



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:57 AM UTC

PDB ID : 4P72 / pdb_00004p72
Title : PheRS in complex with compound 2a
Authors : Ferguson, A.D.
Deposited on : 2014-03-25
Resolution : 2.62 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

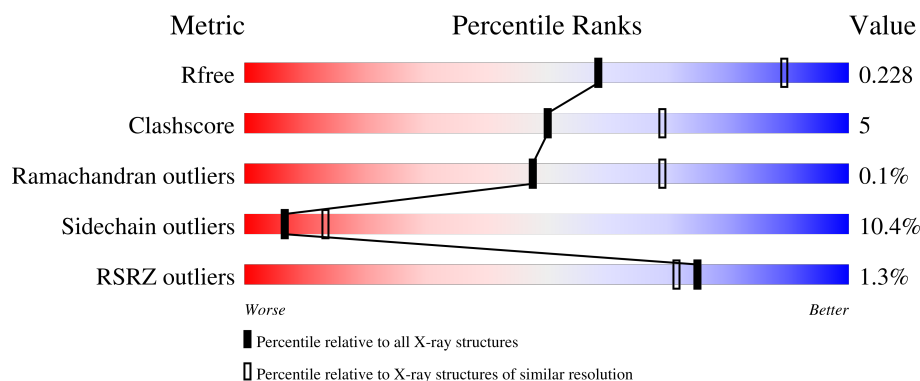
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	792	79% 19% .
1	B	792	80% 17% ..
2	C	338	57% 9% . 30%
2	D	338	4% 59% 11% .. 28%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16183 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.

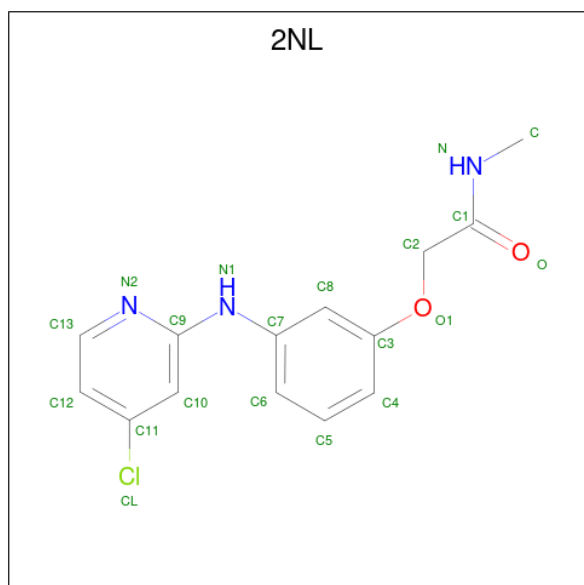
- Molecule 1 is a protein called Phenylalanine-tRNA ligase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	791	Total	C	N	O	S	0	0	0
			6103	3854	1087	1141	21			
1	B	791	Total	C	N	O	S	0	0	0
			6103	3854	1087	1141	21			

- Molecule 2 is a protein called Phenylalanine-tRNA ligase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	235	Total	C	N	O	S	0	0	0
			1897	1203	335	345	14			
2	D	244	Total	C	N	O	S	0	0	0
			1954	1238	345	356	15			

- Molecule 3 is 2-{3-[(4-chloropyridin-2-yl)amino]phenoxy}-N-methylacetamide (CCD ID: 2NL) (formula: C₁₄H₁₄ClN₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total 20	C 14	Cl 1	N 3	O 2	0	0
3	D	1	Total 20	C 14	Cl 1	N 3	O 2	0	0

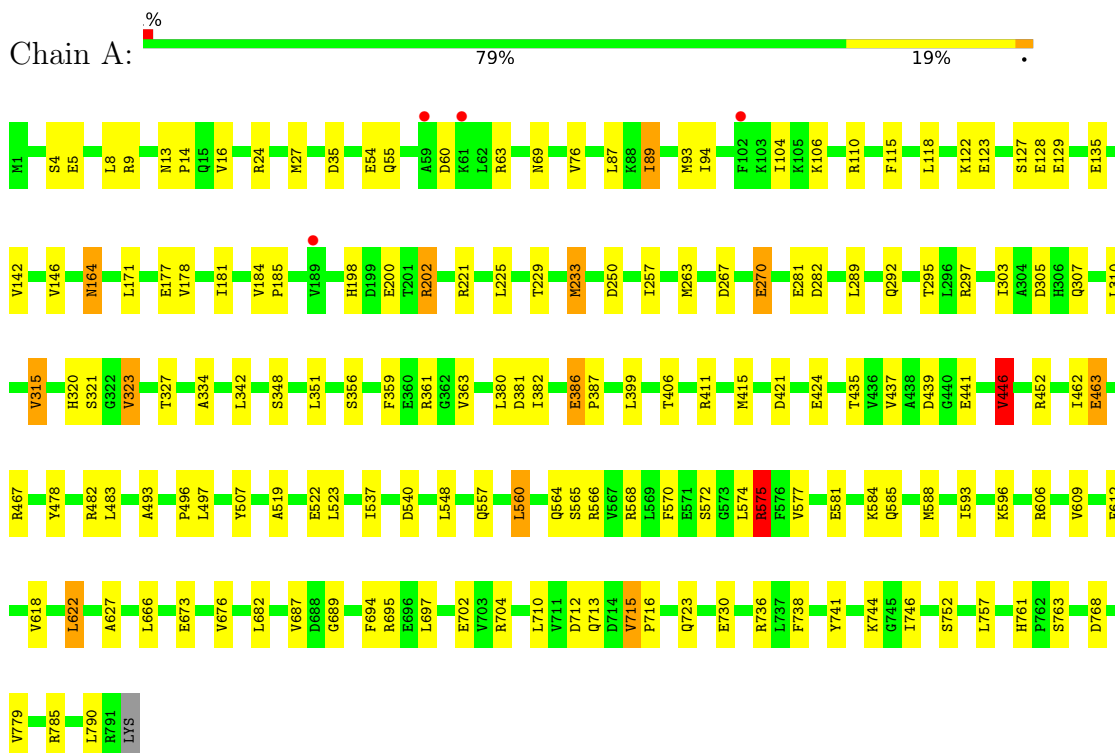
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total 33	O 33	0	0
4	B	43	Total 43	O 43	0	0
4	C	6	Total 6	O 6	0	0
4	D	4	Total 4	O 4	0	0

