



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2023 – 10:40 PM EST

PDB ID : 1ZJ8
Title : Structure of Mycobacterium tuberculosis NirA protein
Authors : Schnell, R.; Sandalova, T.; Hellman, U.; Lindqvist, Y.; Schneider, G.; Structural Proteomics in Europe (SPINE)
Deposited on : 2005-04-28
Resolution : 2.80 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

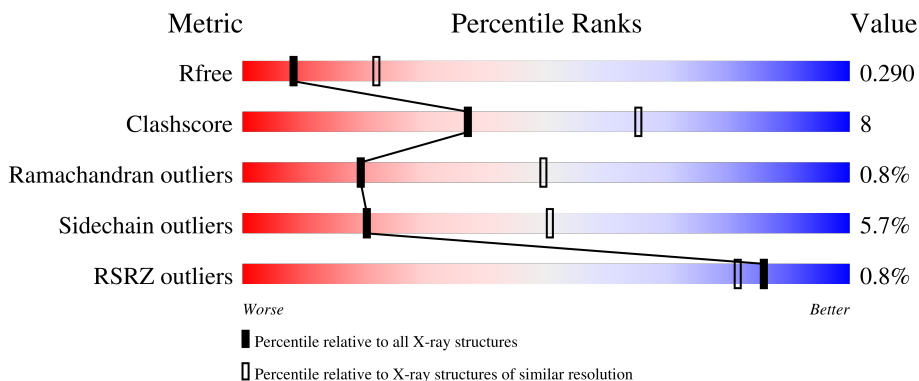
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	566	
1	B	566	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SF4	B	1556	-	-	X	-
4	SRM	B	1557	X	-	-	-

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 8798 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 Probable ferredoxin-dependent nitrite reductase NirA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	546	4316	2714	792	797	13	0	0	0
1	B	546	4316	2714	792	797	13	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP P71753
A	-9	ASP	-	expression tag	UNP P71753
A	-8	VAL	-	expression tag	UNP P71753
A	-7	SER	-	expression tag	UNP P71753
A	-6	HIS	-	expression tag	UNP P71753
A	-5	HIS	-	expression tag	UNP P71753
A	-4	HIS	-	expression tag	UNP P71753
A	-3	HIS	-	expression tag	UNP P71753
A	-2	HIS	-	expression tag	UNP P71753
A	-1	HIS	-	expression tag	UNP P71753
A	0	GLY	-	expression tag	UNP P71753
A	1	MET	-	expression tag	UNP P71753
A	2	ALA	-	expression tag	UNP P71753
B	-10	MET	-	expression tag	UNP P71753
B	-9	ASP	-	expression tag	UNP P71753
B	-8	VAL	-	expression tag	UNP P71753
B	-7	SER	-	expression tag	UNP P71753
B	-6	HIS	-	expression tag	UNP P71753
B	-5	HIS	-	expression tag	UNP P71753
B	-4	HIS	-	expression tag	UNP P71753
B	-3	HIS	-	expression tag	UNP P71753
B	-2	HIS	-	expression tag	UNP P71753
B	-1	HIS	-	expression tag	UNP P71753
B	0	GLY	-	expression tag	UNP P71753
B	1	MET	-	expression tag	UNP P71753

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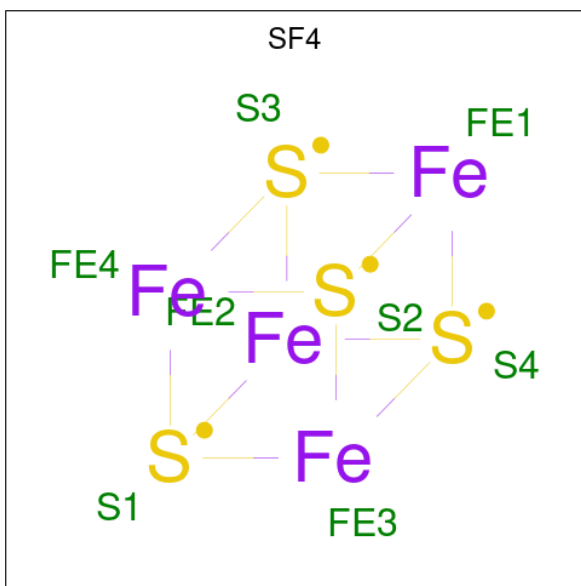
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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	ALA	-	expression tag	UNP P71753

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

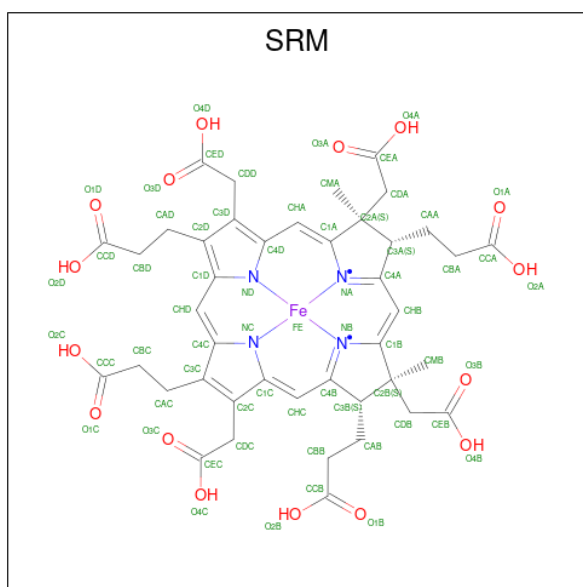
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0

- Molecule 4 is SIROHEME (three-letter code: SRM) (formula: C₄₂H₄₄FeN₄O₁₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
4	B	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		

