



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:31 AM UTC

PDB ID : 4J5X / pdb_00004j5x
Title : Crystal Structure of the SR12813-bound PXR/RXRalpha LBD Heterotrimeric Complex
Authors : Wallace, B.D.; Betts, L.; Redinbo, M.R.
Deposited on : 2013-02-10
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	:	4-5-2 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

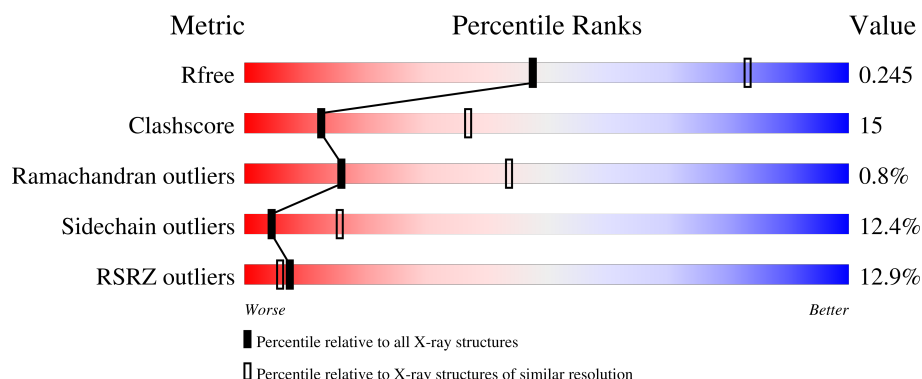
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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	C	264	8% 70% 16% • 10%
1	D	264	7% 64% 23% • 9%
2	A	336	13% 51% 29% 7% • 13%
2	B	336	15% 49% 32% 6% • 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8771 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 Retinoic acid receptor RXR-alpha, Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	239	Total	C	N	O	S	0	0	0
			1898	1215	329	343	11			
1	C	238	Total	C	N	O	S	0	0	0
			1887	1210	326	340	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	463	GLY	-	linker	UNP P19793
D	464	GLY	-	linker	UNP P19793
D	465	SER	-	linker	UNP P19793
D	466	GLY	-	linker	UNP Q15788
D	467	GLY	-	linker	UNP Q15788
C	463	GLY	-	linker	UNP P19793
C	464	GLY	-	linker	UNP P19793
C	465	SER	-	linker	UNP P19793
C	466	GLY	-	linker	UNP Q15788
C	467	GLY	-	linker	UNP Q15788

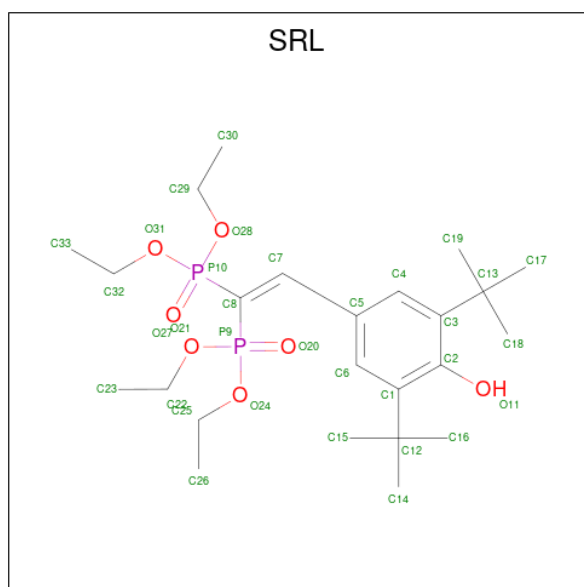
- Molecule 2 is a protein called Nuclear receptor subfamily 1 group I member 2, Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	293	Total	C	N	O	S	0	0	0
			2389	1532	413	426	18			
2	B	293	Total	C	N	O	S	0	0	0
			2371	1519	408	426	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	SER	-	expression tag	UNP O75469
A	128	ASN	-	expression tag	UNP O75469
A	129	ALA	-	expression tag	UNP O75469
A	435	GLY	-	linker	UNP Q15788
A	436	GLY	-	linker	UNP Q15788
A	437	SER	-	linker	UNP Q15788
A	438	GLY	-	linker	UNP Q15788
A	439	GLY	-	linker	UNP Q15788
B	127	SER	-	expression tag	UNP O75469
B	128	ASN	-	expression tag	UNP O75469
B	129	ALA	-	expression tag	UNP O75469
B	435	GLY	-	linker	UNP Q15788
B	436	GLY	-	linker	UNP Q15788
B	437	SER	-	linker	UNP Q15788
B	438	GLY	-	linker	UNP Q15788
B	439	GLY	-	linker	UNP Q15788

- Molecule 3 is [2-(3,5-DI-TERT-BUTYL-4-HYDROXY-PHENYL)-1-(DIETHOXY-PHOSPHORYL)-VINYL]-PHOSPHONIC ACID DIETHYL ESTER (CCD ID: SRL) (formula: $C_{24}H_{42}O_7P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			33	24	7	2		
3	B	1	Total	C	O	P	0	0
			33	24	7	2		

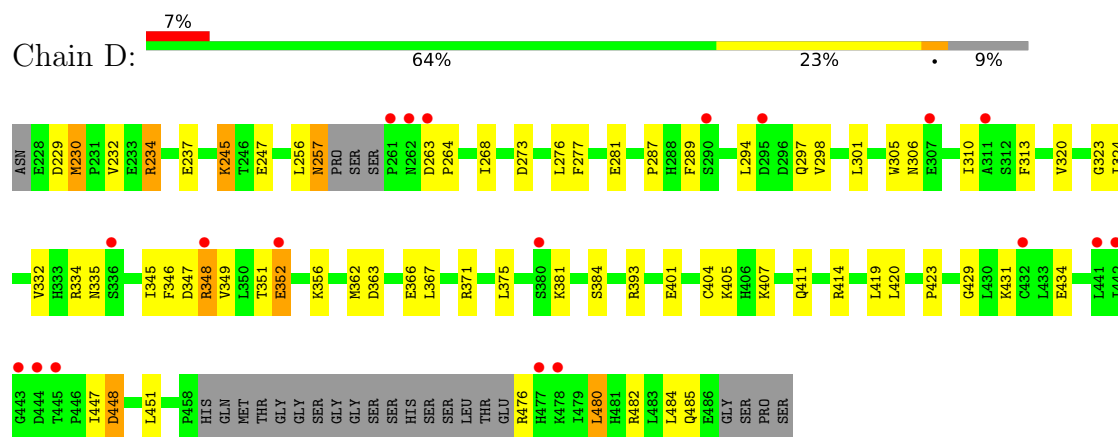
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	44	Total 44	O 44	0	0
4	C	34	Total 34	O 34	0	0
4	A	40	Total 40	O 40	0	0
4	B	42	Total 42	O 42	0	0

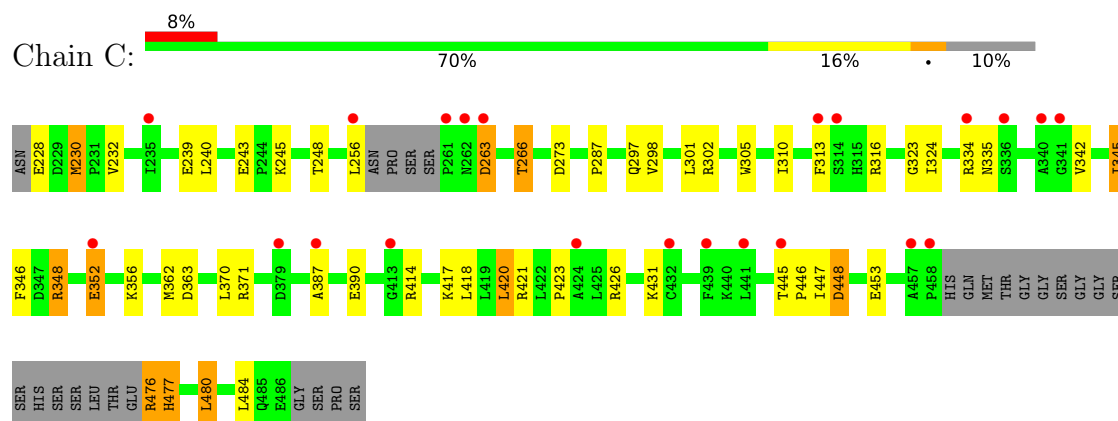
3 Residue-property plots

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.