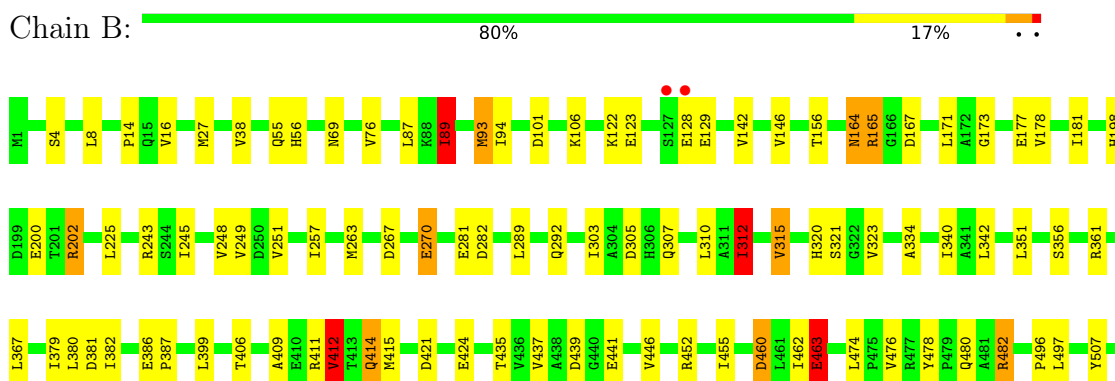
3 Residue-property plots [i](#)

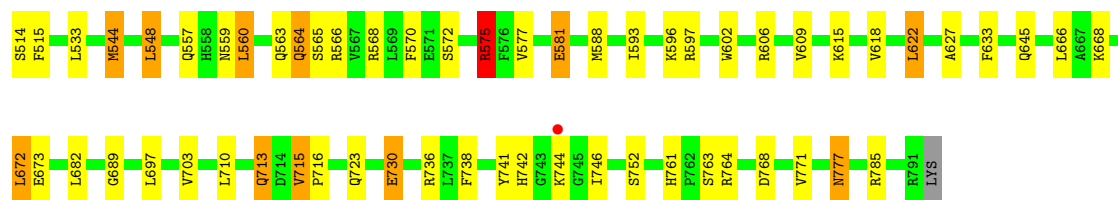
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Phenylalanine-tRNA ligase beta subunit

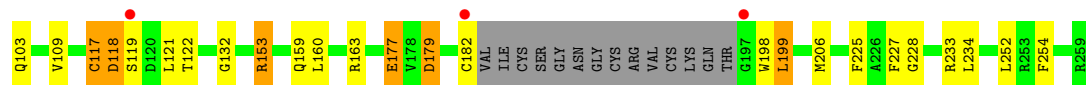
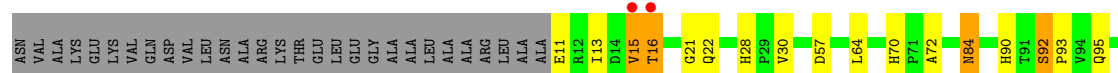
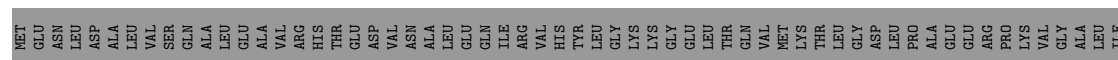


- Molecule 1: Phenylalanine-tRNA ligase beta subunit

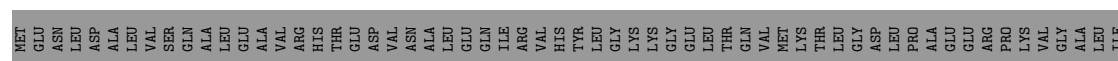




• Molecule 2: Phenylalanine-tRNA ligase alpha subunit



• Molecule 2: Phenylalanine-tRNA ligase alpha subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.30Å 218.83Å 107.63Å 90.00° 101.94° 90.00°	Depositor
Resolution (Å)	75.87 – 2.62 75.87 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.1 (75.87-2.62) 99.7 (75.87-2.62)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.184 , 0.221 0.190 , 0.228	Depositor DCC
R_{free} test set	3822 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16183	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: 2NL

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	0.84	1/6221 (0.0%)	1.30	21/8450 (0.2%)
1	B	0.83	0/6221	1.30	24/8450 (0.3%)
2	C	0.84	0/1946	1.46	13/2628 (0.5%)
2	D	0.88	1/2003 (0.0%)	1.39	16/2706 (0.6%)
All	All	0.84	2/16391 (0.0%)	1.33	74/22234 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	126	MET	SD-CE	-8.95	1.57	1.79
1	A	233	MET	SD-CE	-8.69	1.57	1.79