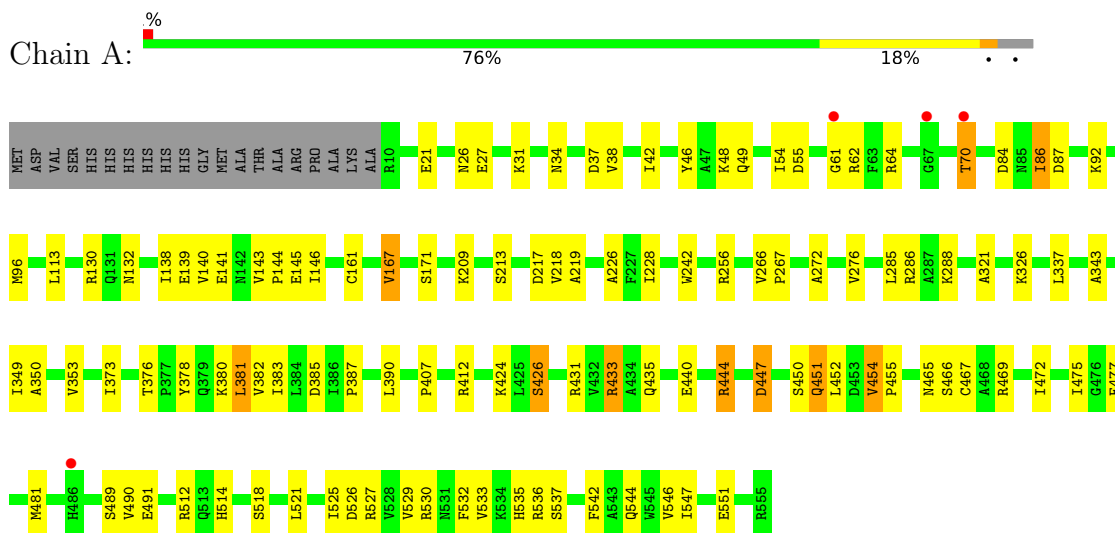
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	15	Total	O	0	0
			15	15		
5	B	7	Total	O	0	0
			7	7		

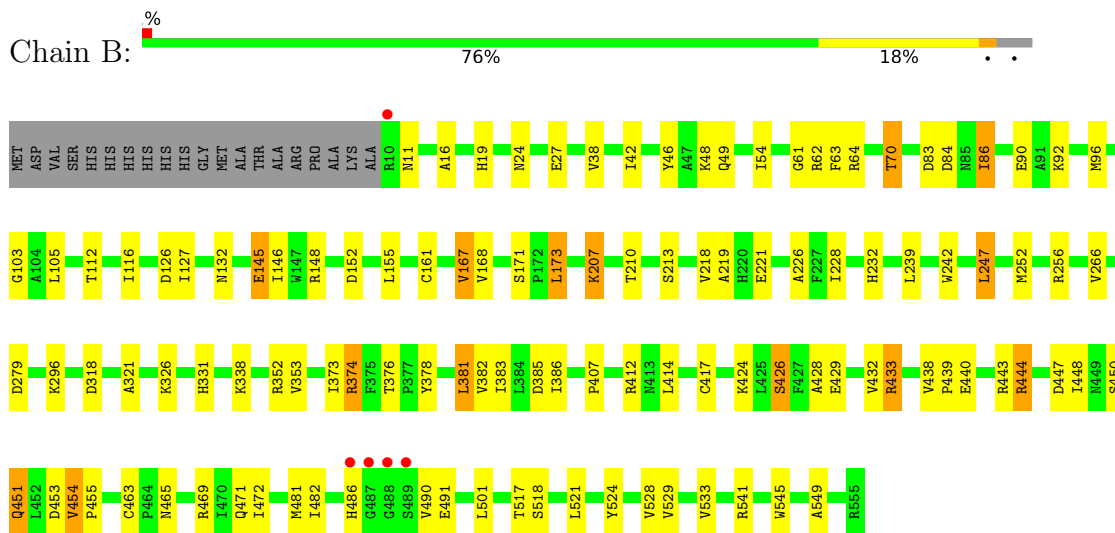
3 Residue-property plots

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: Probable ferredoxin-dependent nitrite reductase NirA



- Molecule 1: Probable ferredoxin-dependent nitrite reductase NirA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.26Å 115.36Å 114.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.65 – 2.80 81.33 – 2.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.65-2.80) 98.7 (81.33-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.58Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.292 0.223 , 0.290	Depositor DCC
R_{free} test set	1778 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtrriage
Anisotropy	0.381	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.019 for -h,l,k	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8798	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SF4, SRM

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	0.61	0/4409	0.72	1/5974 (0.0%)
1	B	0.57	0/4409	0.72	1/5974 (0.0%)
All	All	0.59	0/8818	0.72	2/11948 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	527	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts i

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4316	0	4256	65	0
1	B	4316	0	4256	69	0
2	A	1	0	0	0	0
2	B	1	0	0	1	0
3	A	8	0	0	1	0
3	B	8	0	0	2	0
4	A	63	0	34	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	63	0	34	4	0
5	A	15	0	0	0	0
5	B	7	0	0	1	0
All	All	8798	0	8580	136	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 8.

