.64
1:A:369:CYS:SG	1:A:400:LEU:HD13	2.38	0.64
2:B:341:PRO:HA	2:B:344:GLN:HE21	1.63	0.64
1:C:276:LEU:HB3	1:C:450:PHE:CD2	2.32	0.64
2:D:138:PRO:HG2	2:D:157:LEU:HA	1.80	0.64
2:D:189:ASP:O	2:D:193:LEU:HG	1.98	0.64
2:D:289:ALA:O	2:D:293:GLN:HG3	1.98	0.63
1:A:365:THR:HG21	1:A:403:TYR:CE1	2.34	0.63
1:A:256:LEU:HD11	1:C:338:HIS:HD2	1.64	0.63
2:D:117:LEU:HD12	2:D:261:LEU:CD2	2.28	0.62
1:A:295:ASP:O	1:A:299:ILE:HG13	2.00	0.62
2:B:117:LEU:HB3	2:B:260:VAL:CG1	2.29	0.62
1:C:307:GLU:HB3	1:C:425:LEU:HD21	1.80	0.62
2:B:164:ILE:HD12	2:B:165:ASN:N	2.14	0.62
1:A:276:LEU:HD21	1:A:454:MET:HG3	1.81	0.62
1:C:315:HIS:O	1:C:318:ILE:HG13	2.00	0.62
1:A:236:LEU:O	1:A:240:LEU:HG	1.99	0.62
1:C:227:ASN:N	1:C:399:SER:HG	1.98	0.62
1:A:276:LEU:HB3	1:A:450:PHE:CD2	2.31	0.62
1:A:231:PRO:HG2	1:A:234:ARG:HB2	1.81	0.61
2:B:148:LEU:HB3	2:B:231:ARG:NH1	2.15	0.61
1:C:348:ARG:HG2	1:C:428:ILE:HD11	1.81	0.61
2:D:254:LEU:HB2	2:D:259:TYR:CZ	2.35	0.61
2:D:292:LEU:HD23	2:D:292:LEU:O	2.00	0.61
2:B:200:GLU:HG3	2:B:323:ASN:HD22	1.65	0.61
2:D:154:VAL:HG12	2:D:158:VAL:HG23	1.80	0.61
1:A:317:SER:HA	1:A:325:LEU:HD12	1.83	0.61
2:B:296:ILE:CD1	2:B:309:TYR:HB2	2.28	0.61
1:A:444:ASP:HB3	2:D:348:SER:O	2.01	0.61
2:B:144:HIS:CD2	2:B:223:ARG:HB3	2.35	0.61
1:A:362:MET:HA	1:A:366:GLU:OE2	2.00	0.61
1:C:426:ARG:HH11	2:D:321:SER:HB2	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:MET:HA	2:D:128:MET:HG2	1.83	0.61
2:B:247:GLY:O	2:B:251:LYS:HG3	2.01	0.60
2:D:164:ILE:HD11	5:D:1001[B]:CI2:H42	1.82	0.60
2:D:307:PHE:HB3	2:D:310:ALA:CB	2.31	0.60
1:A:369:CYS:HB3	1:A:400:LEU:HD22	1.83	0.60
1:A:438:PHE:CG	1:C:442:ILE:HD11	2.36	0.60
2:D:249:LEU:HD12	2:D:249:LEU:O	2.01	0.60
1:A:431:LYS:HE3	1:C:442:ILE:O	2.02	0.60
1:A:310:ILE:HA	1:A:313:PHE:CE2	2.37	0.59
1:A:438:PHE:CB	1:C:442:ILE:HD11	2.31	0.59
2:B:208:THR:HG22	2:B:259:TYR:CE2	2.37	0.59
2:D:228:ASP:O	2:D:232:VAL:HG23	2.02	0.59
2:B:146:GLN:CD	2:B:147:PRO:HD2	2.28	0.59
2:B:284:LEU:O	2:B:288:MET:HG2	2.02	0.59
1:C:380:SER:O	1:C:383:LEU:HB2	2.02	0.59
1:A:272:ALA:O	1:A:276:LEU:HB2	2.03	0.59
2:B:187:ILE:HD13	2:B:190:GLN:NE2	2.17	0.59
1:C:250:VAL:HG22	1:C:329:GLY:O	2.02	0.59
1:C:432:CYS:HB3	4:C:1002:F15:C10	2.32	0.59
1:C:262:ASN:HA	1:C:267:ASN:HD21	1.67	0.59
1:C:440:LYS:HB2	1:C:447:ILE:CD1	2.34	0.58
1:C:250:VAL:HG23	1:C:330:LEU:HD12	1.84	0.58
1:A:298:VAL:O	1:A:302:ARG:HB2	2.02	0.58
2:B:261:LEU:HB3	2:B:292:LEU:HD12	1.85	0.58
1:C:252:ALA:HA	1:C:330:LEU:HD11	1.85	0.58
1:C:455:LEU:C	1:C:456:GLU:HG3	2.29	0.58
1:C:320:VAL:HG13	1:C:325:LEU:HD11	1.86	0.58
2:B:177:LYS:HA	2:B:183:ARG:HD3	1.86	0.58
1:C:257:ASN:CG	1:C:257:ASN:O	2.47	0.58
1:C:397:TYR:HB3	2:D:307:PHE:CE2	2.39	0.58
2:D:226:ILE:HG22	6:D:65:HOH:O	2.03	0.58
2:B:169:VAL:HG21	2:B:343:LEU:HD21	1.86	0.58
1:C:334:ARG:HH21	1:C:350:LEU:HD12	1.69	0.57
2:B:286:GLU:O	2:B:290:LEU:HG	2.04	0.57
2:D:129:PHE:CD2	2:D:209:THR:HG21	2.38	0.57
1:A:298:VAL:HG13	3:E:633:LEU:CD2	2.34	0.57
1:A:305:TRP:CD1	1:A:454:MET:HE3	2.39	0.57
2:B:238:PHE:O	2:B:242:LEU:HB3	2.03	0.57
2:D:233:GLY:C	2:D:333:ILE:HD11	2.30	0.57
2:B:226:ILE:HD12	2:B:243:PHE:CD1	2.39	0.57
2:B:301:ARG:HB3	2:B:303:PRO:HD3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:MET:O	1:A:360:MET:HG2	2.05	0.56
1:C:252:ALA:HB2	1:C:330:LEU:CG	2.34	0.56
1:A:315:HIS:HE1	1:A:364:LYS:HG2	1.71	0.56
2:B:242:LEU:HD12	2:B:242:LEU:O	2.05	0.56
1:C:275:GLN:HB3	6:C:55:HOH:O	2.04	0.56
2:B:169:VAL:HG21	2:B:343:LEU:CD2	2.35	0.56
2:D:154:VAL:CG1	2:D:158:VAL:HG23	2.36	0.56
2:B:138:PRO:HG2	2:B:157:LEU:HA	1.88	0.56
2:D:186:PRO:O	2:D:190:GLN:HG3	2.05	0.56
2:D:171:GLN:OE1	2:D:174:LYS:HD2	2.06	0.56
2:D:187:ILE:HA	2:D:190:GLN:HE21	1.71	0.56
1:A:304:GLY:O	1:A:308:LEU:HG	2.06	0.56
1:C:381:LYS:CA	1:C:381:LYS:HE2	2.36	0.55
2:D:269:SER:HB2	2:D:272:ARG:HG2	1.88	0.55
1:C:236:LEU:HD22	1:C:365:THR:OG1	2.06	0.55
3:G:632:ILE:O	3:G:636:LEU:HD13	2.07	0.55
1:A:320:VAL:HG11	1:A:325:LEU:HD21	1.88	0.55
2:B:112:GLU:OE2	2:B:115:ARG:HD3	2.06	0.55
2:B:129:PHE:CD2	2:B:209:THR:HG21	2.41	0.55
2:B:164:ILE:HD12	2:B:164:ILE:C	2.31	0.55