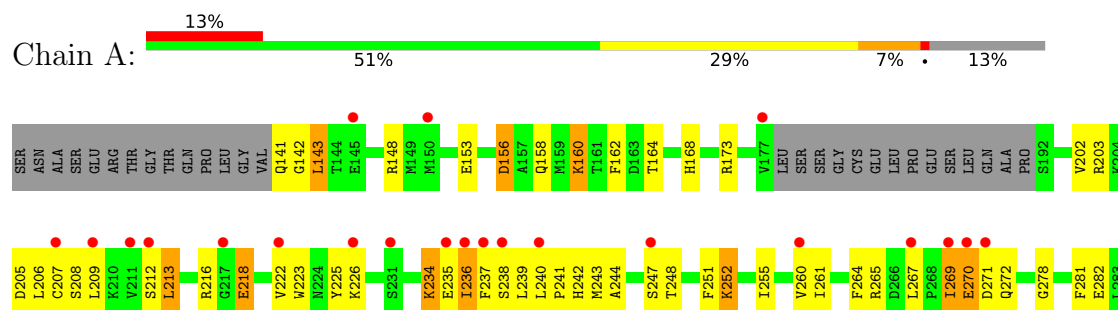
- Molecule 1: Retinoic acid receptor RXR-alpha, Nuclear receptor coactivator 1

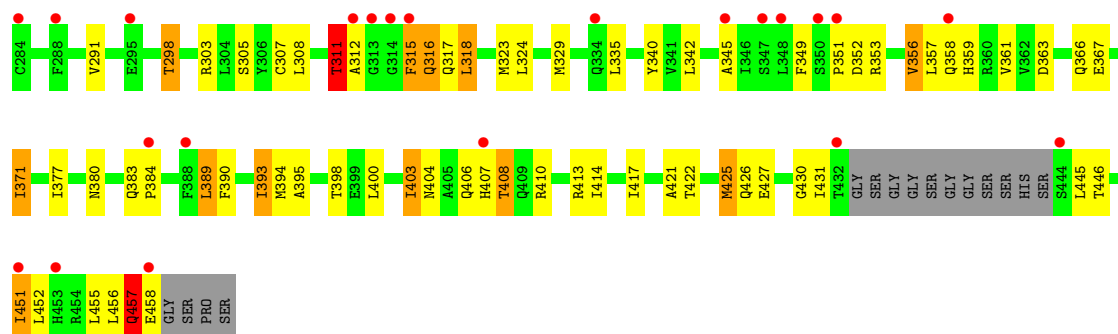


- Molecule 1: Retinoic acid receptor RXR-alpha, Nuclear receptor coactivator 1

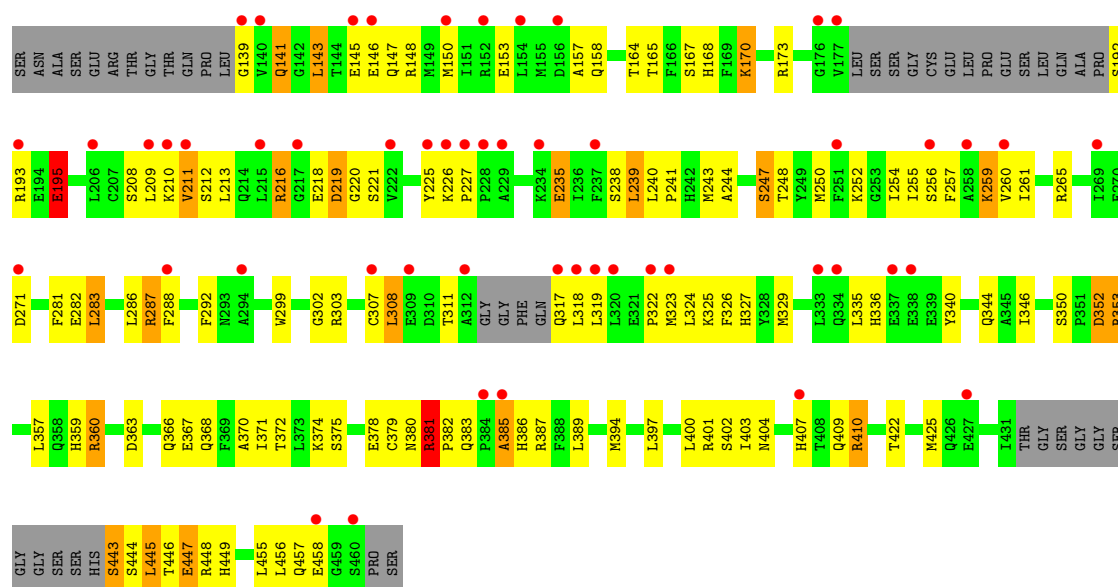


- Molecule 2: Nuclear receptor subfamily 1 group I member 2, Nuclear receptor coactivator 1





- Molecule 2: Nuclear receptor subfamily 1 group I member 2, Nuclear receptor coactivator 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.09Å 120.30Å 175.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.65 – 2.80 45.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.65-2.80) 99.4 (45.65-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.81Å)	Xtriage
Refinement program	PHENIX dev_1037	Depositor
R, R_{free}	0.245 , 0.298 0.248 , 0.245	Depositor DCC
R_{free} test set	1852 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.852	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8771	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1035e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SRL

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	C	0.31	0/1924	0.78	1/2599 (0.0%)
1	D	0.33	0/1935	0.78	1/2614 (0.0%)
2	A	0.34	0/2440	0.85	4/3283 (0.1%)
2	B	0.36	0/2420	0.87	6/3257 (0.2%)
All	All	0.34	0/8719	0.82	12/11753 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	240	LEU	CA-C-N	-8.22	110.48	119.19
2	A	240	LEU	C-N-CA	-8.22	110.48	119.19
2	B	385	ALA	N-CA-C	-7.18	101.65	113.50
2	B	195	GLU	N-CA-C	-7.13	104.39	113.23
2	B	157	ALA	N-CA-C	-6.11	106.36	113.88
2	A	318	LEU	N-CA-C	-5.93	105.89	113.01
2	B	457	GLN	N-CA-C	-5.73	106.63	113.97
1	C	335	ASN	N-CA-C	-5.49	106.51	113.43
2	A	234	LYS	N-CA-C	5.43	118.19	107.98
2	B	208	SER	N-CA-C	-5.29	105.54	113.89
1	D	335	ASN	N-CA-C	-5.11	106.38	113.18
2	B	211	VAL	N-CA-C	5.02	115.87	108.45

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	C	1887	0	1926	39	1
1	D	1898	0	1936	43	1
2	A	2389	0	2402	86	0
2	B	2371	0	2374	105	0
3	A	33	0	42	4	0
3	B	33	0	42	17	0
4	A	40	0	0	13	0
4	B	42	0	0	11	0
4	C	34	0	0	1	0
4	D	44	0	0	9	0
All	All	8771	0	8722	264	1

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 15.