All (136) 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:96:MET:HE1	1:A:146:ILE:HG21	1.62	0.80
1:A:38:VAL:HG21	1:A:62:ARG:HB3	1.65	0.79
1:A:469:ARG:HG2	1:A:472:ILE:HD11	1.66	0.78
1:B:376:THR:HG22	1:B:378:TYR:H	1.54	0.71
1:B:454:VAL:HG21	1:B:541:ARG:HG2	1.71	0.71
1:A:209:LYS:NZ	4:A:557:SRM:O1C	2.23	0.70
4:A:557:SRM:HBD2	4:A:557:SRM:CED	2.22	0.69
1:A:46:TYR:CE1	1:A:54:ILE:HA	2.28	0.69
1:B:11:ASN:OD1	1:B:19:HIS:HB3	1.94	0.68
1:A:481:MET:HE2	1:A:491:GLU:HA	1.73	0.68
1:A:96:MET:CE	1:A:146:ILE:HG21	2.27	0.65
1:A:92:LYS:O	1:A:92:LYS:HG3	1.95	0.65
1:B:426:SER:HB3	3:B:1556:SF4:S2	2.37	0.65
1:B:429:GLU:OE2	1:B:432:VAL:N	2.30	0.65
1:B:239:LEU:HD13	1:B:266:VAL:HG21	1.81	0.63
1:B:46:TYR:CE1	1:B:54:ILE:HA	2.34	0.62
1:B:440:GLU:O	1:B:444:ARG:HB2	2.00	0.61
1:B:381:LEU:N	1:B:381:LEU:HD23	2.16	0.60
1:B:529:VAL:O	1:B:533:VAL:HG23	2.00	0.60
1:A:433:ARG:NH1	1:A:521:LEU:HD12	2.17	0.59
1:B:373:ILE:HD11	1:B:381:LEU:HD12	1.85	0.59
1:A:64:ARG:HB3	1:A:161:CYS:HB3	1.84	0.59
1:A:130:ARG:HE	1:A:167:VAL:HG23	1.68	0.59
1:A:96:MET:HE1	1:A:146:ILE:HD13	1.85	0.58
1:B:70:THR:HG22	1:B:424:LYS:NZ	2.19	0.58
1:A:433:ARG:HH11	1:A:521:LEU:HD12	1.69	0.57
1:B:132:ASN:ND2	4:B:1557:SRM:O1B	2.38	0.56
1:A:529:VAL:O	1:A:533:VAL:HG23	2.05	0.56
1:A:38:VAL:CG2	1:A:62:ARG:HB3	2.35	0.56
1:A:378:TYR:O	1:A:380:LYS:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LEU:N	1:A:381:LEU:HD23	2.20	0.56
1:A:481:MET:HA	1:A:481:MET:CE	2.36	0.55
1:A:387:PRO:HG2	1:A:390:LEU:HD12	1.87	0.55
1:B:207:LYS:NZ	2:B:1558:CL:CL	2.77	0.55
1:A:373:ILE:HD12	1:A:383:ILE:CD1	2.37	0.54
1:A:426:SER:HB3	3:A:556:SF4:S2	2.47	0.54
4:B:1557:SRM:HBD2	4:B:1557:SRM:CED	2.38	0.54
1:A:21:GLU:HA	1:A:21:GLU:OE1	2.07	0.54
1:A:481:MET:CE	1:A:491:GLU:HA	2.38	0.54
1:A:532:PHE:O	1:A:536:ARG:HB2	2.07	0.53
1:A:132:ASN:OD1	1:A:167:VAL:HG11	2.09	0.53
1:A:376:THR:HG22	1:A:378:TYR:H	1.73	0.52
1:B:433:ARG:HH12	1:B:521:LEU:HB2	1.74	0.52
1:B:256:ARG:CD	1:B:321:ALA:HB2	2.40	0.52
1:B:70:THR:HG22	1:B:424:LYS:CE	2.41	0.51
1:B:127:ILE:CD1	1:B:381:LEU:HD22	2.41	0.51
1:B:173:LEU:HD13	1:B:331:HIS:ND1	2.26	0.51
1:A:433:ARG:NH1	1:A:518:SER:O	2.43	0.51
1:A:132:ASN:ND2	4:A:557:SRM:O1B	2.41	0.51
1:A:92:LYS:NZ	1:A:139:GLU:OE1	2.44	0.51
1:A:440:GLU:O	1:A:444:ARG:HB2	2.11	0.50
1:B:42:ILE:HD11	1:B:63:PHE:CE1	2.46	0.50
1:B:112:THR:O	1:B:116:ILE:HG12	2.11	0.50
1:B:376:THR:HG22	1:B:378:TYR:N	2.26	0.50
1:A:38:VAL:HG12	1:A:42:ILE:HG12	1.95	0.49
1:B:221:GLU:HB2	1:B:501:LEU:HD22	1.95	0.49
1:B:168:VAL:HG13	1:B:210:THR:HG22	1.95	0.49
1:B:414:LEU:C	1:B:414:LEU:HD23	2.33	0.49
1:B:417:CYS:HB2	3:B:1556:SF4:S1	2.52	0.49
1:A:34:ASN:HB3	1:A:37:ASP:OD1	2.11	0.49
1:A:380:LYS:C	1:A:381:LEU:HD23	2.33	0.49
1:A:454:VAL:HG22	1:A:455:PRO:HD2	1.95	0.48
1:A:544:GLN:O	1:A:547:ILE:HG12	2.13	0.48
1:B:171:SER:HB2	1:B:213:SER:OG	2.14	0.48
1:B:226:ALA:HB3	1:B:242:TRP:HB2	1.96	0.48
1:A:226:ALA:HB3	1:A:242:TRP:HB2	1.95	0.48
1:B:433:ARG:NH1	1:B:518:SER:O	2.47	0.48
1:A:350:ALA:O	1:A:431:ARG:NH1	2.47	0.48
1:B:96:MET:CE	1:B:146:ILE:HG21	2.43	0.47
1:A:337:LEU:HD11	1:A:343:ALA:HB2	1.96	0.47
1:B:438:VAL:HB	1:B:439:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ILE:HG22	1:A:477:PHE:CE2	2.50	0.47
1:A:285:LEU:HB2	1:A:288:LYS:HB3	1.97	0.47
1:A:542:PHE:O	1:A:546:VAL:HG23	2.15	0.47
1:B:252:MET:HE1	1:B:296:LYS:HB2	1.96	0.47
1:B:481:MET:HA	1:B:481:MET:CE	2.44	0.47
1:B:103:GLY:O	1:B:374:ARG:HA	2.15	0.46
1:B:469:ARG:HG2	1:B:472:ILE:HD11	1.96	0.46
1:B:471:GLN:OE1	1:B:471:GLN:N	2.49	0.46
1:A:490:VAL:HG12	1:A:491:GLU:N	2.30	0.46
1:B:96:MET:HE1	1:B:146:ILE:HG21	1.97	0.46
1:B:145:GLU:OE1	1:B:148:ARG:NH2	2.49	0.46
1:A:34:ASN:O	1:A:37:ASP:OD1	2.34	0.46
1:B:207:LYS:HE3	4:B:1557:SRM:HBD1	1.98	0.46
1:A:450:SER:OG	1:A:451:GLN:NE2	2.48	0.46
1:B:490:VAL:HG12	1:B:491:GLU:N	2.30	0.46
1:A:465:ASN:HB3	4:A:557:SRM:C2D	2.47	0.45
1:A:521:LEU:O	1:A:525:ILE:HG12	2.17	0.45
1:B:247:LEU:CD1	1:B:469:ARG:HG3	2.45	0.45
1:A:27:GLU:O	1:A:31:LYS:HG2	2.16	0.45
1:A:218:VAL:O	1:A:219:ALA:C	2.54	0.45
1:B:70:THR:HG22	1:B:424:LYS:HZ2	1.81	0.45
1:B:482:ILE:HD11	1:B:517:THR:HG22	2.00	0.44
1:B:64:ARG:O	1:B:161:CYS:HB2	2.18	0.44
1:B:83:ASP:O	1:B:86:ILE:HG12	2.17	0.44
1:A:26:ASN:CG	1:A:286:ARG:HE	2.21	0.44
1:B:42:ILE:CD1	1:B:63:PHE:CZ	3.01	0.44
1:B:373:ILE:HD12	1:B:383:ILE:HD13	2.00	0.43
1:A:143:VAL:N	1:A:144:PRO:CD	2.81	0.43
1:A:266:VAL:HB	1:A:267:PRO:HD3	2.00	0.43
1:B:105:LEU:CD2	1:B:155:LEU:HD21	2.49	0.43
1:A:70:THR:HG23	1:A:424:LYS:HD3	2.00	0.43
1:A:447:ASP:OD1	1:A:447:ASP:C	2.57	0.43
1:A:452:LEU:HD23	1:A:452:LEU:HA	1.87	0.42
1:B:433:ARG:HH11	1:B:521:LEU:HD12	1.83	0.42
1:B:383:ILE:CG2	1:B:386:ILE:HD11	2.49	0.42
1:B:38:VAL:HG21	1:B:62:ARG:HB3	2.01	0.42
1:B:70:THR:HG21	1:B:90:GLU:OE2	2.20	0.42
1:B:84:ASP:OD1	1:B:84:ASP:N	2.45	0.42
1:B:465:ASN:HB3	4:B:1557:SRM:C2D	2.49	0.42
1:A:256:ARG:CD	1:A:321:ALA:HB2	2.48	0.42
1:A:526:ASP:O	1:A:530:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:ARG:NH1	1:B:521:LEU:HD12	2.34	0.42
1:A:373:ILE:HD12	1:A:383:ILE:HD13	2.00	0.42
1:B:126:ASP:OD1	1:B:352:ARG:HA	2.19	0.42
1:A:140:VAL:O	1:A:141:GLU:C	2.57	0.41
1:A:407:PRO:HG2	1:A:412:ARG:HB2	2.03	0.41
1:B:16:ALA:HB2	1:B:279:ASP:HB3	2.01	0.41
1:B:167:VAL:HG22	5:B:601:HOH:O	2.21	0.41
1:B:218:VAL:O	1:B:219:ALA:C	2.56	0.41
1:B:70:THR:O	1:B:424:LYS:NZ	2.52	0.41
1:B:454:VAL:HA	1:B:455:PRO:HD3	1.94	0.41
1:A:86:ILE:HD12	1:A:87:ASP:OD2	2.20	0.41
1:A:217:ASP:OD1	1:A:218:VAL:HG13	2.21	0.41
1:B:428:ALA:HA	1:B:491:GLU:OE1	2.21	0.41
1:B:407:PRO:HG2	1:B:412:ARG:HB2	2.03	0.41
1:B:450:SER:OG	1:B:451:GLN:NE2	2.39	0.41
1:A:272:ALA:O	1:A:276:VAL:HG23	2.20	0.41
1:B:524:TYR:O	1:B:528:VAL:HG12	2.20	0.41
1:B:127:ILE:HD13	1:B:381:LEU:HD22	2.03	0.40
1:B:24:ASN:HB2	1:B:27:GLU:H	1.86	0.40
1:B:545:TRP:CE2	1:B:549:ALA:HB2	2.56	0.40
1:A:171:SER:HB2	1:A:213:SER:OG	2.21	0.40
1:A:349:ILE:HG21	1:A:435:GLN:HA	2.04	0.40
1:A:467:CYS:SG	4:A:557:SRM:NC	2.95	0.40
1:B:232:HIS:HE1	1:B:318:ASP:O	2.03	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	544/566 (96%)	509 (94%)	30 (6%)	5 (1%)	17 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	544/566 (96%)	514 (94%)	26 (5%)	4 (1%)	22	53
All	All	1088/1132 (96%)	1023 (94%)	56 (5%)	9 (1%)	19	49