2:B:191:ILE:O	2:B:195:LYS:HG3	2.07	0.55
2:B:107:SER:OG	2:B:110:GLN:HG3	2.06	0.55
1:C:230:MET:HG2	1:C:396:VAL:HG22	1.88	0.55
1:A:362:MET:HE1	1:A:367:LEU:CD1	2.36	0.55
2:B:326:TYR:CZ	5:D:1001[A]:CI2:H25	2.42	0.55
2:D:204:ILE:CD1	2:D:263:ALA:HA	2.36	0.55
2:B:158:VAL:HG22	2:B:232:VAL:HG13	1.89	0.55
2:D:164:ILE:HD12	2:D:164:ILE:C	2.32	0.55
1:A:313:PHE:CD1	1:A:313:PHE:C	2.84	0.54
1:A:423:PRO:O	1:A:426:ARG:HB3	2.07	0.54
1:A:253:ASN:HD22	1:A:262:ASN:HB2	1.70	0.54
2:B:133:VAL:HG11	2:B:221:PRO:HG3	1.89	0.54
2:B:172:VAL:O	2:B:175:PHE:HB3	2.08	0.54
2:B:252:LEU:HB3	2:B:254:LEU:HD21	1.89	0.54
1:C:381:LYS:HE2	1:C:381:LYS:HA	1.88	0.54
2:D:242:LEU:HD12	2:D:242:LEU:O	2.06	0.54
1:A:230:MET:HE3	1:A:396:VAL:HG23	1.89	0.54
2:B:197:ALA:CB	2:B:267:LEU:HA	2.38	0.54
1:C:400:LEU:O	1:C:400:LEU:HD12	2.08	0.54
1:C:432:CYS:HB3	4:C:1002:F15:H5	1.90	0.54
1:A:353:LEU:O	1:A:357:MET:HG3	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:ASN:HD21	1:C:260:SER:HB3	1.72	0.54
2:D:129:PHE:CZ	2:D:206:LEU:HA	2.41	0.54
1:C:276:LEU:HB3	1:C:450:PHE:HD2	1.71	0.54
2:D:117:LEU:CD1	2:D:261:LEU:HD23	2.37	0.54
1:A:255:GLY:HA3	1:A:264:PRO:HD2	1.90	0.54
1:A:362:MET:HE1	1:A:367:LEU:HD13	1.89	0.54
2:B:133:VAL:HG11	2:B:221:PRO:CG	2.38	0.54
2:B:261:LEU:CB	2:B:292:LEU:HD12	2.38	0.54
1:A:452:MET:O	1:A:455:LEU:HD23	2.08	0.53
2:B:178:ASP:O	2:B:179:LEU:HD23	2.08	0.53
1:C:231:PRO:HG2	1:C:234:ARG:HB2	1.89	0.53
1:C:252:ALA:HB2	1:C:330:LEU:HG	1.89	0.53
2:B:289:ALA:O	2:B:293:GLN:HG3	2.07	0.53
2:B:345:GLU:OE1	3:F:689:ILE:HG22	2.08	0.53
2:D:176:THR:HA	2:D:179:LEU:HD12	1.91	0.53
2:B:301:ARG:C	2:B:303:PRO:HD3	2.33	0.53
2:D:181:VAL:HG11	2:D:284:LEU:HD22	1.91	0.53
2:B:197:ALA:HB2	2:B:267:LEU:HA	1.91	0.53
1:C:308:LEU:O	1:C:311:ALA:HB3	2.08	0.53
1:A:360:MET:CE	1:A:362:MET:HB2	2.39	0.52
2:D:207:ASN:CG	2:D:249:LEU:HG	2.33	0.52
1:A:280:VAL:HG11	3:E:636:LEU:HB3	1.90	0.52
1:A:362:MET:HE3	1:A:367:LEU:CB	2.39	0.52
1:C:283:ALA:O	1:C:286:ILE:HB	2.09	0.52
1:C:302:ARG:HD3	3:G:630:HIS:CE1	2.43	0.52
2:B:252:LEU:CB	2:B:254:LEU:HD21	2.40	0.52
1:C:316:ARG:HD2	1:C:325:LEU:O	2.10	0.52
1:C:348:ARG:O	1:C:352:GLU:HB2	2.09	0.52
2:D:200:GLU:HG3	2:D:323:ASN:HB2	1.92	0.52
2:B:302:ARG:O	2:B:302:ARG:CD	2.57	0.52
1:C:276:LEU:CD1	1:C:309:LEU:HD11	2.40	0.52
1:C:362:MET:HE3	1:C:367:LEU:HB2	1.91	0.52
1:C:363:ASP:OD1	1:C:365:THR:HB	2.10	0.52
1:A:288:HIS:HA	1:A:291:GLU:OE1	2.10	0.52
1:C:252:ALA:HB2	1:C:330:LEU:HD21	1.90	0.52
1:A:427:SER:OG	2:B:320:ARG:HD3	2.10	0.51
2:B:117:LEU:HD22	2:B:260:VAL:HG12	1.92	0.51
2:B:189:ASP:OD1	2:B:277:GLN:HG2	2.10	0.51
2:B:309:TYR:O	2:B:313:LEU:HG	2.10	0.51
1:C:403:TYR:C	1:C:403:TYR:CD2	2.89	0.51
1:C:289:PHE:HZ	1:C:301:LEU:HD21	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:ILE:O	1:C:314:SER:HB2	2.11	0.51
1:A:298:VAL:HG13	3:E:633:LEU:HD23	1.93	0.51
2:D:290:LEU:HD23	2:D:293:GLN:NE2	2.26	0.51
2:B:157:LEU:O	2:B:160:HIS:HB3	2.11	0.50
1:C:264:PRO:O	1:C:268:ILE:HG13	2.12	0.50
2:B:206:LEU:HG	2:B:217:PHE:HE2	1.76	0.50
1:C:378:PRO:HA	1:C:383:LEU:HD23	1.93	0.50
1:C:381:LYS:HA	1:C:381:LYS:CE	2.42	0.50
2:B:216:ASN:ND2	2:B:225:THR:HG22	2.26	0.50
1:C:307:GLU:CD	1:C:426:ARG:HA	2.37	0.50
1:C:426:ARG:NH1	2:D:321:SER:HB2	2.26	0.50
1:A:315:HIS:HB2	1:A:367:LEU:HD13	1.94	0.50
1:A:438:PHE:HB2	1:C:442:ILE:HD11	1.93	0.50
1:C:360:MET:O	1:C:361:GLN:C	2.55	0.50
2:D:204:ILE:HD13	2:D:263:ALA:HA	1.93	0.50
1:A:323:GLY:HA3	1:A:331:HIS:NE2	2.26	0.50
1:A:388:GLU:O	1:A:391:ALA:HB3	2.11	0.50
2:B:236:VAL:HG13	2:B:237:GLU:H	1.77	0.50
2:D:144:HIS:CB	2:D:223:ARG:HD2	2.40	0.50
3:H:690:LEU:O	3:H:691:HIS:C	2.55	0.50
1:A:296:ASP:HA	1:A:299:ILE:HD12	1.94	0.50
1:A:282:TRP:O	1:A:286:ILE:HG12	2.11	0.50
1:C:276:LEU:HD23	1:C:450:PHE:CD2	2.47	0.50
1:C:313:PHE:CD1	1:C:313:PHE:C	2.90	0.49
2:D:292:LEU:O	2:D:296:ILE:HG13	2.12	0.49
2:D:236:VAL:O	2:D:240:GLU:HG2	2.12	0.49
2:B:292:LEU:HD23	2:B:292:LEU:C	2.38	0.49
2:D:182:PHE:CE2	2:D:190:GLN:HB3	2.47	0.49
2:D:265:MET:HE3	2:D:289:ALA:HB2	1.94	0.49
1:A:431:LYS:HD3	1:A:434:GLU:OE2	2.13	0.49
2:D:215:GLN:O	2:D:243:PHE:HE2	1.94	0.49