All (264) 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)
2:B:209:LEU:HB3	3:B:501:SRL:H301	1.52	0.89
3:A:501:SRL:H173	3:A:501:SRL:H233	1.55	0.87
2:B:282:GLU:HG3	2:B:404:ASN:HD22	1.44	0.83
1:D:352:GLU:HG2	2:A:352:ASP:HB3	1.64	0.79
2:B:425:MET:HE1	3:B:501:SRL:H191	1.63	0.79
2:A:237:PHE:O	2:A:241:PRO:HD3	1.84	0.78
1:C:420:LEU:HD11	2:B:366:GLN:HG2	1.69	0.74
2:A:216:ARG:NH2	2:A:305:SER:OG	2.21	0.74
2:B:344:GLN:HG2	4:B:641:HOH:O	1.88	0.72
1:D:237:GLU:OE2	4:D:533:HOH:O	2.07	0.71
1:D:352:GLU:OE2	2:A:359:HIS:NE2	2.21	0.70
2:B:212:SER:HB2	2:B:307:CYS:HB3	1.73	0.70
1:C:352:GLU:HG2	2:B:352:ASP:HB3	1.74	0.67
2:B:254:ILE:HD12	2:B:283:LEU:HB3	1.77	0.67
2:B:216:ARG:NH1	2:B:303:ARG:O	2.28	0.67
2:B:283:LEU:HA	4:B:641:HOH:O	1.94	0.67
2:B:209:LEU:HB3	3:B:501:SRL:C30	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:264:PHE:O	2:A:272:GLN:NE2	2.28	0.66
2:B:173:ARG:HE	2:B:241:PRO:HB2	1.59	0.66
3:B:501:SRL:O28	3:B:501:SRL:HC6	1.96	0.66
2:A:390:PHE:H	2:A:393:ILE:HD12	1.61	0.65
1:C:476:ARG:NH1	1:C:477:HIS:O	2.29	0.65
2:A:281:PHE:HE2	2:A:403:ILE:HG22	1.61	0.65
2:B:374:LYS:NZ	4:B:618:HOH:O	2.29	0.65
2:B:281:PHE:CZ	2:B:323:MET:HE1	2.32	0.65
2:A:383:GLN:HB2	2:A:384:PRO:HD3	1.77	0.65
1:D:348:ARG:NH1	2:A:352:ASP:O	2.30	0.65
1:C:448:ASP:OD1	1:C:448:ASP:N	2.29	0.65
1:C:263:ASP:OD2	1:C:266:THR:OG1	2.16	0.64
1:C:302:ARG:HD2	1:C:477:HIS:CD2	2.33	0.64
1:D:393:ARG:NH2	4:D:515:HOH:O	2.30	0.63
1:D:482:ARG:NH1	4:D:526:HOH:O	2.31	0.62
2:A:353:ARG:NH1	4:A:604:HOH:O	2.31	0.62
2:A:318:LEU:HB3	2:A:324:LEU:HD22	1.82	0.62
2:A:342:LEU:HD23	4:A:634:HOH:O	2.00	0.62
1:C:239:GLU:OE1	1:C:371:ARG:NH1	2.33	0.62
2:B:383:GLN:O	2:B:385:ALA:N	2.31	0.61
2:B:139:GLY:HA2	2:B:382:PRO:HD2	1.82	0.60
2:B:219:ASP:OD1	2:B:220:GLY:N	2.35	0.60
2:B:243:MET:O	2:B:247:SER:OG	2.20	0.60
2:B:210:LYS:HE2	2:B:227:PRO:HB2	1.84	0.60
2:B:281:PHE:HE2	2:B:403:ILE:HG22	1.66	0.60
2:B:281:PHE:HZ	2:B:323:MET:HE1	1.65	0.60
2:B:326:PHE:HB2	2:B:403:ILE:HD11	1.84	0.59
3:B:501:SRL:H291	3:B:501:SRL:H153	1.83	0.59
2:A:236:ILE:HD12	2:A:236:ILE:H	1.67	0.59
2:B:260:VAL:O	4:B:628:HOH:O	2.16	0.59
2:B:282:GLU:HG2	2:B:400:LEU:HG	1.85	0.59
1:D:371:ARG:HD2	4:D:538:HOH:O	2.02	0.58
1:D:411:GLN:NE2	4:D:536:HOH:O	2.36	0.58
2:A:345:ALA:HB3	4:A:634:HOH:O	2.04	0.58
2:A:143:LEU:HB2	2:A:148:ARG:HG3	1.85	0.57
1:C:243:GLU:OE2	1:C:316:ARG:NH1	2.33	0.57
2:B:307:CYS:SG	2:B:308:LEU:N	2.77	0.57
2:B:283:LEU:HD12	4:B:641:HOH:O	2.03	0.57
1:D:345:ILE:HD13	1:D:431:LYS:HB3	1.84	0.57
2:B:381:ARG:O	2:B:383:GLN:N	2.35	0.57
2:A:209:LEU:HD13	3:A:501:SRL:H301	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:342:LEU:HA	4:A:634:HOH:O	2.03	0.57
1:D:323:GLY:O	4:D:505:HOH:O	2.18	0.56
2:B:165:THR:HG1	2:B:167:SER:HG	1.52	0.56
2:A:311:THR:OG1	2:A:312:ALA:N	2.37	0.56
1:D:334:ARG:HB3	1:D:346:PHE:CE2	2.41	0.55
2:A:278:GLY:HA3	2:A:353:ARG:HD2	1.89	0.55
1:D:294:LEU:HD21	1:D:485:GLN:HG2	1.87	0.55
1:C:302:ARG:HH11	1:C:477:HIS:CD2	2.24	0.55
2:B:407:HIS:CE1	2:B:410:ARG:HH11	2.25	0.55
2:A:316:GLN:OE1	2:A:317:GLN:N	2.39	0.55
2:B:380:ASN:OD1	2:B:381:ARG:N	2.40	0.54
2:B:235:GLU:O	2:B:238:SER:OG	2.26	0.54
2:B:141:GLN:HE22	2:B:380:ASN:HD22	1.54	0.54
2:B:256:SER:HA	2:B:259:LYS:HB2	1.89	0.54
2:B:360:ARG:NH1	2:B:363:ASP:OD2	2.41	0.54
1:C:453:GLU:CD	1:C:477:HIS:HA	2.33	0.54
2:B:286:LEU:HB2	4:B:641:HOH:O	2.07	0.54
1:D:230:MET:HE2	1:D:287:PRO:HB2	1.90	0.53
2:A:270:GLU:HG2	2:A:445:LEU:HD13	1.89	0.53
2:A:353:ARG:O	2:A:356:VAL:HG12	2.08	0.53
2:B:323:MET:HB2	2:B:407:HIS:HE2	1.74	0.53
1:D:294:LEU:HG	4:D:542:HOH:O	2.08	0.52
1:D:310:ILE:HA	1:D:313:PHE:CD2	2.44	0.52
2:A:351:PRO:HG3	2:A:363:ASP:HA	1.92	0.52
2:B:158:GLN:OE1	2:B:287:ARG:NH1	2.42	0.52
2:B:211:VAL:HG12	2:B:307:CYS:O	2.10	0.52
2:B:170:LYS:NZ	4:B:620:HOH:O	2.35	0.52
2:B:445:LEU:O	2:B:449:HIS:N	2.36	0.52
2:A:239:LEU:O	2:A:243:MET:HG2	2.10	0.52
2:A:352:ASP:OD1	2:A:352:ASP:N	2.41	0.52
2:B:340:TYR:O	2:B:344:GLN:HG3	2.09	0.52
2:A:238:SER:O	2:A:241:PRO:HD2	2.10	0.52
1:C:323:GLY:HA2	1:C:346:PHE:HZ	1.75	0.52
2:A:267:LEU:HB3	4:A:632:HOH:O	2.10	0.52
2:B:146:GLU:OE2	4:B:633:HOH:O	2.19	0.51
2:A:206:LEU:HB3	2:A:236:ILE:HG21	1.91	0.51
2:B:265:ARG:NH2	4:B:628:HOH:O	2.25	0.51
2:A:425:MET:HE3	3:A:501:SRL:C18	2.41	0.51
1:C:421:ARG:NH1	4:C:516:HOH:O	2.43	0.51
2:B:139:GLY:HA2	2:B:382:PRO:CD	2.40	0.51
2:B:213:LEU:HB3	2:B:225:TYR:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:434:GLU:OE2	4:D:518:HOH:O	2.19	0.50
2:A:244:ALA:O	2:A:247:SER:OG	2.20	0.50
1:C:345:ILE:HD13	1:C:431:LYS:HB3	1.92	0.50
1:C:417:LYS:HE2	2:B:367:GLU:HB3	1.92	0.50
2:A:270:GLU:HG2	2:A:445:LEU:HB3	1.94	0.49
2:B:147:GLN:HB3	2:B:372:THR:HG23	1.94	0.49
2:A:242:HIS:HD2	2:A:243:MET:HE3	1.77	0.49
2:B:425:MET:CE	3:B:501:SRL:H191	2.36	0.49
1:D:310:ILE:HA	1:D:313:PHE:CE2	2.47	0.49
1:C:310:ILE:HA	1:C:313:PHE:CE2	2.47	0.49
1:C:426:ARG:HH11	2:B:402:SER:HG	1.60	0.49
2:A:270:GLU:CG	2:A:445:LEU:HB3	2.43	0.49
2:B:363:ASP:O	2:B:367:GLU:HG3	2.12	0.49
1:C:423:PRO:HB2	2:B:401:ARG:HD2	1.94	0.49
2:B:327:HIS:CD2	3:B:501:SRL:H263	2.47	0.49
2:A:173:ARG:HE	2:A:241:PRO:HB3	1.78	0.49
2:B:346:ILE:HG21	2:B:397:LEU:HD13	1.93	0.49
2:B:247:SER:OG	3:B:501:SRL:H171	2.13	0.49
2:A:456:LEU:O	2:A:457:GLN:HB3	2.12	0.49
2:A:234:LYS:HA	2:A:237:PHE:CD2	2.48	0.48
1:D:264:PRO:O	1:D:268:ILE:HG13	2.13	0.48
2:B:143:LEU:HD23	2:B:379:CYS:SG	2.53	0.48
2:B:407:HIS:HA	2:B:410:ARG:HB2	1.94	0.48
1:C:230:MET:HE3	1:C:230:MET:HB2	1.77	0.48
2:B:447:GLU:HG2	2:B:448:ARG:N	2.29	0.48
2:B:443:SER:HB2	2:B:448:ARG:HE	1.79	0.47
1:D:401:GLU:HG2	1:D:405:LYS:HE2	1.96	0.47
2:A:205:ASP:CG	2:A:413:ARG:HH21	2.22	0.47
2:B:218:GLU:CD	2:B:218:GLU:H	2.22	0.47
1:D:447:ILE:HG23	1:D:451:LEU:HD23	1.97	0.47
2:B:381:ARG:N	2:B:382:PRO:HD3	2.29	0.47
1:C:266:THR:HG23	1:C:446:PRO:HD2	1.97	0.47
2:A:158:GLN:O	2:A:162:PHE:N	2.48	0.47
2:B:281:PHE:CE2	2:B:403:ILE:HG22	2.48	0.47