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	447	ASP
1	B	447	ASP
1	B	486	HIS
1	A	61	GLY
1	A	512	ARG
1	A	535	HIS
1	B	61	GLY
1	A	353	VAL
1	B	353	VAL

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	450/465 (97%)	425 (94%)	25 (6%)	21	51
1	B	450/465 (97%)	424 (94%)	26 (6%)	20	50
All	All	900/930 (97%)	849 (94%)	51 (6%)	20	50

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	49	GLN
1	A	55	ASP
1	A	70	THR
1	A	84	ASP
1	A	86	ILE
1	A	113	LEU

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Mol	Chain	Res	Type
1	A	138	ILE
1	A	145	GLU
1	A	167	VAL
1	A	228	ILE
1	A	326	LYS
1	A	381	LEU
1	A	382	VAL
1	A	385	ASP
1	A	426	SER
1	A	433	ARG
1	A	444	ARG
1	A	451	GLN
1	A	454	VAL
1	A	466	SER
1	A	489	SER
1	A	514	HIS
1	A	537	SER
1	A	551	GLU
1	B	48	LYS
1	B	49	GLN
1	B	70	THR
1	B	86	ILE
1	B	92	LYS
1	B	145	GLU
1	B	152	ASP
1	B	167	VAL
1	B	173	LEU
1	B	207	LYS
1	B	228	ILE
1	B	326	LYS
1	B	338	LYS
1	B	374	ARG
1	B	381	LEU
1	B	382	VAL
1	B	385	ASP
1	B	426	SER
1	B	433	ARG
1	B	443	ARG
1	B	444	ARG
1	B	448	ILE
1	B	451	GLN
1	B	453	ASP

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Mol	Chain	Res	Type
1	B	454	VAL
1	B	463	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	232	HIS
1	A	451	GLN
1	A	480	GLN
1	A	544	GLN
1	B	24	ASN
1	B	232	HIS
1	B	235	HIS