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	118	ASP	CA-C-N	16.04	142.44	120.63
2	C	118	ASP	C-N-CA	16.04	142.44	120.63
2	C	119	SER	N-CA-C	11.96	124.31	111.03
2	D	57	ASP	CA-CB-CG	10.70	123.30	112.60
1	A	540	ASP	CA-CB-CG	10.11	122.71	112.60
2	C	57	ASP	CA-CB-CG	9.24	121.84	112.60
1	B	777	ASN	CA-CB-CG	8.26	120.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	177	GLU	CB-CG-CD	7.77	125.81	112.60
1	B	575	ARG	CB-CA-C	-7.63	95.40	109.37
1	B	463	GLU	CB-CG-CD	7.45	125.27	112.60
1	B	89	ILE	N-CA-CB	-7.35	103.78	111.87
2	D	103	GLN	CB-CG-CD	7.17	124.78	112.60
2	C	179	ASP	CA-CB-CG	7.02	119.62	112.60
2	D	179	ASP	CA-CB-CG	6.96	119.56	112.60
2	C	84	ASN	CA-CB-CG	6.77	119.37	112.60
2	D	21	GLY	CA-C-N	6.69	130.38	120.87
2	D	21	GLY	C-N-CA	6.69	130.38	120.87
2	D	16	THR	CA-C-N	6.57	133.12	122.48
2	D	16	THR	C-N-CA	6.57	133.12	122.48
2	D	185	CYS	CA-C-N	6.48	132.10	121.99
2	D	185	CYS	C-N-CA	6.48	132.10	121.99
2	D	121	LEU	N-CA-C	-6.47	101.99	110.53
1	A	575	ARG	N-CA-CB	6.22	120.80	110.85
2	D	84	ASN	CA-CB-CG	6.20	118.80	112.60
2	C	21	GLY	CA-C-N	6.18	129.65	120.87
2	C	21	GLY	C-N-CA	6.18	129.65	120.87
2	C	119	SER	CA-C-O	-6.05	114.67	120.90
1	B	715	VAL	N-CA-CB	5.94	115.60	110.08
2	D	153	ARG	CD-NE-CZ	5.89	132.65	124.40
1	B	738	PHE	CA-CB-CG	5.88	119.68	113.80
1	A	303	ILE	N-CA-C	-5.83	99.47	107.99
1	A	446	VAL	CA-C-N	5.79	127.19	121.57
1	A	446	VAL	C-N-CA	5.79	127.19	121.57
2	D	225	PHE	CA-CB-CG	5.79	119.59	113.80
1	B	281	GLU	N-CA-C	-5.76	101.95	110.48
1	A	281	GLU	N-CA-C	-5.74	101.99	110.48
2	C	225	PHE	CA-CB-CG	5.72	119.52	113.80
1	B	575	ARG	N-CA-CB	-5.70	101.73	110.85
1	B	312	ILE	N-CA-CB	5.68	118.30	111.31
1	B	439	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	715	VAL	N-CA-CB	5.60	115.29	110.08
1	B	412	VAL	N-CA-CB	5.57	117.70	110.57
1	B	303	ILE	N-CA-C	-5.55	99.88	107.99
1	B	496	PRO	CA-C-N	5.54	127.97	120.44
1	B	496	PRO	C-N-CA	5.54	127.97	120.44
1	A	738	PHE	CA-CB-CG	5.47	119.27	113.80
1	B	305	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	55	GLN	CB-CG-CD	5.35	121.69	112.60
2	D	153	ARG	CG-CD-NE	-5.32	100.29	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	LEU	N-CA-C	5.31	117.98	111.82
1	A	496	PRO	CA-C-N	5.31	127.66	120.44
1	A	496	PRO	C-N-CA	5.31	127.66	120.44
1	A	305	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	439	ASP	CA-CB-CG	5.27	117.87	112.60
2	D	44	ILE	CA-CB-CG2	5.23	119.39	110.50
1	A	694	PHE	CA-C-N	5.23	130.37	123.05
1	A	694	PHE	C-N-CA	5.23	130.37	123.05
1	B	267	ASP	N-CA-C	-5.19	101.31	109.25
1	A	35	ASP	CA-CB-CG	5.18	117.78	112.60
2	C	57	ASP	CB-CA-C	-5.18	101.88	110.68
1	A	463	GLU	CB-CG-CD	5.17	121.39	112.60
1	B	94	ILE	CA-C-N	-5.16	117.83	123.30
1	B	94	ILE	C-N-CA	-5.16	117.83	123.30
2	C	16	THR	CB-CA-C	5.12	120.24	111.68
2	D	81	PHE	N-CA-C	-5.11	106.74	113.12
1	A	267	ASP	N-CA-C	-5.10	101.45	109.25
1	B	548	LEU	CA-C-N	5.09	127.08	120.26
1	B	548	LEU	C-N-CA	5.09	127.08	120.26
1	A	612	PHE	CA-CB-CG	-5.06	108.74	113.80
1	B	460	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	548	LEU	CA-C-N	5.02	126.99	120.26
1	A	548	LEU	C-N-CA	5.02	126.99	120.26
1	B	668	LYS	CA-C-N	5.01	127.49	120.28
1	B	668	LYS	C-N-CA	5.01	127.49	120.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	386	GLU	Sidechain

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	6103	0	6136	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6103	0	6136	76	0
2	C	1897	0	1821	26	0
2	D	1954	0	1881	29	0
3	C	20	0	14	3	0
3	D	20	0	14	2	0
4	A	33	0	0	0	0
4	B	43	0	0	0	0
4	C	6	0	0	0	0
4	D	4	0	0	0	0
All	All	16183	0	16002	170	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 5.