2:B:299:TRP:CD2	3:B:501:SRL:H222	2.49	0.47
2:B:352:ASP:OD1	2:B:352:ASP:N	2.25	0.47
2:A:426:GLN:O	2:A:430:GLY:N	2.48	0.47
2:A:235:GLU:O	2:A:238:SER:OG	2.29	0.46
1:D:230:MET:HE3	1:D:230:MET:HB2	1.83	0.46
1:D:345:ILE:O	1:D:349:VAL:HG23	2.15	0.46
2:A:164:THR:HG23	4:A:640:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:426:GLN:HG2	2:A:431:ILE:HB	1.96	0.46
1:C:323:GLY:HA2	1:C:346:PHE:CZ	2.50	0.46
2:A:406:GLN:O	2:A:410:ARG:HB2	2.14	0.46
1:D:245:LYS:O	1:D:245:LYS:NZ	2.40	0.46
2:A:202:VAL:HG13	2:A:414:ILE:HG12	1.96	0.46
2:B:282:GLU:HG3	2:B:404:ASN:ND2	2.23	0.46
2:A:395:ALA:O	2:A:398:THR:OG1	2.30	0.46
2:A:207:CYS:SG	2:A:208:SER:N	2.88	0.46
2:A:223:TRP:CZ3	2:B:225:TYR:HB2	2.51	0.46
2:A:377:ILE:HG21	2:A:389:LEU:HB3	1.97	0.46
2:B:367:GLU:O	2:B:371:ILE:HG13	2.16	0.46
1:D:298:VAL:HG13	1:D:480:LEU:HD13	1.98	0.46
1:C:352:GLU:CD	2:B:359:HIS:HE2	2.23	0.45
2:A:255:ILE:HG22	2:A:456:LEU:HD21	1.97	0.45
2:B:368:GLN:O	2:B:372:THR:OG1	2.26	0.45
1:C:476:ARG:HB2	1:C:477:HIS:H	1.41	0.45
2:A:271:ASP:HB2	4:A:632:HOH:O	2.15	0.45
2:A:451:ILE:O	2:A:455:LEU:HG	2.17	0.45
2:B:322:PRO:HA	2:B:325:LYS:HB3	1.99	0.45
2:B:443:SER:O	2:B:448:ARG:NH1	2.49	0.45
1:D:419:LEU:O	2:A:394:MET:HE2	2.17	0.45
2:A:156:ASP:O	2:A:160:LYS:HB2	2.17	0.45
2:B:141:GLN:NE2	2:B:380:ASN:HD22	2.13	0.45
2:B:407:HIS:CE1	3:B:501:SRL:H141	2.52	0.45
1:D:367:LEU:HD11	4:D:538:HOH:O	2.17	0.45
2:A:141:GLN:HG2	2:A:142:GLY:N	2.31	0.45
2:A:421:ALA:HA	4:A:639:HOH:O	2.15	0.45
1:D:277:PHE:O	1:D:281:GLU:HG2	2.17	0.45
1:D:356:LYS:HA	1:D:356:LYS:HD3	1.68	0.45
2:A:349:PHE:O	2:A:366:GLN:HB2	2.17	0.45
1:C:302:ARG:HD2	1:C:477:HIS:NE2	2.31	0.45
1:C:420:LEU:HA	2:B:394:MET:HE2	1.98	0.45
2:B:346:ILE:HD11	2:B:370:ALA:HA	1.98	0.45
2:B:299:TRP:CG	3:B:501:SRL:H222	2.51	0.45
2:A:141:GLN:HG2	2:A:142:GLY:H	1.81	0.44
2:A:269:ILE:HD12	2:A:270:GLU:H	1.82	0.44
2:B:250:MET:O	2:B:254:ILE:HG12	2.17	0.44
2:B:254:ILE:HG23	2:B:283:LEU:HD23	2.00	0.44
2:A:260:VAL:O	2:A:265:ARG:NH2	2.50	0.44
2:B:239:LEU:HD11	4:B:639:HOH:O	2.18	0.44
2:B:252:LYS:HA	2:B:255:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:501:SRL:H142	3:B:501:SRL:C29	2.48	0.44
1:C:356:LYS:HZ1	2:B:360:ARG:HH22	1.66	0.44
2:B:326:PHE:HB2	2:B:403:ILE:CD1	2.47	0.44
1:D:273:ASP:CG	1:D:448:ASP:HB2	2.43	0.44
2:A:422:THR:OG1	2:A:425:MET:HB2	2.18	0.44
1:D:448:ASP:OD1	1:D:448:ASP:N	2.42	0.44
2:A:216:ARG:HG2	2:A:222:VAL:HG22	1.99	0.44
2:B:244:ALA:O	2:B:248:THR:OG1	2.32	0.44
2:B:299:TRP:CZ2	3:B:501:SRL:H262	2.53	0.44
2:B:380:ASN:C	2:B:382:PRO:HD3	2.43	0.44
1:C:230:MET:HE2	1:C:287:PRO:HB2	1.98	0.44
1:C:414:ARG:O	1:C:418:LEU:HG	2.18	0.44
2:B:219:ASP:OD1	2:B:221:SER:OG	2.31	0.44
1:C:310:ILE:HA	1:C:313:PHE:CD2	2.52	0.43
2:A:218:GLU:H	2:A:218:GLU:HG2	1.66	0.43
2:A:282:GLU:HG3	2:A:400:LEU:HD22	1.99	0.43
1:C:302:ARG:HH11	1:C:477:HIS:HD2	1.64	0.43
1:C:301:LEU:O	1:C:305:TRP:HB3	2.19	0.43
2:A:281:PHE:CE2	2:A:403:ILE:HG22	2.46	0.43
1:C:387:ALA:HA	1:C:390:GLU:HB3	2.00	0.43
2:B:292:PHE:HD1	2:B:299:TRP:CE2	2.37	0.43
1:D:313:PHE:CD1	1:D:313:PHE:C	2.97	0.43
2:B:292:PHE:CD1	2:B:299:TRP:CE2	3.07	0.43
1:C:334:ARG:HB3	1:C:346:PHE:CE2	2.54	0.43
2:B:329:MET:HB3	2:B:329:MET:HE2	1.81	0.43
1:D:257:ASN:OD1	1:D:257:ASN:N	2.52	0.42
1:D:347:ASP:O	1:D:351:THR:HG23	2.18	0.42
2:A:456:LEU:HD22	4:A:638:HOH:O	2.18	0.42
2:A:212:SER:HB2	4:A:626:HOH:O	2.18	0.42
2:A:267:LEU:HD22	4:A:632:HOH:O	2.19	0.42
2:B:380:ASN:OD1	2:B:380:ASN:C	2.61	0.42
1:C:298:VAL:HG13	1:C:480:LEU:HD13	2.01	0.42
2:A:335:LEU:HB2	2:A:340:TYR:CE2	2.54	0.42
2:A:213:LEU:HB3	2:A:225:TYR:HB3	2.01	0.42
2:B:145:GLU:HA	2:B:148:ARG:HD3	2.01	0.42
1:D:276:LEU:HD21	1:D:305:TRP:CE3	2.54	0.42
2:A:452:LEU:HD12	2:A:452:LEU:HA	1.86	0.42
1:C:356:LYS:HA	1:C:356:LYS:HD3	1.79	0.42
2:B:286:LEU:HD12	4:B:641:HOH:O	2.19	0.42
1:D:310:ILE:HD12	1:D:429:GLY:HA2	2.00	0.42
2:B:407:HIS:ND1	3:B:501:SRL:H141	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:HIS:HB3	3:B:501:SRL:H162	2.01	0.42
1:C:273:ASP:CG	1:C:448:ASP:HB2	2.44	0.42
2:A:248:THR:O	2:A:252:LYS:HB2	2.19	0.42
2:A:291:VAL:HG13	4:A:640:HOH:O	2.20	0.42
2:B:336:HIS:CE1	2:B:381:ARG:HH11	2.38	0.42
1:C:370:LEU:HD23	1:C:370:LEU:HA	1.86	0.41
2:A:243:MET:HA	2:A:243:MET:HE2	2.01	0.41
2:A:269:ILE:H	2:A:269:ILE:HG13	1.53	0.41
2:A:298:THR:HB	2:A:307:CYS:HA	2.02	0.41
2:A:367:GLU:O	2:A:371:ILE:HG12	2.19	0.41
2:B:375:SER:HA	2:B:378:GLU:HB3	2.01	0.41
1:C:297:GLN:HB2	1:C:484:LEU:HD13	2.03	0.41
2:A:380:ASN:OD1	2:A:380:ASN:N	2.53	0.41
2:B:383:GLN:O	2:B:386:HIS:N	2.53	0.41
1:D:297:GLN:HB2	1:D:484:LEU:HD13	2.01	0.41
1:D:323:GLY:HA3	1:D:332:VAL:O	2.20	0.41
2:B:193:ARG:C	2:B:195:GLU:H	2.28	0.41
2:A:251:PHE:O	2:A:255:ILE:HG13	2.21	0.41
2:A:394:MET:O	2:A:398:THR:HG23	2.20	0.41
2:B:248:THR:O	2:B:252:LYS:HG2	2.20	0.41
2:B:350:SER:O	2:B:353:ARG:HG3	2.20	0.41
1:D:234:ARG:HE	1:D:234:ARG:HB3	1.54	0.41
1:D:301:LEU:O	1:D:305:TRP:HB3	2.20	0.41
2:B:288:PHE:CD1	3:B:501:SRL:H221	2.56	0.41
1:C:348:ARG:O	1:C:352:GLU:HB2	2.20	0.41
2:B:335:LEU:HB2	2:B:340:TYR:CE2	2.56	0.41
1:D:289:PHE:CD1	1:D:375:LEU:HD21	2.55	0.41
1:D:366:GLU:OE2	1:D:414:ARG:NH2	2.49	0.41
1:D:423:PRO:N	2:A:398:THR:HG22	2.36	0.41
1:C:445:THR:O	1:C:447:ILE:HG13	2.20	0.41
2:A:404:ASN:O	2:A:408:THR:OG1	2.38	0.41
2:A:407:HIS:CE1	3:A:501:SRL:H183	2.55	0.41
2:A:264:PHE:HE1	4:A:638:HOH:O	2.03	0.41
2:A:202:VAL:HG11	2:A:417:ILE:HD11	2.03	0.40
2:B:165:THR:O	2:B:302:GLY:HA3	2.21	0.40
2:B:259:LYS:HE3	2:B:456:LEU:C	2.46	0.40
2:B:283:LEU:HA	2:B:283:LEU:HD12	1.93	0.40
1:D:306:ASN:O	1:D:310:ILE:HG13	2.21	0.40
2:B:257:PHE:O	2:B:261:ILE:HG12	2.21	0.40
2:A:315:PHE:HD1	2:A:315:PHE:HA	1.73	0.40
3:B:501:SRL:H291	3:B:501:SRL:H142	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:261:ILE:O	2:A:265:ARG:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:GLU:OE2	1:C:248:THR:OG1[1_665]	2.13	0.07