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SF4	A	556	1	0,12,12	-	-	-		
4	SRM	B	1557	-	68,70,70	1.44	10 (14%)	81,112,112	2.06	20 (24%)
4	SRM	A	557	-	68,70,70	1.49	13 (19%)	81,112,112	2.00	25 (30%)
3	SF4	B	1556	1	0,12,12	-	-	-		

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
3	SF4	A	556	1	-	-	0/6/5/5
3	SF4	B	1556	1	-	-	0/6/5/5
4	SRM	B	1557	-	1/1/19/23	12/38/126/126	-
4	SRM	A	557	-	-	12/38/126/126	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	557	SRM	C4C-C3C	-4.30	1.37	1.45
4	B	1557	SRM	C4C-C3C	-4.25	1.37	1.45
4	B	1557	SRM	C1C-C2C	-3.58	1.38	1.45
4	A	557	SRM	CHA-C1A	3.34	1.41	1.35
4	A	557	SRM	C1C-C2C	-3.34	1.39	1.45
4	B	1557	SRM	CHD-C4C	2.97	1.39	1.35
4	B	1557	SRM	CHA-C1A	2.93	1.40	1.35
4	A	557	SRM	CHD-C4C	2.91	1.39	1.35
4	A	557	SRM	C4B-NB	-2.67	1.33	1.35
4	A	557	SRM	CMA-C2A	-2.54	1.50	1.54
4	B	1557	SRM	O2C-CCC	-2.45	1.22	1.30
4	B	1557	SRM	CMA-C2A	-2.39	1.50	1.54
4	A	557	SRM	C1C-NC	-2.29	1.35	1.39
4	B	1557	SRM	O4C-CEC	-2.29	1.23	1.30
4	A	557	SRM	O2B-CCB	-2.26	1.23	1.30
4	A	557	SRM	CMB-C2B	-2.25	1.50	1.54
4	B	1557	SRM	O4A-CEA	-2.18	1.23	1.30
4	B	1557	SRM	C2A-C3A	-2.17	1.49	1.55
4	A	557	SRM	CDB-C2B	-2.15	1.49	1.56
4	A	557	SRM	O4B-CEB	-2.14	1.23	1.30
4	A	557	SRM	C2A-C3A	-2.11	1.49	1.55
4	A	557	SRM	CAA-C3A	-2.10	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1557	SRM	O2B-CCB	-2.08	1.23	1.30

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1557	SRM	C3D-CDD-CED	7.36	123.01	114.21
4	A	557	SRM	C3D-CDD-CED	7.35	123.01	114.21
4	B	1557	SRM	CAC-C3C-C2C	-6.46	115.89	129.51
4	B	1557	SRM	CAC-C3C-C4C	5.28	134.84	124.89
4	A	557	SRM	CAC-C3C-C2C	-5.00	118.96	129.51
4	B	1557	SRM	CBD-CAD-C2D	4.59	120.44	112.62
4	A	557	SRM	CAC-C3C-C4C	4.05	132.53	124.89
4	B	1557	SRM	C4D-CHA-C1A	-4.04	122.11	130.12
4	A	557	SRM	CBA-CAA-C3A	-3.95	103.32	114.73
4	A	557	SRM	CBD-CAD-C2D	3.51	118.60	112.62
4	A	557	SRM	C2C-C1C-NC	3.41	113.64	110.32
4	A	557	SRM	C1C-C2C-C3C	-3.41	102.92	106.86
4	A	557	SRM	CAD-CBD-CCD	3.36	123.17	113.76
4	A	557	SRM	C4D-CHA-C1A	-3.29	123.61	130.12
4	B	1557	SRM	CBA-CAA-C3A	-3.21	105.45	114.73
4	B	1557	SRM	CAD-CBD-CCD	3.14	122.55	113.76
4	B	1557	SRM	CAB-C3B-C4B	-3.10	105.72	111.19
4	A	557	SRM	CAB-C3B-C4B	-3.10	105.72	111.19
4	B	1557	SRM	C1C-C2C-C3C	-3.06	103.32	106.86
4	B	1557	SRM	O2D-CCD-CBD	2.95	123.52	114.03
4	A	557	SRM	CEC-CDC-C2C	2.92	121.37	113.79
4	A	557	SRM	C4C-NC-C1C	-2.88	102.53	105.35
4	B	1557	SRM	C2C-C1C-NC	2.86	113.11	110.32
4	A	557	SRM	CBC-CAC-C3C	2.77	120.33	112.63
4	B	1557	SRM	CBC-CAC-C3C	2.77	120.31	112.63
4	A	557	SRM	CAA-C3A-C4A	2.71	115.96	111.19
4	B	1557	SRM	C4C-NC-C1C	-2.64	102.76	105.35
4	B	1557	SRM	C2B-C1B-CHB	2.46	125.78	123.54
4	A	557	SRM	C2B-C1B-NB	2.44	115.13	111.21
4	A	557	SRM	CDD-C3D-C4D	-2.41	123.70	127.36
4	B	1557	SRM	O4D-CED-O3D	-2.37	117.38	123.30
4	B	1557	SRM	CAC-CBC-CCC	-2.34	108.56	113.60
4	A	557	SRM	O4D-CED-O3D	-2.34	117.48	123.30
4	B	1557	SRM	O2B-CCB-CBB	2.32	121.47	114.03
4	A	557	SRM	O2D-CCD-CBD	2.29	121.37	114.03
4	B	1557	SRM	CMA-C2A-CDA	2.27	114.55	110.80
4	A	557	SRM	CAC-CBC-CCC	-2.24	108.79	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	557	SRM	O2B-CCB-CBB	2.23	121.18	114.03
4	B	1557	SRM	CHC-C1C-C2C	-2.22	121.34	124.94
4	A	557	SRM	CHC-C1C-C2C	-2.19	121.39	124.94
4	B	1557	SRM	CEC-CDC-C2C	2.18	119.45	113.79
4	A	557	SRM	O2B-CCB-O1B	-2.14	117.96	123.30
4	A	557	SRM	O4A-CEA-CDA	2.08	121.02	114.35
4	A	557	SRM	C2A-C3A-C4A	2.03	103.50	100.90
4	A	557	SRM	CMB-C2B-C3B	2.00	115.78	112.08