1:A:276:LEU:HD21	1:A:454:MET:CG	2.43	0.49
1:C:238:ALA:O	1:C:242:VAL:HG23	2.11	0.49
2:B:216:ASN:CG	2:B:225:THR:HG22	2.37	0.49
1:C:381:LYS:HE2	1:C:381:LYS:N	2.27	0.49
1:C:289:PHE:CZ	1:C:301:LEU:HD21	2.47	0.49
3:E:638:GLN:O	3:E:639:GLU:O	2.31	0.49
1:A:230:MET:SD	1:A:287:PRO:HG2	2.53	0.49
1:A:383:LEU:HD23	1:A:386:PRO:HA	1.94	0.49
2:D:255:GLN:H	2:D:258:GLU:HB2	1.78	0.49
2:B:260:VAL:O	2:B:263:ALA:HB3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ALA:HA	1:A:262:ASN:HD22	1.77	0.48
1:A:362:MET:HE3	1:A:367:LEU:CA	2.43	0.48
2:B:106:LEU:O	2:B:107:SER:O	2.32	0.48
1:C:438:PHE:C	1:C:438:PHE:CD2	2.91	0.48
1:A:346:PHE:HE1	1:A:350:LEU:HD11	1.78	0.48
1:C:230:MET:HE3	1:C:396:VAL:HG23	1.95	0.48
2:D:262:LEU:HD12	2:D:262:LEU:C	2.38	0.48
1:C:234:ARG:HA	1:C:237:GLU:HB3	1.96	0.48
1:C:430:LEU:HD11	2:D:321:SER:HA	1.95	0.48
2:D:113:LEU:HD23	2:D:291:THR:CG2	2.36	0.48
2:D:301:ARG:C	2:D:303:PRO:CD	2.87	0.48
2:B:121:HIS:HD2	2:B:125:MET:HE3	1.78	0.48
1:C:257:ASN:ND2	1:C:260:SER:HB3	2.28	0.48
3:H:685:GLU:O	3:H:685:GLU:HG3	2.14	0.48
2:B:200:GLU:CG	2:B:323:ASN:HD22	2.27	0.48
2:B:334:GLN:HB3	6:B:56:HOH:O	2.13	0.48
1:C:378:PRO:HD2	1:C:393:ARG:HH11	1.79	0.48
2:D:202:CYS:O	2:D:206:LEU:HB2	2.13	0.48
1:A:406:HIS:O	1:A:409:PRO:HD3	2.13	0.48
2:D:333:ILE:HB	2:D:336:LEU:HD23	1.95	0.48
2:B:152:ALA:HB1	2:B:153:PRO:HD2	1.96	0.47
1:C:231:PRO:HG3	1:C:234:ARG:HD3	1.95	0.47
1:C:335:ASN:O	1:C:339:SER:HB3	2.14	0.47
1:C:252:ALA:HB2	1:C:330:LEU:CD2	2.44	0.47
1:A:255:GLY:HA3	1:A:264:PRO:CD	2.43	0.47
2:D:199:VAL:HB	2:D:323:ASN:ND2	2.30	0.47
1:A:287:PRO:O	1:A:288:HIS:HB2	2.14	0.47
1:A:274:LYS:HE2	1:A:327:ALA:O	2.15	0.47
2:B:301:ARG:C	2:B:303:PRO:CD	2.88	0.47
1:C:282:TRP:CH2	1:C:371:ARG:HB3	2.50	0.47
1:C:348:ARG:HD3	1:C:428:ILE:HG12	1.97	0.47
1:C:400:LEU:HD11	1:C:418:LEU:CD2	2.45	0.47
1:C:406:HIS:O	1:C:409:PRO:HD3	2.13	0.47
1:A:447:ILE:HG23	1:A:451:LEU:HD23	1.97	0.47
1:C:309:LEU:HD22	6:C:55:HOH:O	2.13	0.47
1:C:361:GLN:HE21	1:C:361:GLN:HB3	1.59	0.47
1:A:262:ASN:C	1:A:267:ASN:HD21	2.22	0.47
2:B:252:LEU:HB3	2:B:308:LEU:HD11	1.96	0.47
2:D:193:LEU:HD21	2:D:281:ILE:HD13	1.97	0.47
2:D:196:GLY:HA3	2:D:272:ARG:HD2	1.97	0.47
2:B:138:PRO:HB2	2:B:140:HIS:CE1	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:MET:O	2:B:289:ALA:C	2.58	0.47
1:C:258:PRO:HA	1:C:263:ASP:OD2	2.14	0.47
1:C:287:PRO:O	1:C:288:HIS:HB2	2.15	0.46
2:B:236:VAL:HG12	6:B:21:HOH:O	2.14	0.46
2:B:117:LEU:CD1	2:B:261:LEU:HD23	2.45	0.46
2:B:169:VAL:CG2	2:B:343:LEU:HD21	2.45	0.46
1:C:255:GLY:C	1:C:257:ASN:H	2.24	0.46
2:D:150:THR:HB	2:D:151:LEU:HD22	1.97	0.46
2:D:187:ILE:HD13	2:D:190:GLN:NE2	2.30	0.46
1:A:258:PRO:HA	1:A:263:ASP:OD1	2.15	0.46
1:A:412:PRO:C	1:A:414:ARG:H	2.24	0.46
2:B:197:ALA:HB1	2:B:201:ILE:HD11	1.96	0.46
1:C:338:HIS:HE1	1:C:347:ASP:OD1	1.98	0.46
1:A:302:ARG:HG2	6:E:25:HOH:O	2.16	0.46
2:B:120:ALA:CB	2:B:178:ASP:HB3	2.41	0.46
2:B:154:VAL:HG23	6:B:14:HOH:O	2.15	0.46
2:D:133:VAL:HA	2:D:137:PRO:HG3	1.98	0.46
2:D:197:ALA:O	2:D:201:ILE:HG13	2.15	0.46
2:B:129:PHE:CE2	2:B:206:LEU:HA	2.51	0.46
2:B:234:PHE:O	2:B:235:GLN:C	2.58	0.46
2:B:290:LEU:HD23	2:B:293:GLN:NE2	2.30	0.46
3:G:635:ARG:O	3:G:639:GLU:HG2	2.16	0.46
1:A:249:TYR:HE2	1:A:325:LEU:HB3	1.77	0.46
1:A:360:MET:O	1:A:361:GLN:C	2.59	0.46
2:D:164:ILE:HA	2:D:167:PHE:HB3	1.98	0.46
2:D:165:ASN:C	2:D:165:ASN:HD22	2.23	0.46
1:C:252:ALA:CB	1:C:330:LEU:HD21	2.46	0.46
1:C:362:MET:CE	1:C:367:LEU:HB2	2.46	0.46
2:D:328:TYR:O	2:D:331:GLN:HB2	2.15	0.46
1:A:354:VAL:O	1:A:355:SER:C	2.56	0.46
1:A:430:LEU:HD11	2:B:321:SER:HA	1.97	0.46
1:A:455:LEU:HD23	1:A:455:LEU:H	1.81	0.46
2:B:148:LEU:HB3	2:B:231:ARG:HH12	1.78	0.46
1:C:353:LEU:O	1:C:357:MET:HG3	2.16	0.46
2:B:164:ILE:CD1	5:D:1001[A]:CI2:H42	2.37	0.45
2:B:253:GLN:C	2:B:254:LEU:HD23	2.41	0.45
2:B:314:GLY:O	2:B:318:GLU:HG2	2.17	0.45
3:F:686:ARG:O	3:F:687:HIS:C	2.59	0.45
3:H:689:ILE:O	3:H:692:ARG:HB3	2.16	0.45
1:A:399:SER:O	1:A:402:ALA:HB3	2.16	0.45
2:B:306:ARG:HG3	2:B:307:PHE:N	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:VAL:CG2	1:C:399:SER:HB3	2.45	0.45