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	C	232/264 (88%)	220 (95%)	10 (4%)	2 (1%)	14	41
1	D	233/264 (88%)	222 (95%)	10 (4%)	1 (0%)	30	60
2	A	287/336 (85%)	263 (92%)	22 (8%)	2 (1%)	18	47
2	B	285/336 (85%)	253 (89%)	29 (10%)	3 (1%)	11	36
All	All	1037/1200 (86%)	958 (92%)	71 (7%)	8 (1%)	16	44

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	457	GLN
2	B	219	ASP
2	B	381	ARG
1	C	263	ASP
2	A	311	THR
2	B	141	GLN
1	D	263	ASP
1	C	342	VAL

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	C	205/227 (90%)	187 (91%)	18 (9%)	9	29
1	D	207/227 (91%)	186 (90%)	21 (10%)	7	23
2	A	262/295 (89%)	226 (86%)	36 (14%)	3	13
2	B	260/295 (88%)	219 (84%)	41 (16%)	2	9
All	All	934/1044 (90%)	818 (88%)	116 (12%)	4	16

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	229	ASP
1	D	230	MET
1	D	232	VAL
1	D	234	ARG
1	D	245	LYS
1	D	256	LEU
1	D	257	ASN
1	D	320	VAL
1	D	324	ILE
1	D	348	ARG
1	D	352	GLU
1	D	362	MET
1	D	363	ASP
1	D	381	LYS
1	D	384	SER
1	D	404	CYS
1	D	407	LYS
1	D	420	LEU
1	D	448	ASP
1	D	476	ARG
1	D	480	LEU
1	C	228	GLU
1	C	230	MET
1	C	232	VAL

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Mol	Chain	Res	Type
1	C	240	LEU
1	C	245	LYS
1	C	256	LEU
1	C	266	THR
1	C	324	ILE
1	C	345	ILE
1	C	348	ARG
1	C	352	GLU
1	C	362	MET
1	C	363	ASP
1	C	420	LEU
1	C	448	ASP
1	C	476	ARG
1	C	477	HIS
1	C	480	LEU
2	A	143	LEU
2	A	153	GLU
2	A	156	ASP
2	A	160	LYS
2	A	168	HIS
2	A	203	ARG
2	A	213	LEU
2	A	218	GLU
2	A	226	LYS
2	A	236	ILE
2	A	252	LYS
2	A	269	ILE
2	A	270	GLU
2	A	298	THR
2	A	303	ARG
2	A	308	LEU
2	A	311	THR
2	A	315	PHE
2	A	316	GLN
2	A	323	MET
2	A	329	MET
2	A	356	VAL
2	A	357	LEU
2	A	358	GLN
2	A	361	VAL
2	A	371	ILE
2	A	389	LEU

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Mol	Chain	Res	Type
2	A	393	ILE
2	A	403	ILE
2	A	408	THR
2	A	425	MET
2	A	427	GLU
2	A	446	THR
2	A	451	ILE
2	A	457	GLN
2	A	458	GLU
2	B	143	LEU
2	B	150	MET
2	B	153	GLU
2	B	164	THR
2	B	168	HIS
2	B	170	LYS
2	B	192	SER
2	B	195	GLU
2	B	216	ARG
2	B	226	LYS
2	B	235	GLU
2	B	239	LEU
2	B	240	LEU
2	B	247	SER
2	B	259	LYS
2	B	271	ASP
2	B	283	LEU
2	B	287	ARG
2	B	308	LEU
2	B	311	THR
2	B	317	GLN
2	B	318	LEU
2	B	319	LEU
2	B	324	LEU
2	B	352	ASP
2	B	353	ARG
2	B	357	LEU
2	B	360	ARG
2	B	381	ARG
2	B	387	ARG
2	B	389	LEU
2	B	409	GLN
2	B	410	ARG