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1557	SRM	NC

All (24) torsion outliers are listed below:

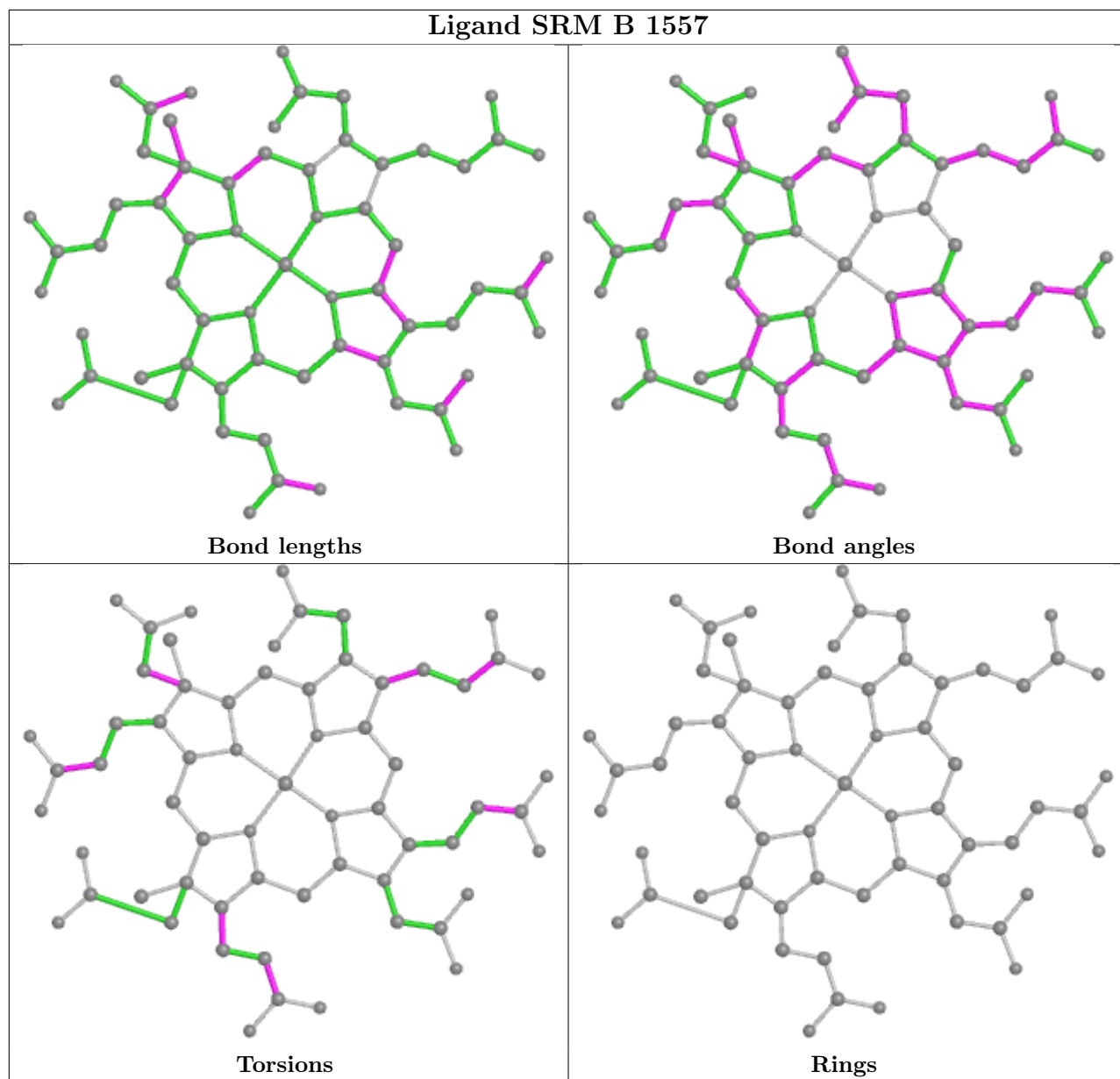
Mol	Chain	Res	Type	Atoms
4	A	557	SRM	C1A-C2A-CDA-CEA
4	A	557	SRM	CMA-C2A-CDA-CEA
4	A	557	SRM	C3D-C2D-CAD-CBD
4	B	1557	SRM	C1A-C2A-CDA-CEA
4	B	1557	SRM	CMA-C2A-CDA-CEA
4	B	1557	SRM	C3D-C2D-CAD-CBD
4	A	557	SRM	C4B-C3B-CAB-CBB
4	B	1557	SRM	C4B-C3B-CAB-CBB
4	B	1557	SRM	CAD-CBD-CCD-O2D
4	A	557	SRM	CAC-CBC-CCC-O2C
4	A	557	SRM	CAD-CBD-CCD-O2D
4	A	557	SRM	CAB-CBB-CCB-O2B
4	B	1557	SRM	CAD-CBD-CCD-O1D
4	A	557	SRM	C3A-C2A-CDA-CEA
4	A	557	SRM	CAC-CBC-CCC-O1C
4	A	557	SRM	CAB-CBB-CCB-O1B
4	A	557	SRM	CAD-CBD-CCD-O1D
4	B	1557	SRM	CAC-CBC-CCC-O1C
4	A	557	SRM	C3A-CAA-CBA-CCA
4	B	1557	SRM	CAC-CBC-CCC-O2C
4	B	1557	SRM	CAB-CBB-CCB-O2B
4	B	1557	SRM	CAB-CBB-CCB-O1B
4	B	1557	SRM	CAA-CBA-CCA-O2A
4	B	1557	SRM	CAA-CBA-CCA-O1A