All (170) 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:C:228:GLY:HA3	3:C:301:2NL:H1	1.45	0.97
1:A:566:ARG:HH12	2:C:22:GLN:HE22	1.09	0.93
1:B:559:ASN:HD21	2:D:252:LEU:H	1.23	0.85
1:B:312:ILE:HG12	1:B:315:VAL:HG13	1.59	0.84
1:B:761:HIS:HD2	1:B:763:SER:H	1.28	0.81
1:A:761:HIS:HD2	1:A:763:SER:H	1.27	0.81
1:A:566:ARG:HH12	2:C:22:GLN:NE2	1.79	0.80
1:A:198:HIS:HD2	1:A:200:GLU:H	1.26	0.80
1:B:463:GLU:HG2	2:D:174:PRO:HB3	1.64	0.78
1:B:198:HIS:HD2	1:B:200:GLU:H	1.29	0.77
1:B:564:GLN:HG2	2:D:252:LEU:HD12	1.68	0.75
1:A:483:LEU:HB3	2:D:44:ILE:CG1	2.17	0.74
1:A:695:ARG:H	2:D:257:GLN:HE22	1.34	0.74
1:A:779:VAL:HG11	1:A:790:LEU:HD21	1.71	0.70
1:A:94:ILE:O	1:A:104:ILE:O	2.12	0.68
1:B:564:GLN:HE21	2:D:252:LEU:HB2	1.57	0.68
2:D:28:HIS:HD2	2:D:30:VAL:H	1.42	0.67
1:A:483:LEU:HB3	2:D:44:ILE:HG13	1.76	0.67
1:B:615:LYS:NZ	2:C:16:THR:HG22	2.09	0.67
1:B:514:SER:H	2:D:126:MET:CE	2.09	0.66
2:C:70:HIS:HD2	2:C:72:ALA:H	1.41	0.66
2:C:28:HIS:HD2	2:C:30:VAL:H	1.43	0.65
2:D:70:HIS:HD2	2:D:72:ALA:H	1.43	0.65
2:D:167:SER:HB2	2:D:177:GLU:HG3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:VAL:HG11	1:B:771:VAL:HG21	1.77	0.65
1:A:564:GLN:HE21	2:C:252:LEU:HB2	1.63	0.64
1:B:69:ASN:HD22	1:B:93:MET:HE3	1.63	0.62
1:A:359:PHE:CE1	1:A:363:VAL:HG21	2.33	0.62
1:A:359:PHE:CD1	1:A:363:VAL:HG21	2.35	0.61
1:B:514:SER:H	2:D:126:MET:HE1	1.65	0.60
1:B:559:ASN:ND2	2:D:252:LEU:H	1.98	0.60
1:A:779:VAL:CG1	1:A:790:LEU:HD21	2.33	0.58
1:B:581:GLU:H	1:B:581:GLU:CD	2.11	0.58
1:B:557:GLN:HE21	1:B:672:LEU:HD12	1.68	0.57
3:D:301:2NL:N2	3:D:301:2NL:H8	2.19	0.57
1:B:409:ALA:HA	1:B:412:VAL:HG13	1.87	0.56
1:A:200:GLU:OE1	1:A:221:ARG:HD3	2.05	0.56
1:B:310:LEU:HD22	1:B:321:SER:HB3	1.87	0.56
1:B:615:LYS:HZ2	2:C:16:THR:HG22	1.70	0.56
1:A:106:LYS:HE3	1:A:115:PHE:CE1	2.41	0.56
1:B:164:ASN:HD22	1:B:164:ASN:H	1.53	0.56
2:C:233:ARG:HH11	2:C:233:ARG:HG3	1.71	0.55
1:A:323:VAL:HG22	1:A:327:THR:HG21	1.88	0.55
1:B:312:ILE:HG12	1:B:315:VAL:CG1	2.34	0.55
1:B:251:VAL:HG21	1:B:379:ILE:HG13	1.89	0.55
1:B:597:ARG:HA	1:B:609:VAL:CG1	2.36	0.55
1:A:702:GLU:H	1:B:563:GLN:HE22	1.54	0.54
1:A:310:LEU:HD22	1:A:321:SER:HB3	1.88	0.54
1:B:414:GLN:HG3	1:B:415:MET:N	2.22	0.54
1:B:713:GLN:HB2	1:B:742:HIS:HE1	1.73	0.54
2:C:132:GLY:HA3	2:C:227:PHE:CZ	2.42	0.54
1:A:493:ALA:O	1:A:687:VAL:HG12	2.09	0.53
3:C:301:2NL:N2	3:C:301:2NL:H8	2.23	0.53
1:A:177:GLU:OE2	1:A:467:ARG:NH1	2.41	0.53
2:D:132:GLY:HA3	2:D:227:PHE:CZ	2.42	0.53
1:B:8:LEU:HD21	1:B:178:VAL:HG21	1.90	0.53
1:A:482:ARG:HD2	1:B:478:TYR:O	2.09	0.52
1:A:741:TYR:HB3	1:A:752:SER:HB3	1.91	0.52
1:B:697:LEU:HD11	2:C:254:PHE:HB2	1.92	0.52