1:C:280:VAL:HG11	3:G:636:LEU:HB3	1.97	0.45
2:D:159:THR:O	2:D:163:ASP:CG	2.59	0.45
2:D:308:LEU:HA	2:D:308:LEU:HD12	1.69	0.45
3:G:638:GLN:O	3:G:639:GLU:O	2.34	0.45
1:A:236:LEU:HB2	1:A:365:THR:OG1	2.16	0.45
1:C:349:VAL:O	1:C:353:LEU:HB2	2.17	0.45
1:C:432:CYS:HB3	4:C:1002:F15:H33	1.98	0.45
2:D:341:PRO:O	2:D:344:GLN:HB3	2.17	0.45
1:A:351:THR:O	1:A:351:THR:HG22	2.15	0.45
1:C:355:SER:O	1:C:358:ARG:HB3	2.16	0.45
2:D:118:LEU:HD12	2:D:260:VAL:HG21	1.97	0.45
2:D:176:THR:O	2:D:179:LEU:HB2	2.17	0.45
1:A:433:LEU:O	1:A:434:GLU:C	2.59	0.45
2:B:191:ILE:HG22	2:B:195:LYS:HD2	1.99	0.45
2:B:201:ILE:O	2:B:205:VAL:HG23	2.16	0.45
2:D:256:GLU:HB3	2:D:257:PRO:CD	2.47	0.45
1:C:238:ALA:HB2	1:C:285:ARG:O	2.15	0.45
2:D:262:LEU:HD22	2:D:312:LEU:HD22	1.98	0.45
2:B:270:PRO:HD2	2:B:285:GLN:NE2	2.32	0.45
1:A:264:PRO:O	1:A:265:VAL:C	2.58	0.45
1:C:446:PRO:HA	6:C:44:HOH:O	2.16	0.45
1:A:259:SER:CA	3:H:685:GLU:HG2	2.47	0.45
1:A:360:MET:SD	1:A:418:LEU:HD12	2.57	0.45
2:B:309:TYR:CE2	2:B:313:LEU:HD11	2.52	0.45
2:D:125:MET:C	2:D:127:THR:H	2.25	0.45
1:A:397:TYR:CZ	2:B:310:ALA:HB1	2.52	0.44
2:B:143:ILE:O	2:B:143:ILE:CG2	2.58	0.44
2:B:118:LEU:HA	2:B:121:HIS:HB3	1.99	0.44
2:B:161:PHE:HE2	5:D:1001[A]:CI2:H52	1.80	0.44
2:D:161:PHE:O	2:D:165:ASN:HB2	2.16	0.44
1:A:266:THR:O	1:A:270:GLN:HG3	2.18	0.44
1:A:352:GLU:HB2	1:A:428:ILE:HD11	1.99	0.44
1:A:402:ALA:O	1:A:406:HIS:HB3	2.17	0.44
2:B:307:PHE:HB3	2:B:310:ALA:HB3	1.99	0.44
1:C:306:ASN:O	1:C:310:ILE:HG13	2.17	0.44
2:D:153:PRO:O	2:D:156:PRO:HD2	2.18	0.44
1:C:252:ALA:CA	1:C:330:LEU:HD11	2.46	0.44
1:C:422:LEU:HB2	1:C:423:PRO:HD3	2.00	0.44
1:A:279:LEU:HD11	1:A:308:LEU:CD1	2.41	0.44
2:B:124:HIS:HE1	2:B:178:ASP:OD2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:ARG:O	2:B:303:PRO:HD2	2.18	0.44
1:C:230:MET:HG3	1:C:235:ILE:HD11	1.98	0.44
1:C:390:GLU:O	1:C:390:GLU:HG2	2.18	0.44
2:D:106:LEU:HA	2:D:110:GLN:OE1	2.17	0.44
3:F:696:GLU:O	3:F:697:GLY:C	2.60	0.44
1:A:362:MET:CE	1:A:367:LEU:HB2	2.43	0.44
1:C:400:LEU:HD11	1:C:418:LEU:HD23	2.00	0.44
1:A:453:GLU:OE1	3:E:632:ILE:HG13	2.18	0.44
2:B:292:LEU:HD22	2:B:309:TYR:HD1	1.81	0.44
1:C:289:PHE:HE2	3:G:637:LEU:HD21	1.81	0.44
1:C:397:TYR:HB3	2:D:307:PHE:CZ	2.52	0.44
1:C:408:TYR:HA	1:C:410:GLU:OE1	2.18	0.44
1:A:242:VAL:HG21	1:A:282:TRP:CD1	2.53	0.44
1:A:360:MET:HE2	1:A:362:MET:HB2	1.98	0.44
1:A:438:PHE:CE1	1:A:442:ILE:HD12	2.53	0.44
2:B:214:THR:O	2:B:215:GLN:HB3	2.17	0.44
2:B:217:PHE:O	2:B:223:ARG:HA	2.17	0.44
1:C:324:ILE:HD11	1:C:350:LEU:HD23	2.00	0.44
1:C:362:MET:HE3	1:C:367:LEU:CA	2.47	0.44
1:C:363:ASP:OD1	1:C:366:GLU:HG3	2.18	0.44
1:C:370:LEU:HD23	1:C:400:LEU:CD2	2.48	0.44
1:C:376:PHE:HB3	1:C:393:ARG:HB2	1.99	0.44
2:D:140:HIS:CD2	2:D:148:LEU:HB2	2.53	0.43
1:A:315:HIS:ND1	1:A:367:LEU:HD22	2.33	0.43
1:C:276:LEU:HB3	1:C:450:PHE:CE2	2.53	0.43
2:D:138:PRO:HG2	2:D:157:LEU:CA	2.46	0.43
1:A:236:LEU:HG	1:A:240:LEU:HD11	2.00	0.43
2:B:164:ILE:HG12	5:D:1001[A]:CI2:H41	2.00	0.43
2:B:335:GLY:O	2:B:338:ALA:HB3	2.18	0.43
1:A:333:HIS:HD2	1:A:335:ASN:HB2	1.83	0.43
1:A:402:ALA:O	1:A:406:HIS:CB	2.67	0.43
1:C:250:VAL:O	1:C:330:LEU:HD12	2.18	0.43
2:D:200:GLU:HG2	2:D:319:LEU:O	2.17	0.43
1:A:422:LEU:HB2	1:A:423:PRO:HD3	2.01	0.43
2:B:249:LEU:HD12	2:B:249:LEU:O	2.18	0.43
2:D:129:PHE:O	2:D:219:CYS:HB3	2.19	0.43
2:D:125:MET:HG2	2:D:171:GLN:HB3	2.00	0.43
1:A:302:ARG:HA	1:A:454:MET:HE1	2.01	0.43
2:B:278:ARG:O	2:B:278:ARG:HG2	2.18	0.43
1:A:276:LEU:O	1:A:279:LEU:HB3	2.19	0.43
1:C:272:ALA:HB2	4:C:1002:F15:C6	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:130:GLU:CD	2:D:130:GLU:H	2.27	0.43
2:D:155:LEU:HB3	2:D:156:PRO:HD3	2.01	0.43
1:A:284:LYS:C	1:A:286:ILE:H	2.27	0.42
1:C:365:THR:HG21	1:C:403:TYR:CE1	2.54	0.42
2:D:288:MET:O	2:D:289:ALA:C	2.61	0.42
1:A:279:LEU:HD21	1:A:305:TRP:HA	2.01	0.42
1:A:437:PHE:O	1:A:440:LYS:HB3	2.18	0.42
2:B:140:HIS:CE1	2:B:148:LEU:HD13	2.55	0.42
2:B:261:LEU:HD13	2:B:292:LEU:HB2	2.01	0.42
1:A:257:ASN:HA	1:A:258:PRO:HD3	1.87	0.42
2:D:186:PRO:HG3	2:D:277:GLN:HG2	2.01	0.42