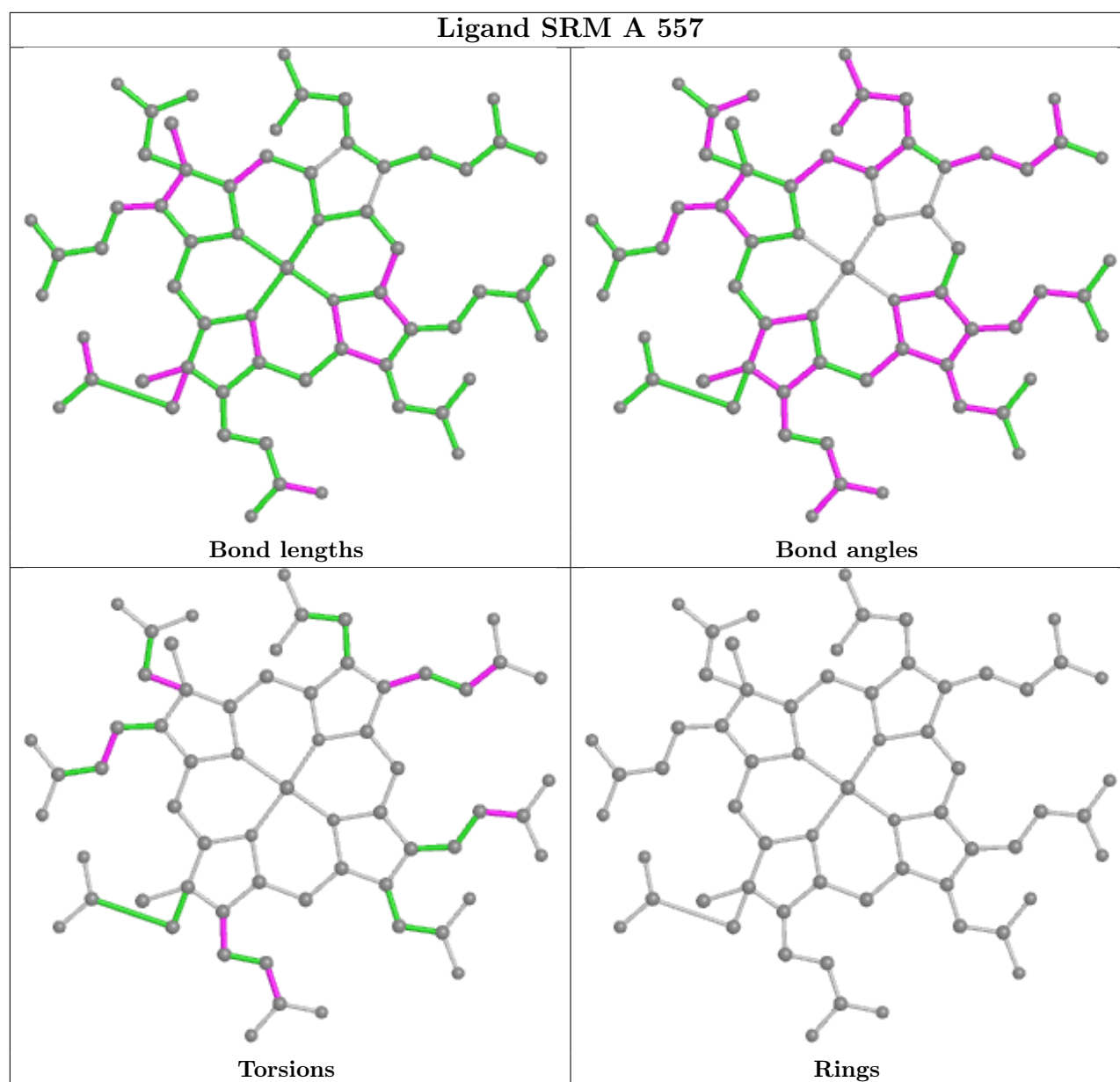
There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	556	SF4	1	0
4	B	1557	SRM	4	0
4	A	557	SRM	5	0
3	B	1556	SF4	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	546/566 (96%)	-0.29	4 (0%) 87 84	27, 43, 68, 83	0
1	B	546/566 (96%)	-0.32	5 (0%) 84 80	27, 43, 68, 82	0
All	All	1092/1132 (96%)	-0.30	9 (0%) 86 81	27, 43, 68, 83	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	487	GLY	4.8
1	A	61	GLY	3.6
1	A	486	HIS	3.2
1	B	10	ARG	2.9
1	A	67	GLY	2.7
1	B	488	GLY	2.5
1	B	489	SER	2.3
1	A	70	THR	2.0
1	B	486	HIS	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.

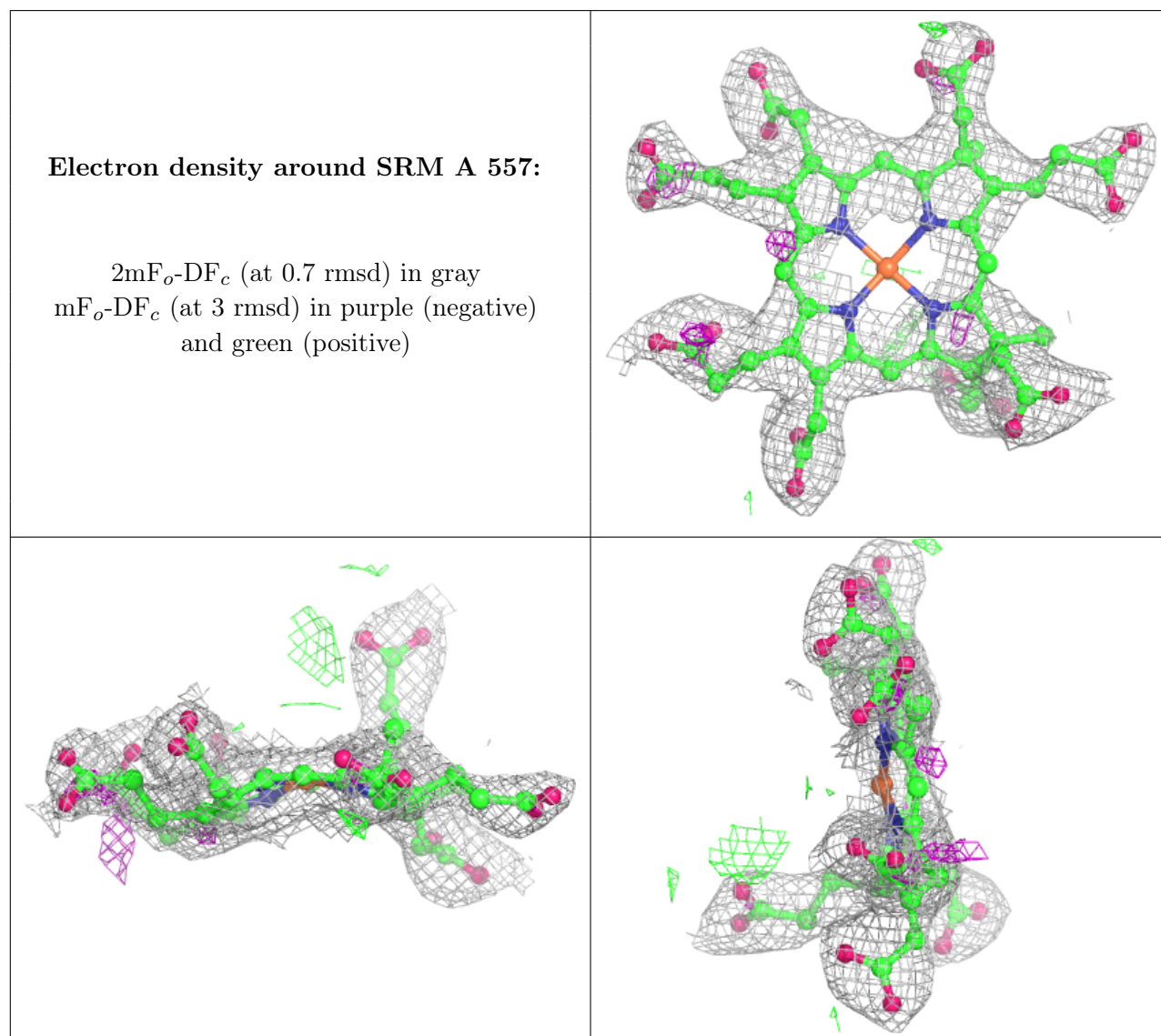
6.4 Ligands [i](#)

