Full wwPDB X-ray Structure Validation Report ⓘ

Apr 30, 2024 – 04:44 pm BST

PDB ID	:	8RKQ
Title	:	Structure of human DELTA-1-PYRROLINE-5-CARBOXYLATE DEHYDROGENASE (ALDH4A1) complexed with the molecular tweezer CLR01
Authors	:	Porfetye, A.T.; Vetter, I.R.
Deposited on	:	2023-12-28
Resolution	:	2.60 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:

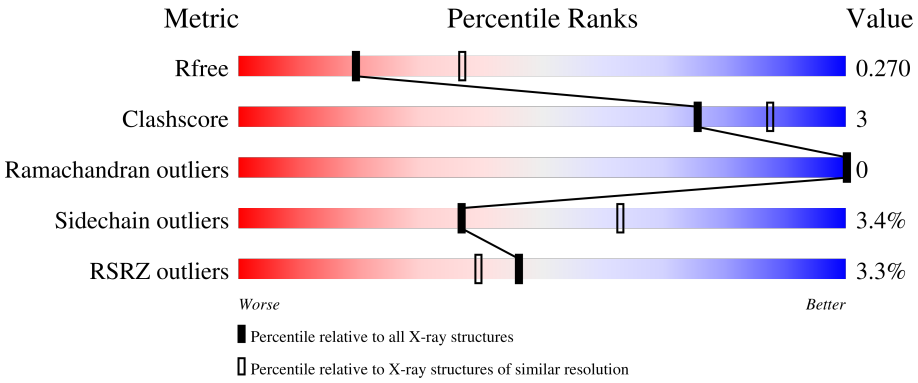
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	567	89% 7% .
1	B	567	% 87% 8% .
1	C	567	4% 85% 10% . .
1	D	567	7% 84% 12% .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16936 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 Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4228	2700	726	786	16			
1	B	543	Total	C	N	O	S	0	0	0
			4203	2685	721	782	15			
1	C	543	Total	C	N	O	S	0	0	0
			4199	2683	720	781	15			
1	D	543	Total	C	N	O	S	0	0	0
			4199	2683	720	781	15			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	initiating methionine	UNP P30038
A	-2	GLY	-	expression tag	UNP P30038
A	-1	SER	-	expression tag	UNP P30038
A	0	SER	-	expression tag	UNP P30038
A	1	HIS	-	expression tag	UNP P30038
A	2	HIS	-	expression tag	UNP P30038
A	3	HIS	-	expression tag	UNP P30038
A	4	HIS	-	expression tag	UNP P30038
A	5	HIS	-	expression tag	UNP P30038
A	6	HIS	-	expression tag	UNP P30038
A	7	SER	-	expression tag	UNP P30038
A	8	SER	-	expression tag	UNP P30038
A	9	GLY	-	expression tag	UNP P30038
A	10	LEU	-	expression tag	UNP P30038
A	11	VAL	-	expression tag	UNP P30038
A	12	PRO	-	expression tag	UNP P30038
A	13	ARG	-	expression tag	UNP P30038
A	14	GLY	-	expression tag	UNP P30038
A	15	SER	-	expression tag	UNP P30038
A	16	HIS	-	expression tag	UNP P30038
A	17	MET	-	expression tag	UNP P30038