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Mol	Chain	Res	Type
2	B	422	THR
2	B	443	SER
2	B	444	SER
2	B	445	LEU
2	B	446	THR
2	B	447	GLU
2	B	455	LEU
2	B	458	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	275	GLN
1	D	288	HIS
1	C	253	ASN
1	C	275	GLN
1	C	477	HIS
2	A	141	GLN
2	A	201	GLN
2	A	366	GLN
2	B	141	GLN
2	B	201	GLN
2	B	214	GLN
2	B	366	GLN
2	B	404	ASN

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

2 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
3	SRL	B	501	-	30,33,33	1.74	6 (20%)	40,50,50	2.11	11 (27%)
3	SRL	A	501	-	30,33,33	1.27	4 (13%)	40,50,50	1.79	12 (30%)

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	SRL	B	501	-	-	12/36/44/44	0/1/1/1
3	SRL	A	501	-	-	8/36/44/44	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	SRL	C13-C3	-4.49	1.47	1.54
3	B	501	SRL	P10-O27	4.24	1.51	1.46
3	A	501	SRL	P10-O27	2.90	1.50	1.46
3	B	501	SRL	C4-C5	-2.85	1.34	1.39
3	B	501	SRL	P9-O24	2.80	1.64	1.57
3	A	501	SRL	P9-O20	2.77	1.49	1.46
3	B	501	SRL	C5-C7	2.62	1.51	1.46
3	B	501	SRL	C12-C1	-2.46	1.50	1.54
3	A	501	SRL	C13-C3	-2.33	1.50	1.54
3	A	501	SRL	C5-C7	2.30	1.51	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	SRL	C4-C3-C2	6.64	122.91	116.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	SRL	C3-C2-C1	-6.21	116.89	122.61
3	A	501	SRL	O31-P10-O27	-3.76	105.37	115.00
3	A	501	SRL	C3-C2-C1	-3.57	119.32	122.61
3	A	501	SRL	O24-P9-O21	3.50	112.00	102.13
3	B	501	SRL	C12-C1-C2	3.23	125.33	121.98
3	A	501	SRL	C4-C3-C2	3.12	119.70	116.87
3	A	501	SRL	C12-C1-C2	3.05	125.14	121.98
3	A	501	SRL	C16-C12-C1	2.87	116.33	110.87
3	B	501	SRL	C16-C12-C1	2.79	116.17	110.87
3	B	501	SRL	C19-C13-C3	-2.51	106.08	110.87
3	A	501	SRL	O31-P10-O28	2.48	109.13	102.13
3	A	501	SRL	O28-P10-O27	-2.47	108.68	115.00
3	B	501	SRL	O28-P10-O27	-2.40	108.84	115.00
3	B	501	SRL	C4-C3-C13	-2.31	114.47	120.19
3	B	501	SRL	C19-C13-C18	2.25	115.04	108.36
3	B	501	SRL	C15-C12-C1	-2.22	106.64	110.87
3	A	501	SRL	C18-C13-C17	-2.12	102.05	108.36
3	A	501	SRL	O21-P9-O20	-2.06	109.71	115.00
3	B	501	SRL	O21-C22-C23	2.02	122.85	110.80
3	A	501	SRL	C6-C1-C2	2.01	118.70	116.87
3	A	501	SRL	C19-C13-C18	2.00	114.31	108.36
3	B	501	SRL	C6-C5-C7	2.00	128.11	120.79

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	SRL	C4-C5-C7-C8
3	A	501	SRL	C6-C5-C7-C8
3	A	501	SRL	C5-C7-C8-P9
3	A	501	SRL	C5-C7-C8-P10
3	A	501	SRL	C7-C8-P9-O21
3	A	501	SRL	C7-C8-P10-O28
3	B	501	SRL	C5-C7-C8-P9
3	B	501	SRL	C5-C7-C8-P10
3	B	501	SRL	C7-C8-P10-O28
3	B	501	SRL	C7-C8-P10-O31
3	B	501	SRL	C2-C1-C12-C16
3	B	501	SRL	C2-C1-C12-C14
3	B	501	SRL	C2-C1-C12-C15
3	B	501	SRL	C6-C1-C12-C16
3	A	501	SRL	C22-O21-P9-C8

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Mol	Chain	Res	Type	Atoms
3	B	501	SRL	C25-O24-P9-C8
3	B	501	SRL	C6-C1-C12-C14
3	B	501	SRL	C22-O21-P9-O24
3	B	501	SRL	C6-C1-C12-C15
3	A	501	SRL	C22-O21-P9-O24

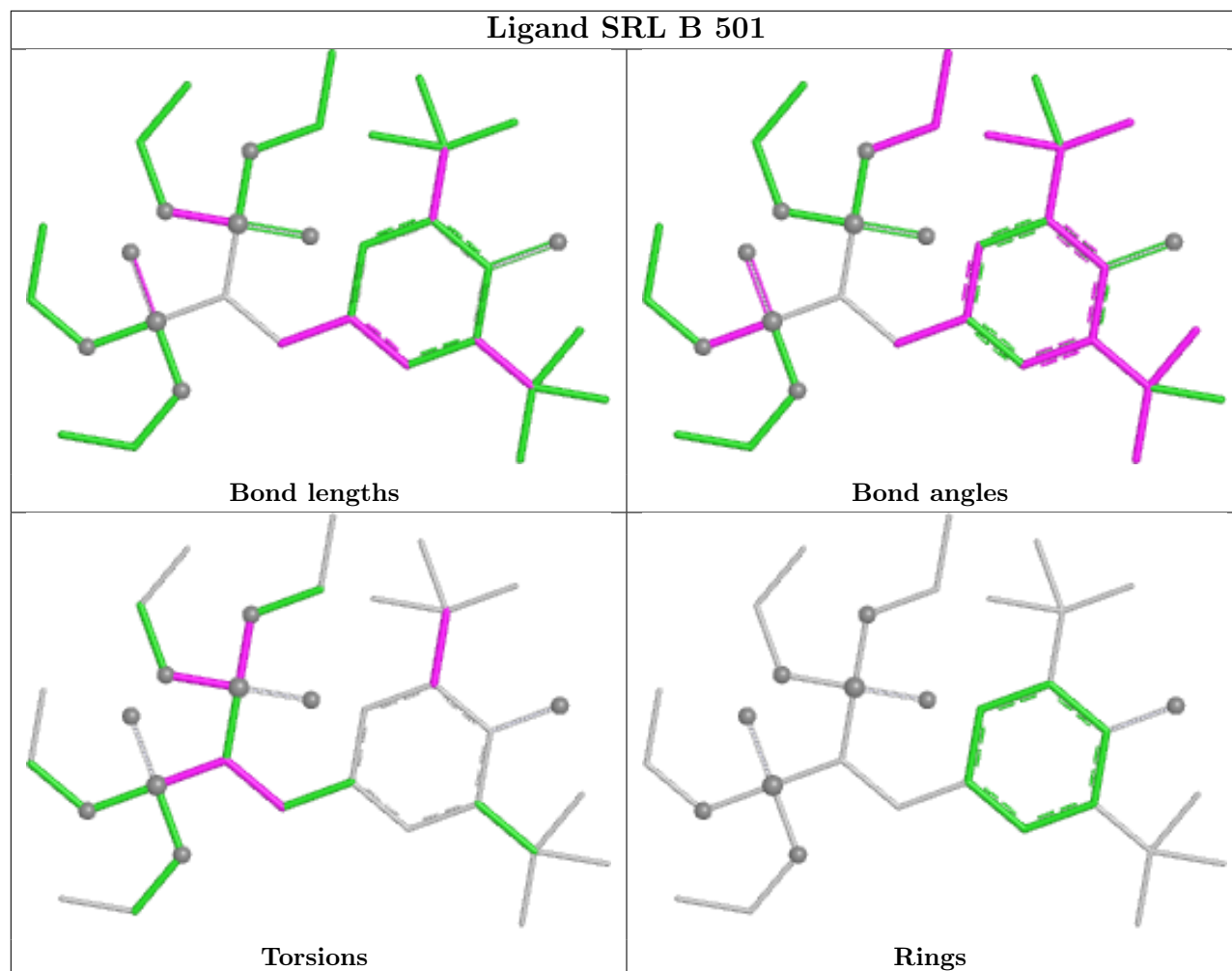
There are no ring outliers.