2:D:292:LEU:HD23	2:D:296:ILE:HG13	2.01	0.42
2:D:302:ARG:O	2:D:302:ARG:CD	2.67	0.42
3:F:689:ILE:HG13	3:F:692:ARG:CZ	2.49	0.42
2:D:117:LEU:HD23	2:D:117:LEU:HA	1.81	0.42
3:G:633:LEU:HD12	3:G:633:LEU:O	2.19	0.42
1:A:232:VAL:HG13	1:A:365:THR:HG23	2.01	0.42
1:C:345:ILE:HG23	1:C:346:PHE:N	2.35	0.42
1:C:376:PHE:CB	1:C:393:ARG:HB2	2.50	0.42
2:D:333:ILE:HG22	2:D:336:LEU:HB2	2.02	0.42
1:A:358:ARG:C	1:A:360:MET:H	2.28	0.42
1:A:442:ILE:O	1:A:443:GLY:C	2.63	0.42
2:B:129:PHE:CZ	2:B:205:VAL:HG12	2.55	0.42
1:C:271:ALA:HB2	1:C:328:THR:CG2	2.45	0.42
1:C:333:HIS:C	1:C:335:ASN:H	2.27	0.42
1:C:378:PRO:C	1:C:380:SER:H	2.27	0.42
1:C:374:VAL:HG12	1:C:375:LEU:N	2.35	0.42
2:D:287:GLU:HB3	2:D:288:MET:HE2	2.00	0.42
2:B:194:LEU:HA	2:B:194:LEU:HD12	1.60	0.42
2:B:270:PRO:HB2	2:B:278:ARG:CG	2.50	0.42
1:A:334:ARG:O	1:A:337:ALA:HB3	2.20	0.42
1:C:243:GLU:HA	1:C:244:PRO:HD3	1.76	0.42
1:A:283:ALA:O	1:A:286:ILE:HB	2.20	0.41
1:C:305:TRP:O	1:C:309:LEU:HG	2.20	0.41
3:H:691:HIS:O	3:H:695:GLN:HG2	2.20	0.41
1:A:239:GLU:HA	1:A:239:GLU:OE1	2.20	0.41
1:A:280:VAL:O	1:A:283:ALA:HB3	2.20	0.41
2:B:148:LEU:HD23	2:B:231:ARG:NH2	2.35	0.41
1:C:230:MET:HG2	1:C:396:VAL:CG2	2.50	0.41
1:C:362:MET:HE1	1:C:367:LEU:HD12	2.02	0.41
1:C:365:THR:HG21	1:C:403:TYR:CD1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:214:THR:O	2:D:215:GLN:CB	2.67	0.41
2:D:327:GLY:O	2:D:331:GLN:HG2	2.20	0.41
1:C:366:GLU:HB3	1:C:418:LEU:HD21	2.02	0.41
2:D:316:LEU:O	2:D:320:ARG:HG3	2.20	0.41
1:C:374:VAL:O	1:C:375:LEU:C	2.63	0.41
1:C:411:GLN:HA	1:C:412:PRO:HD3	1.68	0.41
2:D:141:LEU:HB3	2:D:222:LEU:HD22	2.02	0.41
1:A:233:GLU:O	1:A:237:GLU:HB2	2.21	0.41
1:A:272:ALA:HB2	4:A:1003:F15:H29	2.02	0.41
2:D:161:PHE:CZ	2:D:234:PHE:HZ	2.37	0.41
2:B:137:PRO:HG2	2:B:142:PHE:CZ	2.56	0.41
2:B:165:ASN:HD22	2:B:165:ASN:HA	1.65	0.41
1:C:370:LEU:HD11	1:C:418:LEU:O	2.21	0.41
1:C:457:ALA:HA	1:C:458:PRO:HD3	1.90	0.41
2:D:125:MET:CE	2:D:205:VAL:HG21	2.51	0.41
1:A:315:HIS:CD2	1:A:362:MET:HE2	2.56	0.41
2:B:334:GLN:O	2:B:336:LEU:N	2.50	0.41
2:D:139:ALA:HA	2:D:142:PHE:HD2	1.85	0.41
1:A:300:LEU:HD22	1:A:375:LEU:O	2.20	0.41
1:A:393:ARG:NH2	2:B:311:LYS:HA	2.36	0.41
2:B:316:LEU:HD23	2:B:316:LEU:HA	1.93	0.41
1:C:449:THR:OG1	1:C:450:PHE:N	2.51	0.41
1:C:227:ASN:HB2	1:C:228:GLU:H	1.55	0.41
1:A:414:ARG:HG3	1:A:414:ARG:NH1	2.36	0.40
1:A:439:PHE:HB3	1:A:445:THR:HB	2.03	0.40
2:B:129:PHE:HE2	2:B:206:LEU:HA	1.84	0.40
1:C:276:LEU:HD13	1:C:309:LEU:HD11	2.02	0.40
2:D:301:ARG:C	2:D:303:PRO:HD2	2.46	0.40
2:D:340:MET:HA	2:D:341:PRO:HD2	1.83	0.40
1:A:242:VAL:HG21	1:A:282:TRP:HD1	1.86	0.40
1:A:345:ILE:O	1:A:349:VAL:HG23	2.20	0.40
2:B:245:PHE:CE1	2:B:315:LEU:HD22	2.56	0.40
2:B:301:ARG:O	2:B:303:PRO:CD	2.69	0.40
1:C:390:GLU:O	1:C:394:GLU:HG2	2.21	0.40
1:C:391:ALA:O	1:C:394:GLU:HB2	2.21	0.40
2:D:181:VAL:HG12	2:D:284:LEU:HD13	2.02	0.40
1:A:411:GLN:HG3	1:A:411:GLN:O	2.21	0.40
2:B:236:VAL:HG13	2:B:237:GLU:N	2.36	0.40
1:A:272:ALA:HB2	4:A:1003:F15:C8	2.52	0.40
1:A:282:TRP:CZ3	1:A:375:LEU:HD22	2.56	0.40
2:D:245:PHE:CZ	2:D:319:LEU:HG	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:636:LEU:C	3:G:638:GLN:H	2.30	0.40
1:A:307:GLU:HB3	1:A:425:LEU:HD21	2.04	0.40
2:B:154:VAL:HG12	2:B:158:VAL:HG23	2.02	0.40
2:B:170:LEU:CD2	2:B:342:LEU:HD22	2.52	0.40
2:D:171:GLN:HA	2:D:174:LYS:HB2	2.04	0.40
2:D:254:LEU:HD12	2:D:258:GLU:C	2.46	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	230/236 (98%)	180 (78%)	38 (16%)	12 (5%)	1	3
1	C	230/236 (98%)	182 (79%)	35 (15%)	13 (6%)	1	2
2	B	244/246 (99%)	209 (86%)	29 (12%)	6 (2%)	4	11
2	D	244/246 (99%)	213 (87%)	26 (11%)	5 (2%)	6	16
3	E	8/13 (62%)	6 (75%)	2 (25%)	0	100	100
3	F	10/13 (77%)	4 (40%)	6 (60%)	0	100	100
3	G	10/13 (77%)	7 (70%)	3 (30%)	0	100	100
3	H	10/13 (77%)	6 (60%)	4 (40%)	0	100	100
All	All	986/1016 (97%)	807 (82%)	143 (14%)	36 (4%)	2	6

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	449	THR
2	B	107	SER
2	B	198	ALA
1	C	412	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	449	THR
2	D	305	ASP
1	A	285	ARG
1	A	443	GLY
2	B	335	GLY
1	C	361	GLN
1	A	360	MET