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	MET	-	initiating methionine	UNP P30038
B	-2	GLY	-	expression tag	UNP P30038
B	-1	SER	-	expression tag	UNP P30038
B	0	SER	-	expression tag	UNP P30038
B	1	HIS	-	expression tag	UNP P30038
B	2	HIS	-	expression tag	UNP P30038
B	3	HIS	-	expression tag	UNP P30038
B	4	HIS	-	expression tag	UNP P30038
B	5	HIS	-	expression tag	UNP P30038
B	6	HIS	-	expression tag	UNP P30038
B	7	SER	-	expression tag	UNP P30038
B	8	SER	-	expression tag	UNP P30038
B	9	GLY	-	expression tag	UNP P30038
B	10	LEU	-	expression tag	UNP P30038
B	11	VAL	-	expression tag	UNP P30038
B	12	PRO	-	expression tag	UNP P30038
B	13	ARG	-	expression tag	UNP P30038
B	14	GLY	-	expression tag	UNP P30038
B	15	SER	-	expression tag	UNP P30038
B	16	HIS	-	expression tag	UNP P30038
B	17	MET	-	expression tag	UNP P30038
C	-3	MET	-	initiating methionine	UNP P30038
C	-2	GLY	-	expression tag	UNP P30038
C	-1	SER	-	expression tag	UNP P30038
C	0	SER	-	expression tag	UNP P30038
C	1	HIS	-	expression tag	UNP P30038
C	2	HIS	-	expression tag	UNP P30038
C	3	HIS	-	expression tag	UNP P30038
C	4	HIS	-	expression tag	UNP P30038
C	5	HIS	-	expression tag	UNP P30038
C	6	HIS	-	expression tag	UNP P30038
C	7	SER	-	expression tag	UNP P30038
C	8	SER	-	expression tag	UNP P30038
C	9	GLY	-	expression tag	UNP P30038
C	10	LEU	-	expression tag	UNP P30038
C	11	VAL	-	expression tag	UNP P30038
C	12	PRO	-	expression tag	UNP P30038
C	13	ARG	-	expression tag	UNP P30038
C	14	GLY	-	expression tag	UNP P30038
C	15	SER	-	expression tag	UNP P30038
C	16	HIS	-	expression tag	UNP P30038
C	17	MET	-	expression tag	UNP P30038

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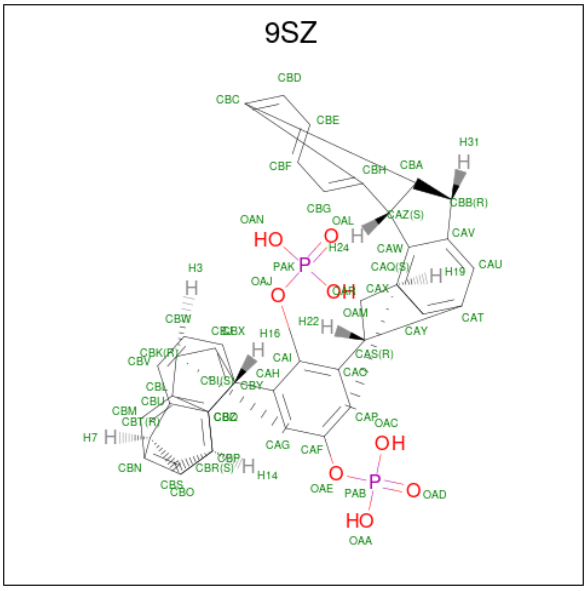
Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	MET	-	initiating methionine	UNP P30038
D	-2	GLY	-	expression tag	UNP P30038
D	-1	SER	-	expression tag	UNP P30038
D	0	SER	-	expression tag	UNP P30038
D	1	HIS	-	expression tag	UNP P30038
D	2	HIS	-	expression tag	UNP P30038
D	3	HIS	-	expression tag	UNP P30038
D	4	HIS	-	expression tag	UNP P30038
D	5	HIS	-	expression tag	UNP P30038
D	6	HIS	-	expression tag	UNP P30038
D	7	SER	-	expression tag	UNP P30038
D	8	SER	-	expression tag	UNP P30038
D	9	GLY	-	expression tag	UNP P30038
D	10	LEU	-	expression tag	UNP P30038
D	11	VAL	-	expression tag	UNP P30038
D	12	PRO	-	expression tag	UNP P30038
D	13	ARG	-	expression tag	UNP P30038
D	14	GLY	-	expression tag	UNP P30038
D	15	SER	-	expression tag	UNP P30038
D	16	HIS	-	expression tag	UNP P30038
D	17	MET	-	expression tag	UNP P30038

- Molecule 2 is (1R,5S,9S,16R,20R,24S,28S,35R)-3,22-Bis(dihydroxyphosphoryloxy)tridecacyclo[22.14.1.15,20.19,16.128,35.02,23.04,21.06,19.08,17.010,15.025,38.027,36.029,34]dotetraconta-2(23),3,6,8(17),10,12,14,18,21,25,27(36),29,31,33,37-pentadecaene (three-letter code: 9SZ) (formula: $C_{42}H_{32}O_8P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			52	42	8	2		

- Molecule 3 is water.