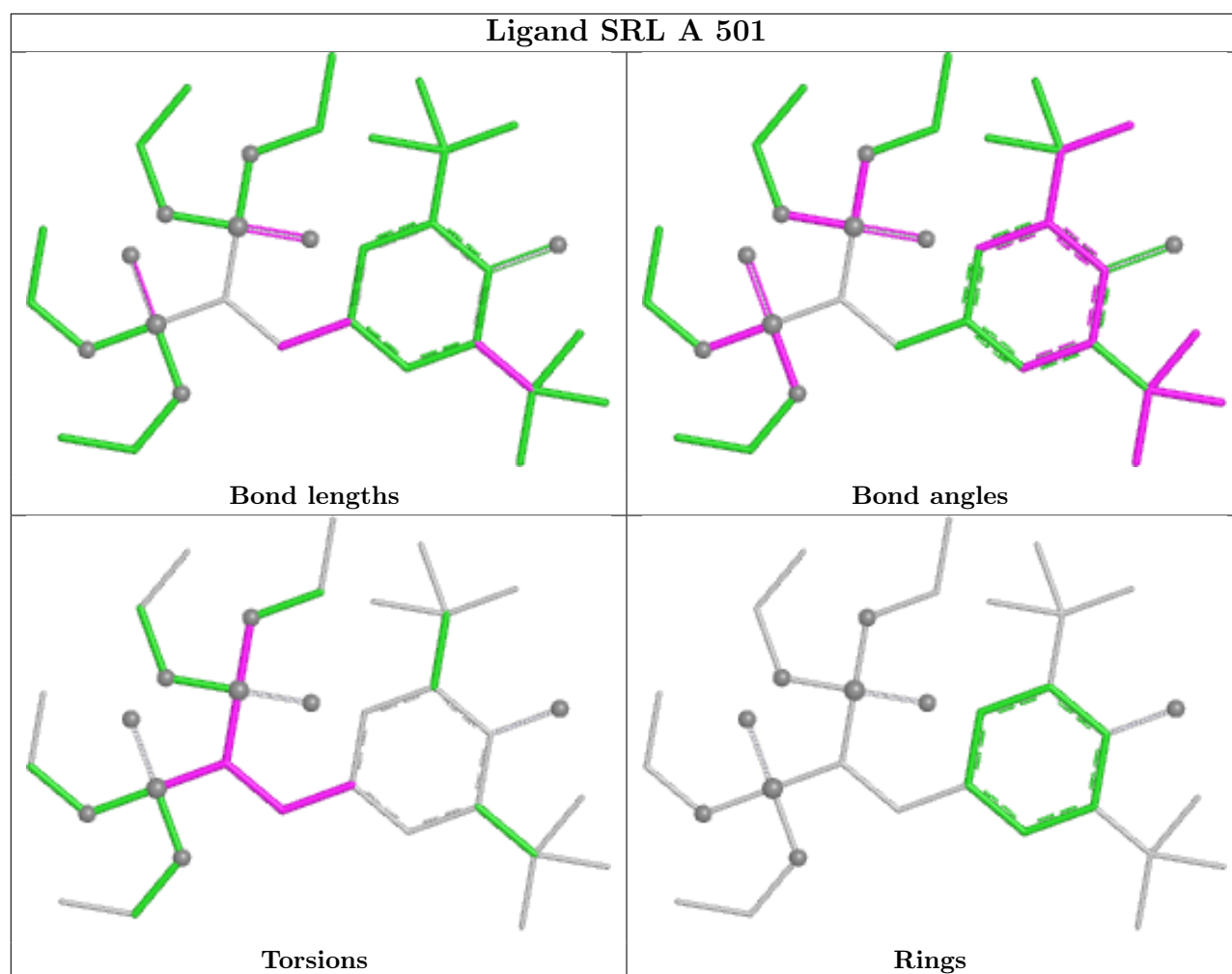
2 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	SRL	17	0
3	A	501	SRL	4	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.

Ligand SRL B 501





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	C	238/264 (90%)	0.99	22 (9%)	14 10	28, 47, 73, 123	0
1	D	239/264 (90%)	0.88	19 (7%)	18 13	30, 46, 79, 101	0
2	A	293/336 (87%)	1.11	44 (15%)	5 4	28, 54, 90, 128	0
2	B	293/336 (87%)	1.20	52 (17%)	4 3	33, 55, 93, 111	0
All	All	1063/1200 (88%)	1.05	137 (12%)	7 6	28, 51, 87, 128	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	236	ILE	5.2
2	A	237	PHE	5.0
2	B	229	ALA	4.2
2	A	150	MET	4.2
1	C	387	ALA	4.0
2	B	217	GLY	4.0
2	A	177	VAL	4.0
2	B	323	MET	3.9
2	B	140	VAL	3.8
2	A	211	VAL	3.8
1	C	261	PRO	3.8
2	B	139	GLY	3.7
1	C	432	CYS	3.7
1	D	477	HIS	3.6
1	D	445	THR	3.6
1	C	340	ALA	3.5
1	C	457	ALA	3.5
1	D	261	PRO	3.4
1	D	432	CYS	3.4
2	B	150	MET	3.4
2	A	347	SER	3.4

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Mol	Chain	Res	Type	RSRZ
2	A	351	PRO	3.3
2	B	317	GLN	3.3
1	C	256	LEU	3.3
2	B	269	ILE	3.3
2	B	211	VAL	3.3
2	A	432	THR	3.3
2	B	193	ARG	3.1
1	C	262	ASN	3.1
1	C	439	PHE	3.1
2	B	177	VAL	3.1
1	C	352	GLU	3.1
1	D	441	LEU	3.1
2	B	384	PRO	3.1
1	D	352	GLU	3.1
2	B	320	LEU	3.0
1	D	295	ASP	2.9
2	A	238	SER	2.9
2	B	319	LEU	2.9
2	A	345	ALA	2.9
2	A	271	ASP	2.9
1	D	348	ARG	2.8
2	A	288	PHE	2.8
1	C	263	ASP	2.8
1	D	263	ASP	2.8
2	B	460	SER	2.8
2	B	176	GLY	2.8
2	A	260	VAL	2.7
1	C	441	LEU	2.7
2	A	350	SER	2.7
2	B	227	PRO	2.7
2	B	458	GLU	2.7
2	B	318	LEU	2.7
2	B	156	ASP	2.7
2	A	312	ALA	2.7
2	A	388	PHE	2.6
2	B	228	PRO	2.6
2	A	145	GLU	2.6
2	A	458	GLU	2.6
2	B	333	LEU	2.6
2	B	385	ALA	2.6
2	A	269	ILE	2.6
1	D	311	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	A	247	SER	2.6
2	B	210	LYS	2.6
2	A	270	GLU	2.6
2	A	384	PRO	2.5
2	A	315	PHE	2.5
2	B	312	ALA	2.5
2	B	407	HIS	2.5
2	B	322	PRO	2.5
2	A	295	GLU	2.5
2	B	145	GLU	2.5
2	A	453	HIS	2.5
2	B	154	LEU	2.4
2	B	237	PHE	2.4
2	A	313	GLY	2.4
2	B	146	GLU	2.4
2	B	225	TYR	2.4
1	C	424	ALA	2.4
2	B	215	LEU	2.4
1	D	442	ILE	2.3
1	C	341	GLY	2.3
1	C	379	ASP	2.3
2	A	207	CYS	2.3
2	B	334	GLN	2.3
1	C	235	ILE	2.3
2	A	226	LYS	2.3
1	C	313	PHE	2.3
2	B	288	PHE	2.3
2	A	240	LEU	2.3
2	A	358	GLN	2.3
2	A	212	SER	2.3
2	A	267	LEU	2.3
2	B	226	LYS	2.3
1	D	380	SER	2.3
1	C	413	GLY	2.3
2	B	258	ALA	2.2
2	B	309	GLU	2.2
2	A	209	LEU	2.2
2	B	234	LYS	2.2
1	C	445	THR	2.2
1	C	458	PRO	2.2
1	D	336	SER	2.2
2	B	251	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	A	235	GLU	2.2
1	D	262	ASN	2.2
2	A	407	HIS	2.2
2	B	222	VAL	2.2
1	D	307	GLU	2.2
2	A	451	ILE	2.2
2	A	334	GLN	2.2
2	A	222	VAL	2.2
1	C	314	SER	2.2
2	A	231	SER	2.2
2	B	427	GLU	2.2
1	D	478	LYS	2.1
2	B	209	LEU	2.1
2	A	444	SER	2.1
2	B	307	CYS	2.1
2	B	294	ALA	2.1
2	B	260	VAL	2.1
2	A	217	GLY	2.1
2	B	206	LEU	2.1
2	B	271	ASP	2.1
1	D	443	GLY	2.1
1	C	334	ARG	2.1
2	B	152	ARG	2.1
1	D	290	SER	2.0
1	D	444	ASP	2.0
2	B	337	GLU	2.0
1	C	336	SER	2.0
2	B	256	SER	2.0
2	A	284	CYS	2.0
2	A	348	LEU	2.0
2	A	314	GLY	2.0
2	B	338	GLU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