1:A:229:THR:HG23	1:A:233:MET:HE2	1.92	0.52
1:A:164:ASN:H	1:A:164:ASN:HD22	1.56	0.52
1:B:741:TYR:HB3	1:B:752:SER:HB3	1.91	0.52
2:C:199:LEU:HD23	2:C:233:ARG:HH22	1.74	0.52
1:A:8:LEU:HD21	1:A:178:VAL:HG21	1.91	0.51
1:A:233:MET:CE	1:A:250:ASP:HB3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:163:ARG:HB3	2:D:179:ASP:HB2	1.93	0.51
1:A:87:LEU:HD21	1:A:135:GLU:HG2	1.92	0.51
1:A:89:ILE:HD13	1:A:118:LEU:HD22	1.92	0.51
1:B:476:VAL:HG13	2:D:146:GLY:HA2	1.91	0.51
2:C:163:ARG:HB3	2:C:179:ASP:HB2	1.93	0.51
1:A:380:LEU:HD11	1:A:387:PRO:HG3	1.93	0.50
1:B:380:LEU:HD11	1:B:387:PRO:HG3	1.94	0.50
1:A:483:LEU:HB3	2:D:44:ILE:HG12	1.90	0.50
2:C:64:LEU:HD11	2:C:92:SER:HB2	1.94	0.50
1:B:597:ARG:HA	1:B:609:VAL:HG12	1.94	0.50
1:B:716:PRO:HA	2:C:15:VAL:HG21	1.94	0.49
2:C:28:HIS:CD2	2:C:30:VAL:H	2.27	0.49
1:A:478:TYR:O	1:B:482:ARG:HG3	2.12	0.49
2:D:64:LEU:HD11	2:D:92:SER:HB2	1.94	0.49
1:B:38:VAL:HG12	1:B:156:THR:HG23	1.93	0.49
1:B:575:ARG:HG3	1:B:588:MET:SD	2.53	0.49
1:A:575:ARG:HD2	1:A:577:VAL:HG23	1.95	0.48
1:A:716:PRO:HA	2:D:15:VAL:HG21	1.95	0.48
1:B:533:LEU:HG	1:B:544:MET:HE3	1.94	0.48
1:A:177:GLU:O	1:A:181:ILE:HG13	2.13	0.48
1:B:713:GLN:HB2	1:B:742:HIS:CE1	2.48	0.48
1:A:415:MET:HG2	1:A:462:ILE:HG21	1.94	0.48
2:D:28:HIS:CD2	2:D:30:VAL:H	2.27	0.48
1:B:55:GLN:HE21	1:B:56:HIS:N	2.12	0.48
1:A:229:THR:CG2	1:A:233:MET:HE2	2.45	0.47
1:A:537:ILE:HD13	2:C:117:CYS:O	2.14	0.47
1:A:519:ALA:O	1:A:523:LEU:CD2	2.63	0.47
1:B:198:HIS:HD2	1:B:200:GLU:N	2.06	0.47
1:A:69:ASN:HD22	1:A:93:MET:HE1	1.79	0.47
1:B:575:ARG:HD2	1:B:577:VAL:HG23	1.96	0.47
1:B:618:VAL:HG12	1:B:622:LEU:HD22	1.96	0.47
1:A:452:ARG:HA	1:A:452:ARG:HD2	1.83	0.46
1:A:270:GLU:HG2	1:A:320:HIS:O	2.15	0.46
1:A:297:ARG:NH1	1:A:348:SER:HB2	2.30	0.46
1:A:415:MET:SD	2:C:206:MET:HG3	2.55	0.46
1:A:618:VAL:HG12	1:A:622:LEU:HD22	1.98	0.46
1:B:270:GLU:HG2	1:B:320:HIS:O	2.16	0.46
2:C:199:LEU:HD23	2:C:233:ARG:NH2	2.30	0.46
1:B:202:ARG:HD3	1:B:202:ARG:HA	1.77	0.46
1:B:315:VAL:HB	1:B:356:SER:HB3	1.97	0.46
2:D:167:SER:CB	2:D:177:GLU:HG3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:VAL:HB	1:A:356:SER:HB3	1.98	0.45
1:B:575:ARG:HG3	1:B:588:MET:CG	2.47	0.45
1:A:5:GLU:HG2	1:A:9:ARG:HD2	1.99	0.45
1:A:435:THR:O	1:A:446:VAL:HA	2.16	0.45
1:A:519:ALA:O	1:A:523:LEU:HD22	2.16	0.45
1:B:435:THR:O	1:B:446:VAL:HA	2.16	0.45
1:A:507:TYR:HB3	1:A:570:PHE:HD2	1.82	0.45
1:A:574:LEU:HD13	1:A:585:GLN:HB3	1.98	0.45
1:B:507:TYR:HB3	1:B:570:PHE:HD2	1.81	0.45
2:D:92:SER:N	2:D:93:PRO:HD2	2.31	0.45
1:B:615:LYS:HZ1	2:C:16:THR:HG22	1.80	0.44
1:A:627:ALA:HB2	1:A:689:GLY:HA2	1.99	0.44
2:C:153:ARG:HG2	2:C:159:GLN:HA	1.99	0.44