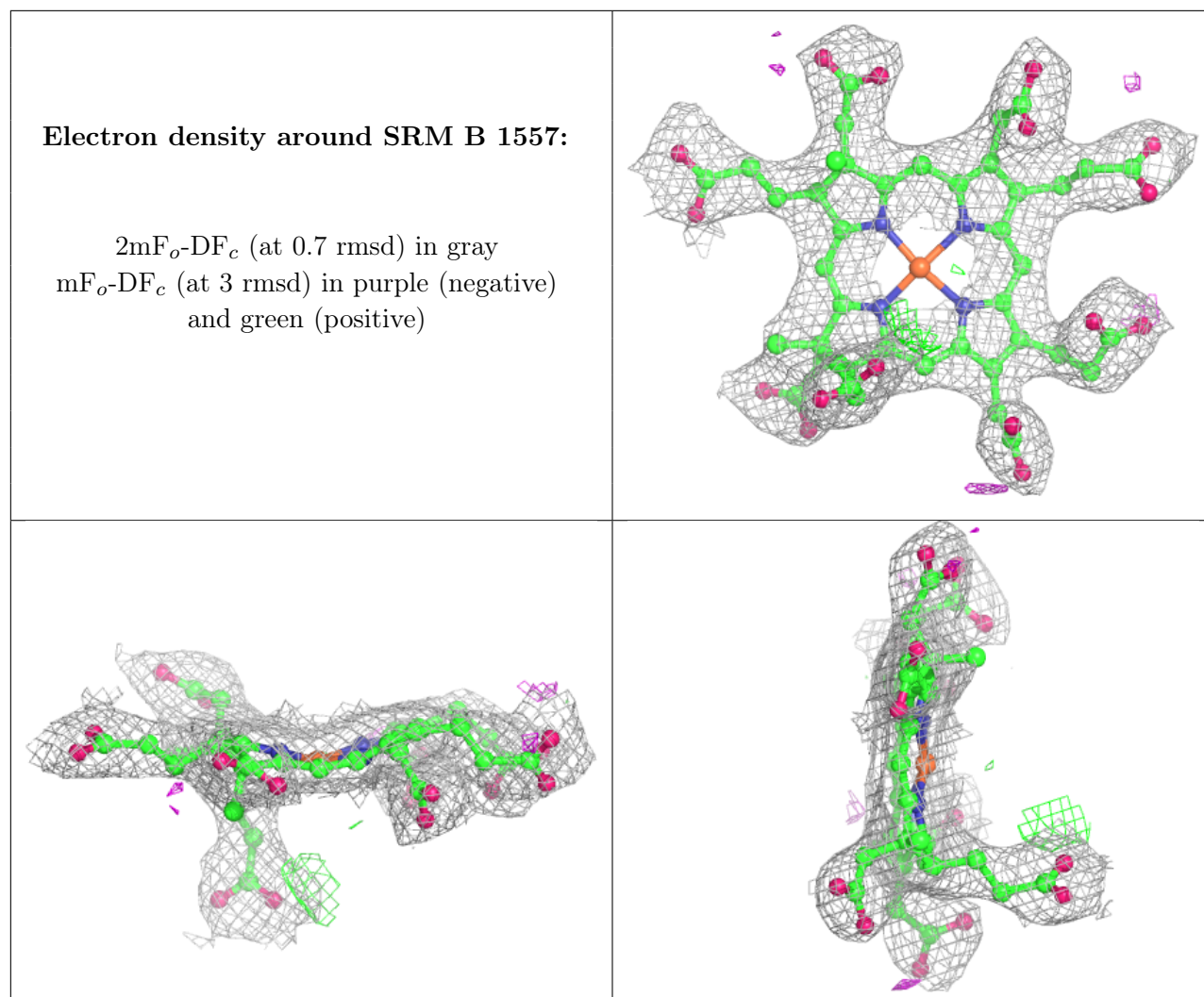
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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(Å ²)	Q<0.9
2	CL	A	558	1/1	0.86	0.20	43,43,43,43	0
2	CL	B	1558	1/1	0.91	0.10	27,27,27,27	0
4	SRM	A	557	63/63	0.95	0.23	28,36,42,47	0
4	SRM	B	1557	63/63	0.96	0.17	28,34,42,46	0
3	SF4	A	556	8/8	0.97	0.09	44,46,48,50	0
3	SF4	B	1556	8/8	0.99	0.11	30,32,33,33	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.