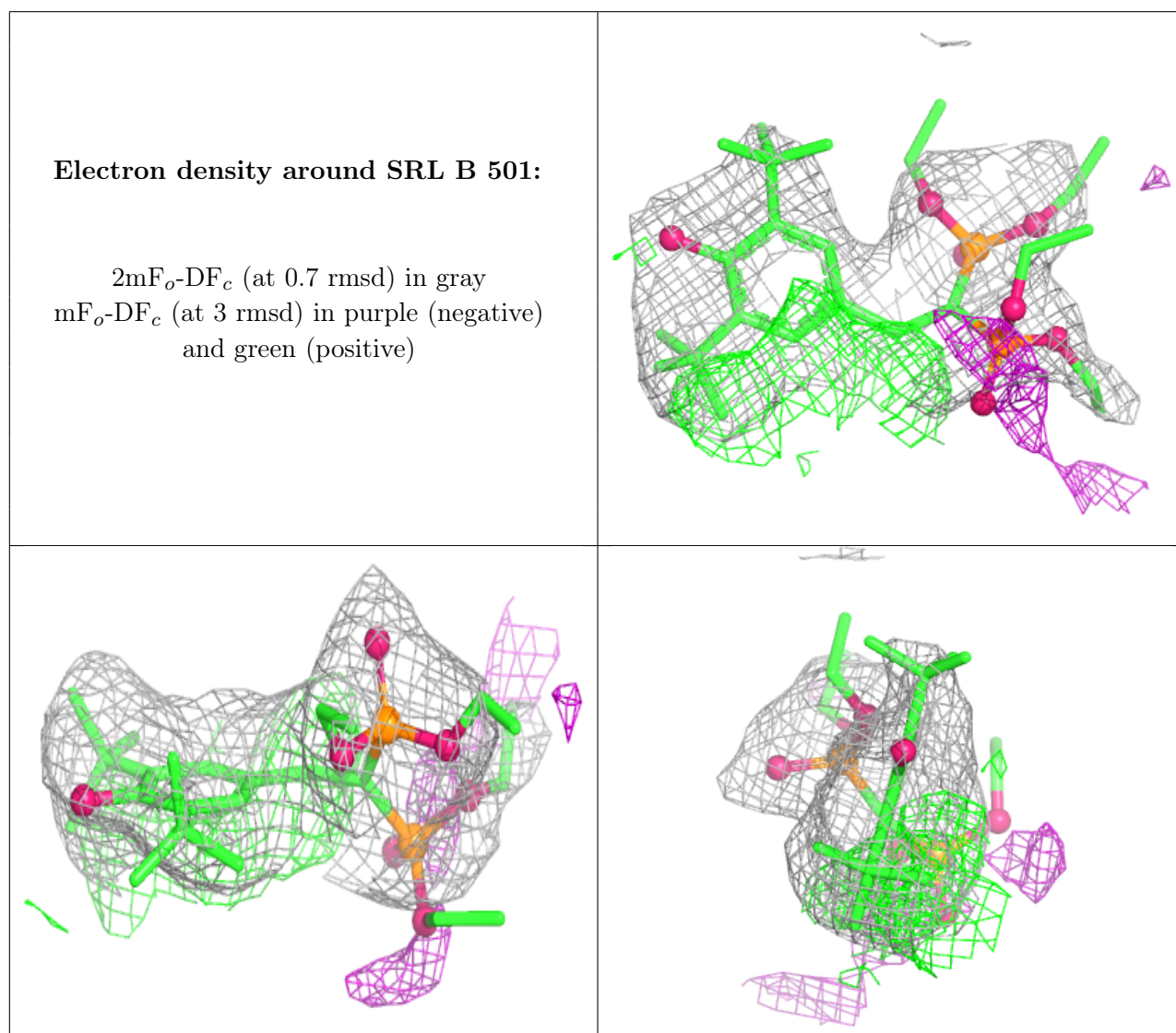
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
3	SRL	B	501	33/33	0.77	0.30	56,88,109,114	0
3	SRL	A	501	33/33	0.84	0.26	57,80,95,114	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.

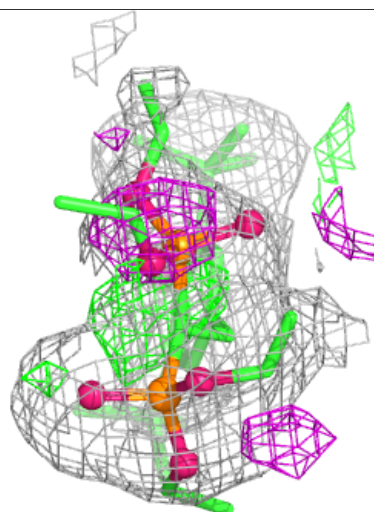
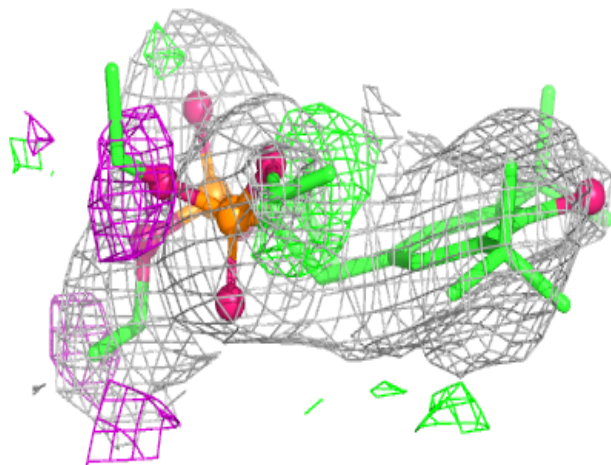
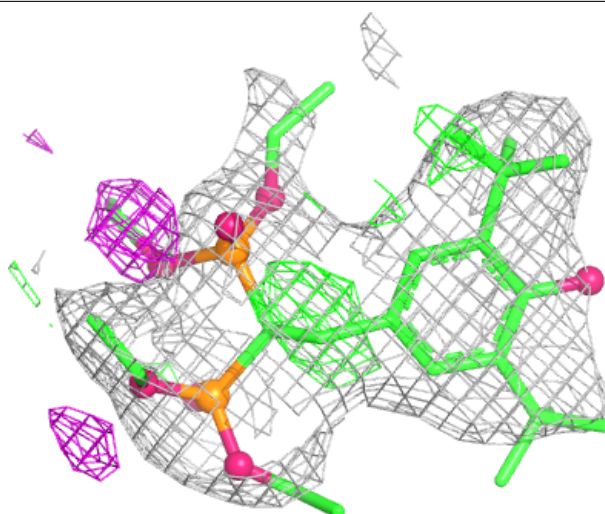
Electron density around SRL B 501:

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 SRL A 501:

$2mF_o-DF_c$ (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.