1:A:202:ARG:HD3	1:A:202:ARG:HA	1.75	0.44
3:D:301:2NL:N2	3:D:301:2NL:C6	2.81	0.44
1:B:627:ALA:HB2	1:B:689:GLY:HA2	2.00	0.44
1:A:13:ASN:O	1:A:184:VAL:HG21	2.17	0.44
1:A:575:ARG:HG2	1:A:588:MET:CG	2.48	0.44
1:A:566:ARG:HD2	1:A:596:LYS:O	2.18	0.44
1:B:415:MET:HG2	1:B:462:ILE:HG21	2.00	0.44
2:C:92:SER:N	2:C:93:PRO:HD2	2.33	0.43
1:A:9:ARG:NH1	1:A:16:VAL:O	2.49	0.43
1:B:165:ARG:HH22	1:B:177:GLU:CD	2.26	0.43
1:B:514:SER:H	2:D:126:MET:HE3	1.83	0.43
1:B:514:SER:N	2:D:126:MET:HE1	2.30	0.43
2:C:182:CYS:C	2:C:199:LEU:HD12	2.44	0.43
1:B:474:LEU:HB2	2:D:145:LYS:HE2	2.01	0.43
1:B:761:HIS:CD2	1:B:763:SER:H	2.20	0.43
1:A:198:HIS:HD2	1:A:200:GLU:N	2.03	0.43
1:B:177:GLU:O	1:B:181:ILE:HG12	2.19	0.43
1:B:597:ARG:HA	1:B:609:VAL:HG13	2.00	0.43
1:A:359:PHE:CD1	1:A:363:VAL:CG2	3.01	0.43
1:B:167:ASP:O	1:B:173:GLY:HA3	2.19	0.42
1:B:87:LEU:HD13	1:B:89:ILE:HD13	2.01	0.42
1:B:515:PHE:HB3	1:B:544:MET:HE1	2.00	0.42
1:A:568:ARG:HA	1:A:593:ILE:HG22	2.02	0.42
1:B:165:ARG:HA	1:B:165:ARG:HD2	1.76	0.42
3:C:301:2NL:N2	3:C:301:2NL:C6	2.82	0.42
1:B:14:PRO:HB2	1:B:16:VAL:HG22	2.01	0.42
1:B:572:SER:HA	1:B:588:MET:O	2.20	0.42
1:B:263:MET:HE3	1:B:334:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ARG:HG2	1:A:588:MET:HG3	2.02	0.41
1:B:476:VAL:HG13	2:D:146:GLY:CA	2.49	0.41
1:B:566:ARG:HD2	1:B:596:LYS:O	2.20	0.41
1:A:557:GLN:HA	1:A:560:LEU:HB2	2.01	0.41
1:B:602:TRP:CD1	2:D:18:PRO:HD2	2.55	0.41
1:B:557:GLN:HA	1:B:560:LEU:HB2	2.03	0.41
2:D:153:ARG:HG3	2:D:158:LYS:O	2.19	0.41
1:A:263:MET:HE3	1:A:334:ALA:HB2	2.03	0.41
1:A:712:ASP:O	1:A:715:VAL:HG12	2.20	0.41
1:A:14:PRO:HB2	1:A:16:VAL:HG22	2.02	0.41
1:A:572:SER:HA	1:A:588:MET:O	2.20	0.41
1:B:478:TYR:HE1	2:D:150:GLU:HG2	1.86	0.41
1:B:730:GLU:CD	1:B:730:GLU:H	2.29	0.41
1:A:704:ARG:HA	1:A:757:LEU:O	2.21	0.41
1:B:248:VAL:O	1:B:251:VAL:HG22	2.21	0.40
2:C:163:ARG:HB2	2:C:198:TRP:CZ3	2.56	0.40
2:C:199:LEU:CD2	2:C:233:ARG:HH22	2.34	0.40
1:B:715:VAL:HA	1:B:716:PRO:HD3	2.00	0.40
1:B:455:ILE:HD13	1:B:460:ASP:HB3	2.03	0.40
1:B:568:ARG:HA	1:B:593:ILE:HG22	2.02	0.40
1:A:184:VAL:CG2	1:A:185:PRO:HD2	2.50	0.40
1:A:593:ILE:HD12	1:A:609:VAL:HG21	2.03	0.40
1:B:633:PHE:HB3	2:C:16:THR:HG21	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	789/792 (100%)	770 (98%)	19 (2%)	0	100	100
1	B	789/792 (100%)	772 (98%)	17 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	231/338 (68%)	220 (95%)	10 (4%)	1 (0%)	30	49
2	D	240/338 (71%)	228 (95%)	10 (4%)	2 (1%)	16	31
All	All	2049/2260 (91%)	1990 (97%)	56 (3%)	3 (0%)	48	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	120	ASP
2	C	122	THR
2	D	122	THR