2	B	300	GLN
1	C	288	HIS
1	C	312	SER
1	C	387	ALA
2	D	147	PRO
1	A	412	PRO
2	B	302	ARG
2	B	330	ILE
1	C	285	ARG
1	C	303	ALA
1	C	359	ASP
1	C	367	LEU
2	D	107	SER
2	D	302	ARG
1	A	264	PRO
1	A	306	ASN
1	C	304	GLY
2	D	134	GLN
1	A	361	GLN
1	A	304	GLY
1	A	342	VAL
1	A	242	VAL
1	A	354	VAL
1	C	287	PRO
1	C	442	ILE

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	200/204 (98%)	190 (95%)	10 (5%)	22	48
1	C	200/204 (98%)	192 (96%)	8 (4%)	28	56
2	B	219/219 (100%)	207 (94%)	12 (6%)	19	45
2	D	219/219 (100%)	212 (97%)	7 (3%)	34	64
3	E	9/12 (75%)	8 (89%)	1 (11%)	6	15
3	F	10/12 (83%)	10 (100%)	0	100	100
3	G	11/12 (92%)	10 (91%)	1 (9%)	9	22
3	H	11/12 (92%)	11 (100%)	0	100	100
All	All	879/894 (98%)	840 (96%)	39 (4%)	25	53

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	ARG
1	A	302	ARG
1	A	324	ILE
1	A	365	THR
1	A	370	LEU
1	A	381	LYS
1	A	397	TYR
1	A	431	LYS
1	A	444	ASP
1	A	450	PHE
2	B	134	GLN
2	B	144	HIS
2	B	150	THR
2	B	151	LEU
2	B	165	ASN
2	B	184	SER
2	B	194	LEU
2	B	227	GLU
2	B	242	LEU
2	B	259	TYR
2	B	304	ARG
2	B	321	SER
1	C	229	ASP
1	C	251	GLU
1	C	314	SER
1	C	339	SER
1	C	350	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	351	THR
1	C	361	GLN
1	C	404	CYS
2	D	128	MET
2	D	146	GLN
2	D	213	GLN
2	D	240	GLU
2	D	294	SER
2	D	296	ILE
2	D	321	SER
3	E	632	ILE
3	G	629	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	262	ASN
1	A	267	ASN
1	A	270	GLN
1	A	275	GLN
1	A	288	HIS
1	A	306	ASN
1	A	315	HIS
1	A	333	HIS
1	A	338	HIS
1	A	361	GLN
1	A	377	ASN
2	B	105	GLN
2	B	121	HIS
2	B	124	HIS
2	B	131	GLN
2	B	144	HIS
2	B	146	GLN
2	B	190	GLN
2	B	203	HIS
2	B	244	HIS
2	B	246	HIS
2	B	277	GLN
2	B	323	ASN
2	B	344	GLN
1	C	267	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	270	GLN
1	C	275	GLN
1	C	335	ASN
1	C	338	HIS
1	C	361	GLN
1	C	377	ASN
1	C	406	HIS
2	D	105	GLN
2	D	124	HIS
2	D	140	HIS
2	D	146	GLN
2	D	190	GLN
2	D	283	GLN
2	D	299	GLN
2	D	331	GLN
3	E	638	GLN
3	F	691	HIS
3	F	695	GLN
3	H	695	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	F15	C	1002	-	16,16,16	1.38	3 (18%)	16,16,16	0.86	0
5	CI2	D	1001[A]	-	26,26,26	1.26	4 (15%)	42,42,42	1.59	8 (19%)
5	CI2	D	1001[B]	-	26,26,26	1.24	4 (15%)	42,42,42	1.35	9 (21%)
4	F15	A	1003	-	16,16,16	1.49	3 (18%)	16,16,16	1.41	2 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	F15	C	1002	-	-	8/14/14/14	-
5	CI2	D	1001[A]	-	-	0/4/62/62	0/4/4/4
5	CI2	D	1001[B]	-	-	0/4/62/62	0/4/4/4
4	F15	A	1003	-	-	7/14/14/14	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	F15	C4-C1	4.14	1.60	1.50
4	C	1002	F15	C4-C1	3.36	1.58	1.50
5	D	1001[A]	CI2	C8-C19	2.98	1.59	1.53
5	D	1001[B]	CI2	C12-C13	2.88	1.55	1.50
5	D	1001[A]	CI2	C20-C19	2.58	1.58	1.53
5	D	1001[A]	CI2	C22-C4	-2.42	1.52	1.56
5	D	1001[A]	CI2	C21-C20	2.38	1.58	1.53
4	C	1002	F15	C5-C4	2.38	1.60	1.52
5	D	1001[B]	CI2	C8-C19	2.19	1.57	1.53
4	C	1002	F15	O2-C1	-2.16	1.23	1.30
4	A	1003	F15	C5-C4	2.07	1.59	1.52
5	D	1001[B]	CI2	C9-C8	2.05	1.57	1.53
4	A	1003	F15	O2-C1	-2.04	1.24	1.30
5	D	1001[B]	CI2	C15-C13	2.01	1.54	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1001[A]	CI2	C10-C11-C12	-3.62	106.11	111.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1001[A]	CI2	C6-C7-C22	3.09	107.48	103.84
5	D	1001[A]	CI2	C4-C22-C7	-2.99	96.60	99.72
5	D	1001[B]	CI2	C6-C7-C22	2.76	107.08	103.84
5	D	1001[A]	CI2	C21-C22-C7	2.71	111.30	107.25
5	D	1001[A]	CI2	C23-C22-C21	-2.65	106.69	110.61
5	D	1001[B]	CI2	C4-C22-C7	-2.65	96.95	99.72
5	D	1001[B]	CI2	C12-C11-C17	2.60	115.15	112.75
5	D	1001[B]	CI2	C18-C17-C11	-2.51	106.24	110.44
4	A	1003	F15	C8-C5-C4	2.49	122.29	113.13
4	A	1003	F15	O2-C1-C4	2.48	121.85	114.00
5	D	1001[A]	CI2	C15-C13-C12	2.42	119.56	115.89
5	D	1001[B]	CI2	C19-C17-C11	2.26	111.65	108.51
5	D	1001[B]	CI2	C5-C4-C22	2.16	106.15	104.21
5	D	1001[B]	CI2	C15-C16-C17	2.15	116.12	113.44
5	D	1001[A]	CI2	C23-C22-C7	2.14	115.55	111.68
5	D	1001[B]	CI2	C23-C22-C7	2.13	115.54	111.68
5	D	1001[A]	CI2	C9-C8-C7	-2.07	108.65	112.08
5	D	1001[B]	CI2	C10-C11-C12	-2.04	108.31	111.17

There are no chirality outliers.