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	645/646 (100%)	578 (90%)	67 (10%)	7	13
1	B	645/646 (100%)	569 (88%)	76 (12%)	5	10
2	C	205/287 (71%)	188 (92%)	17 (8%)	10	22
2	D	211/287 (74%)	193 (92%)	18 (8%)	10	21
All	All	1706/1866 (91%)	1528 (90%)	178 (10%)	7	13

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	24	ARG
1	A	27	MET
1	A	54	GLU
1	A	60	ASP
1	A	63	ARG
1	A	76	VAL
1	A	89	ILE
1	A	110	ARG

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Mol	Chain	Res	Type
1	A	122	LYS
1	A	123	GLU
1	A	127	SER
1	A	128	GLU
1	A	129	GLU
1	A	142	VAL
1	A	146	VAL
1	A	164	ASN
1	A	171	LEU
1	A	202	ARG
1	A	225	LEU
1	A	257	ILE
1	A	270	GLU
1	A	282	ASP
1	A	289	LEU
1	A	292	GLN
1	A	295	THR
1	A	307	GLN
1	A	315	VAL
1	A	323	VAL
1	A	342	LEU
1	A	351	LEU
1	A	361	ARG
1	A	381	ASP
1	A	382	ILE
1	A	386	GLU
1	A	399	LEU
1	A	406	THR
1	A	411	ARG
1	A	421	ASP
1	A	424	GLU
1	A	437	VAL
1	A	441	GLU
1	A	446	VAL
1	A	463	GLU
1	A	497	LEU
1	A	522	GLU
1	A	560	LEU
1	A	565	SER
1	A	575	ARG
1	A	581	GLU
1	A	584	LYS

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Mol	Chain	Res	Type
1	A	606	ARG
1	A	622	LEU
1	A	666	LEU
1	A	673	GLU
1	A	676	VAL
1	A	682	LEU
1	A	697	LEU
1	A	710	LEU
1	A	713	GLN
1	A	723	GLN
1	A	730	GLU
1	A	736	ARG
1	A	744	LYS
1	A	746	ILE
1	A	768	ASP
1	A	785	ARG
1	B	4	SER
1	B	27	MET
1	B	76	VAL
1	B	89	ILE
1	B	93	MET
1	B	101	ASP
1	B	106	LYS
1	B	122	LYS
1	B	123	GLU
1	B	128	GLU
1	B	129	GLU
1	B	142	VAL
1	B	146	VAL
1	B	164	ASN
1	B	165	ARG
1	B	171	LEU
1	B	202	ARG
1	B	225	LEU
1	B	243	ARG
1	B	245	ILE
1	B	249	VAL
1	B	257	ILE
1	B	270	GLU
1	B	282	ASP
1	B	289	LEU
1	B	292	GLN

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Mol	Chain	Res	Type
1	B	307	GLN
1	B	312	ILE
1	B	315	VAL
1	B	323	VAL
1	B	340	ILE
1	B	342	LEU
1	B	351	LEU
1	B	361	ARG
1	B	381	ASP
1	B	382	ILE
1	B	386	GLU
1	B	399	LEU
1	B	406	THR
1	B	411	ARG
1	B	412	VAL
1	B	414	GLN
1	B	421	ASP
1	B	424	GLU
1	B	437	VAL
1	B	441	GLU
1	B	452	ARG
1	B	463	GLU
1	B	480	GLN
1	B	482	ARG
1	B	497	LEU
1	B	544	MET
1	B	548	LEU
1	B	560	LEU
1	B	564	GLN
1	B	565	SER
1	B	575	ARG
1	B	581	GLU
1	B	606	ARG
1	B	622	LEU
1	B	645	GLN
1	B	666	LEU
1	B	672	LEU
1	B	673	GLU
1	B	682	LEU
1	B	710	LEU
1	B	713	GLN
1	B	723	GLN

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Mol	Chain	Res	Type
1	B	730	GLU
1	B	736	ARG
1	B	744	LYS
1	B	746	ILE
1	B	764	ARG
1	B	768	ASP
1	B	777	ASN
1	B	785	ARG
2	C	11	GLU
2	C	13	ILE
2	C	15	VAL
2	C	84	ASN
2	C	90	HIS
2	C	92	SER
2	C	95	GLN
2	C	103	GLN
2	C	109	VAL
2	C	117	CYS
2	C	118	ASP
2	C	121	LEU
2	C	153	ARG
2	C	160	LEU
2	C	177	GLU
2	C	199	LEU
2	C	234	LEU
2	D	8	LEU
2	D	15	VAL
2	D	20	ARG
2	D	44	ILE
2	D	57	ASP
2	D	84	ASN
2	D	90	HIS
2	D	92	SER
2	D	95	GLN
2	D	103	GLN
2	D	109	VAL
2	D	117	CYS
2	D	122	THR
2	D	153	ARG
2	D	160	LEU
2	D	184	ILE
2	D	199	LEU

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Mol	Chain	Res	Type
2	D	234	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	144	GLN
1	A	164	ASN
1	A	198	HIS
1	A	352	HIS
1	A	558	HIS
1	A	564	GLN
1	A	723	GLN
1	A	742	HIS
1	A	761	HIS
1	A	776	GLN
1	B	66	GLN
1	B	164	ASN
1	B	198	HIS
1	B	508	GLN
1	B	557	GLN
1	B	559	ASN
1	B	563	GLN
1	B	564	GLN
1	B	723	GLN
1	B	742	HIS
1	B	760	GLN
1	B	761	HIS
1	B	776	GLN
2	C	22	GLN
2	C	28	HIS
2	C	70	HIS
2	C	84	ASN
2	C	95	GLN
2	C	103	GLN
2	C	123	HIS
2	C	223	GLN
2	D	28	HIS
2	D	70	HIS
2	D	84	ASN
2	D	95	GLN
2	D	123	HIS

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Mol	Chain	Res	Type
2	D	159	GLN
2	D	181	GLN
2	D	257	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	2NL	C	301	-	21,21,21	0.31	0	25,27,27	0.72	0
3	2NL	D	301	-	21,21,21	0.31	0	25,27,27	0.60	0

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	2NL	C	301	-	-	2/11/11/11	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2NL	D	301	-	-	0/11/11/11	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