All (15) torsion outliers are listed below:

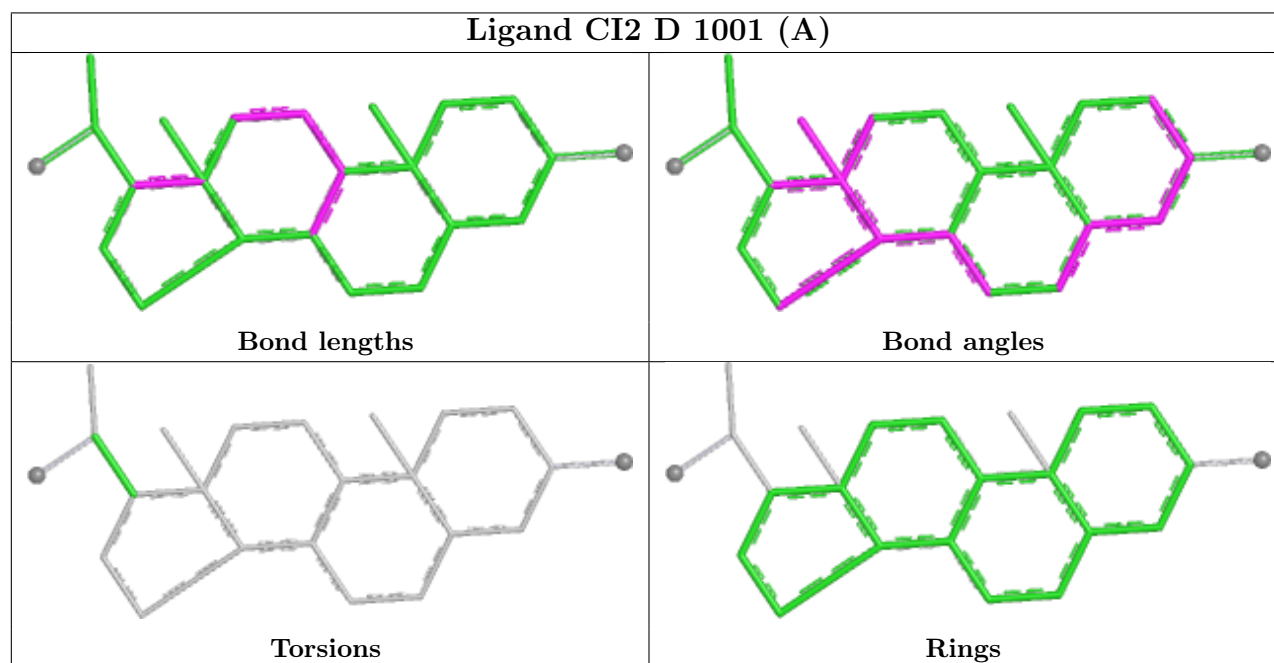
Mol	Chain	Res	Type	Atoms
4	A	1003	F15	C9-C10-C11-C12
4	A	1003	F15	C11-C10-C9-C7
4	C	1002	F15	C7-C6-C8-C5
4	C	1002	F15	C9-C10-C11-C12
4	A	1003	F15	C6-C7-C9-C10
4	C	1002	F15	C13-C2-C3-C14
4	C	1002	F15	C1-C4-C5-C8
4	A	1003	F15	C12-C13-C2-C3
4	A	1003	F15	C8-C6-C7-C9
4	C	1002	F15	C15-C14-C3-C2
4	A	1003	F15	O2-C1-C4-C5
4	A	1003	F15	O3-C1-C4-C5
4	C	1002	F15	C6-C7-C9-C10
4	C	1002	F15	O2-C1-C4-C5
4	C	1002	F15	O3-C1-C4-C5

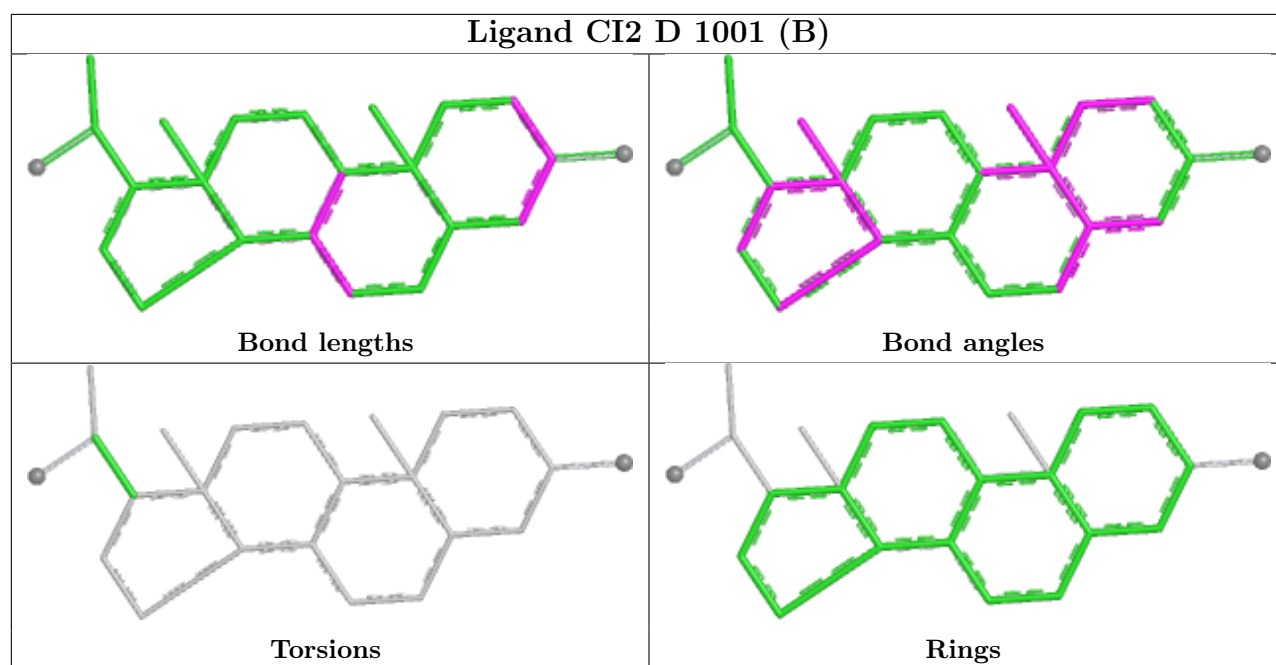
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1002	F15	4	0
5	D	1001[A]	CI2	5	0
5	D	1001[B]	CI2	2	0
4	A	1003	F15	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	232/236 (98%)	-1.23	0 100 100	45, 87, 131, 154	0
1	C	232/236 (98%)	-1.32	0 100 100	44, 82, 111, 130	0
2	B	246/246 (100%)	-1.24	0 100 100	55, 82, 140, 177	0
2	D	246/246 (100%)	-1.30	0 100 100	56, 82, 135, 173	0
3	E	10/13 (76%)	-0.99	0 100 100	112, 123, 125, 127	0
3	F	12/13 (92%)	-1.10	0 100 100	99, 105, 132, 134	0
3	G	12/13 (92%)	-1.13	0 100 100	115, 123, 132, 144	0
3	H	12/13 (92%)	-0.82	0 100 100	130, 134, 145, 148	0
All	All	1002/1016 (98%)	-1.26	0 100 100	44, 84, 134, 177	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

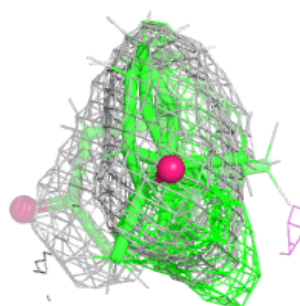
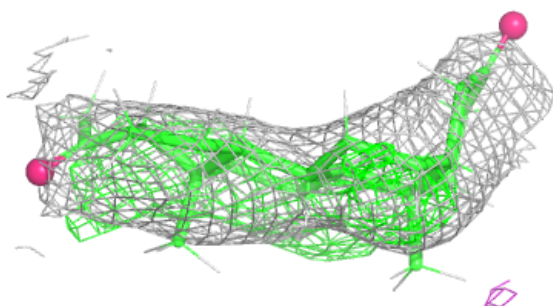
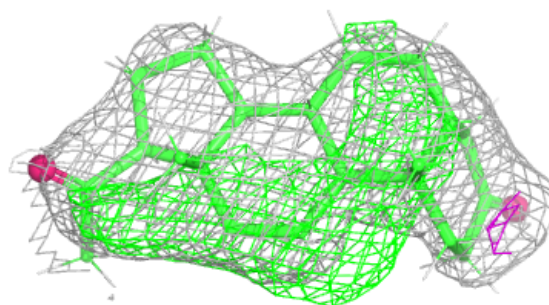
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

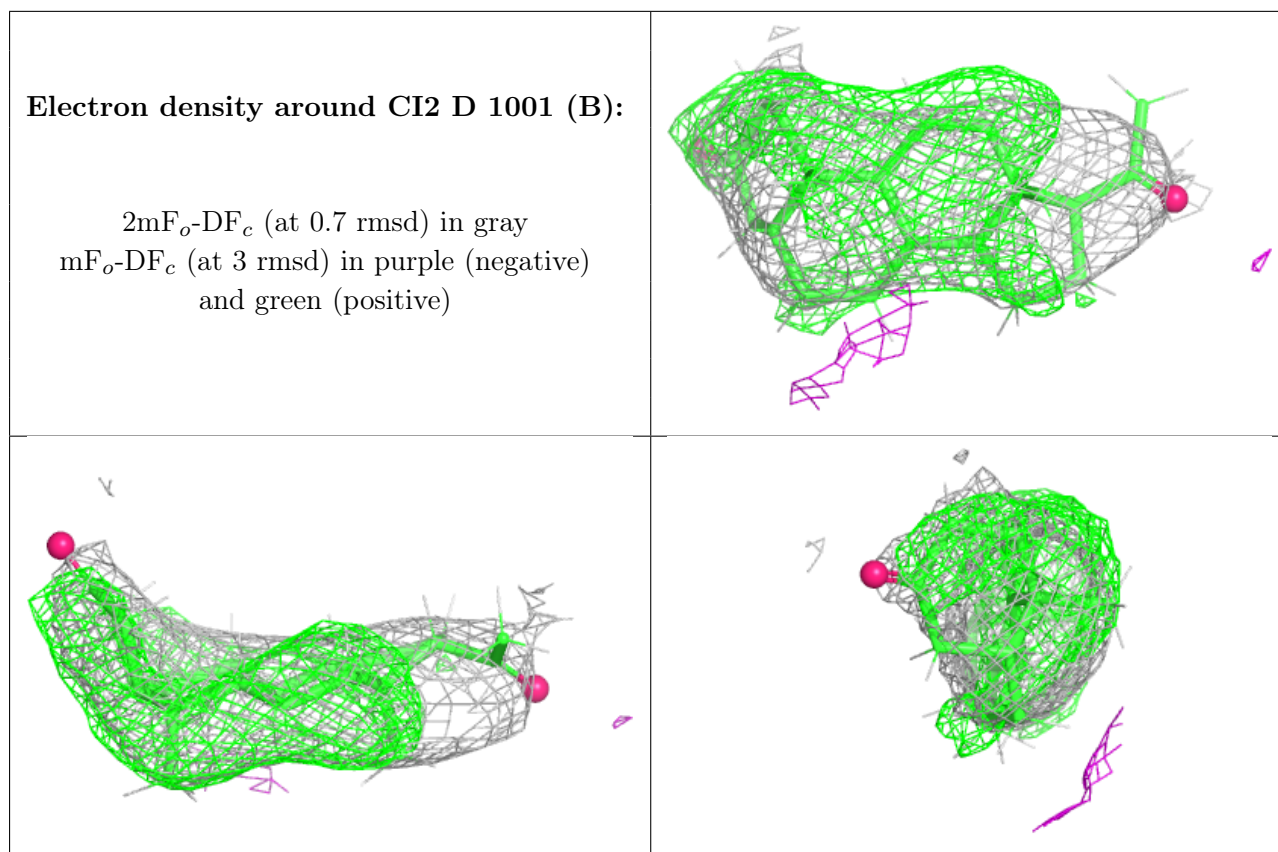
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	F15	A	1003	17/17	0.99	0.07	71,81,83,83	0
4	F15	C	1002	17/17	0.99	0.07	95,99,107,107	0
5	CI2	D	1001[A]	23/23	1.00	0.09	83,86,87,87	55
5	CI2	D	1001[B]	23/23	1.00	0.09	98,100,100,101	55

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 CI2 D 1001 (A):

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.