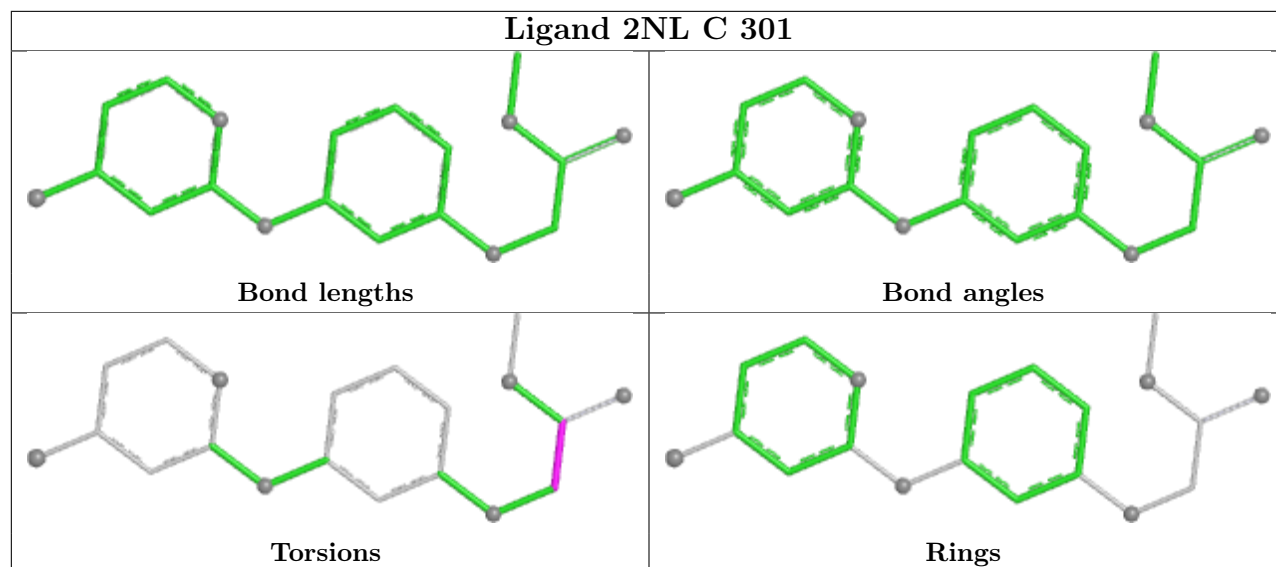
Mol	Chain	Res	Type	Atoms
3	C	301	2NL	N-C1-C2-O1
3	C	301	2NL	O-C1-C2-O1

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	2NL	3	0
3	D	301	2NL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	791/792 (99%)	-0.17	4 (0%) 87 85	33, 51, 84, 107	0
1	B	791/792 (99%)	-0.26	3 (0%) 88 86	29, 49, 82, 107	0
2	C	235/338 (69%)	-0.14	5 (2%) 63 59	38, 49, 78, 112	0
2	D	244/338 (72%)	-0.01	14 (5%) 29 24	35, 50, 88, 114	0
All	All	2061/2260 (91%)	-0.18	26 (1%) 75 71	29, 50, 83, 114	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	8	LEU	5.1
2	D	16	THR	3.7
2	C	16	THR	3.7
2	C	182	CYS	3.6
2	D	15	VAL	3.1
2	D	184	ILE	3.1
2	D	188	ASN	2.9
1	A	102	PHE	2.9
2	D	9	ALA	2.8
2	D	185	CYS	2.6
2	C	15	VAL	2.5
2	D	186	SER	2.5
2	C	197	GLY	2.5
2	D	183	VAL	2.4
2	D	119	SER	2.4
1	B	128	GLU	2.3
2	D	118	ASP	2.3
1	A	59	ALA	2.3
2	D	122	THR	2.3
2	D	121	LEU	2.3
1	A	61	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	197	GLY	2.2
1	B	127	SER	2.1
1	B	744	LYS	2.1
2	C	119	SER	2.0
1	A	189	VAL	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](#)

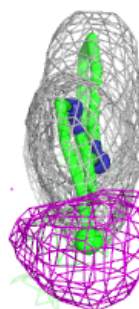
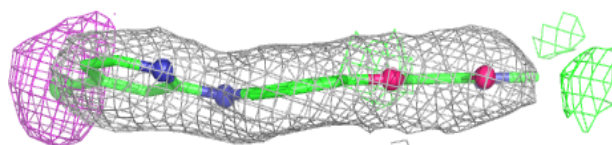
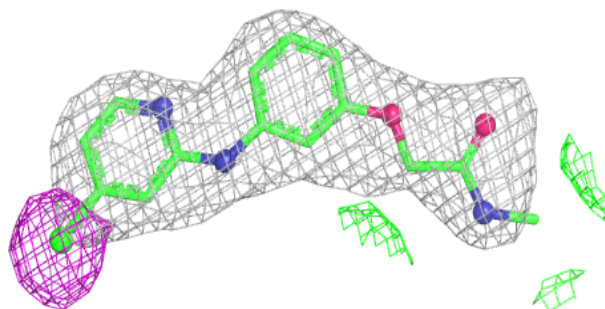
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	2NL	C	301	20/20	0.88	0.12	32,42,57,75	0
3	2NL	D	301	20/20	0.89	0.12	39,46,62,77	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 2NL C 301:

$2mF_o-DF_c$ (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.