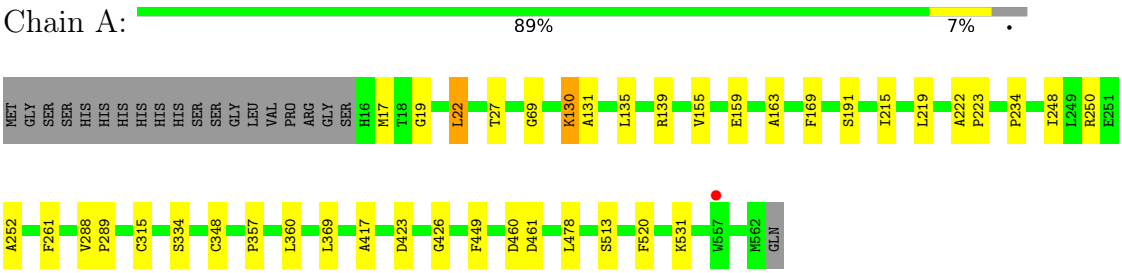
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	21	Total	O	0	0
			21	21		
3	C	3	Total	O	0	0
			3	3		
3	D	7	Total	O	0	0
			7	7		

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.

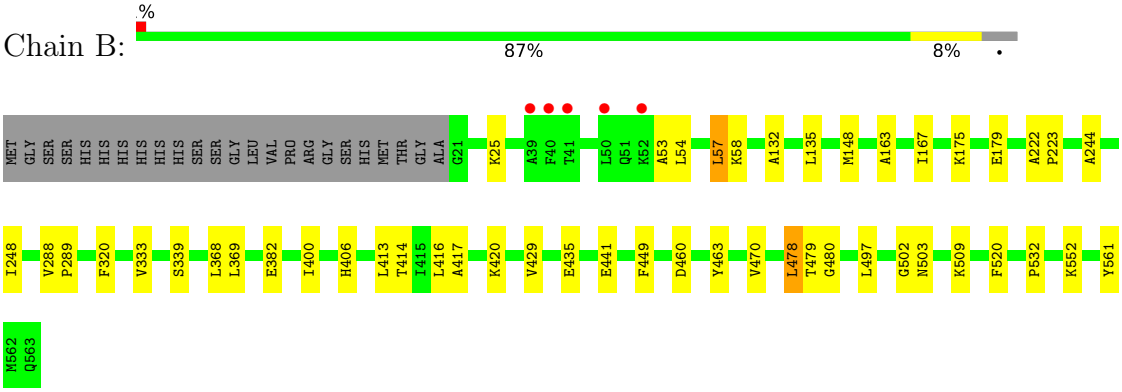
• Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial

Chain A:



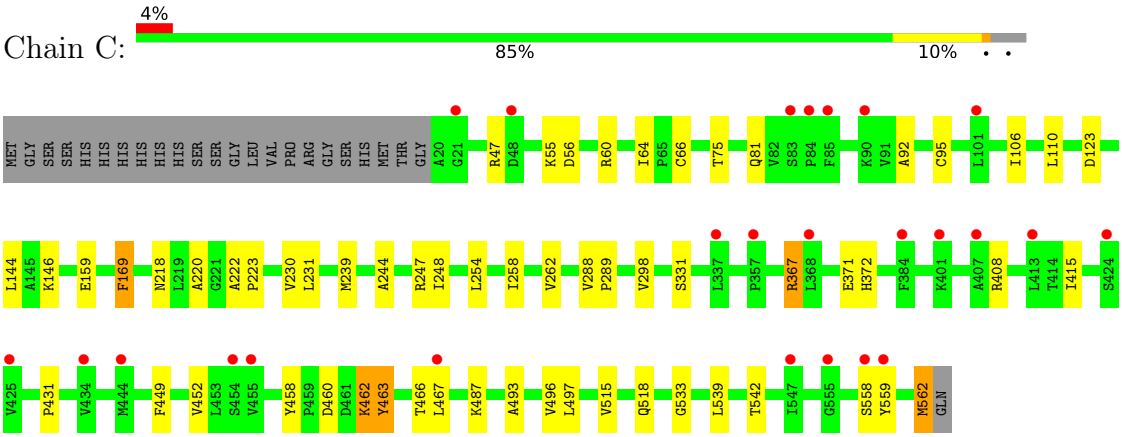
• Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial

Chain B:



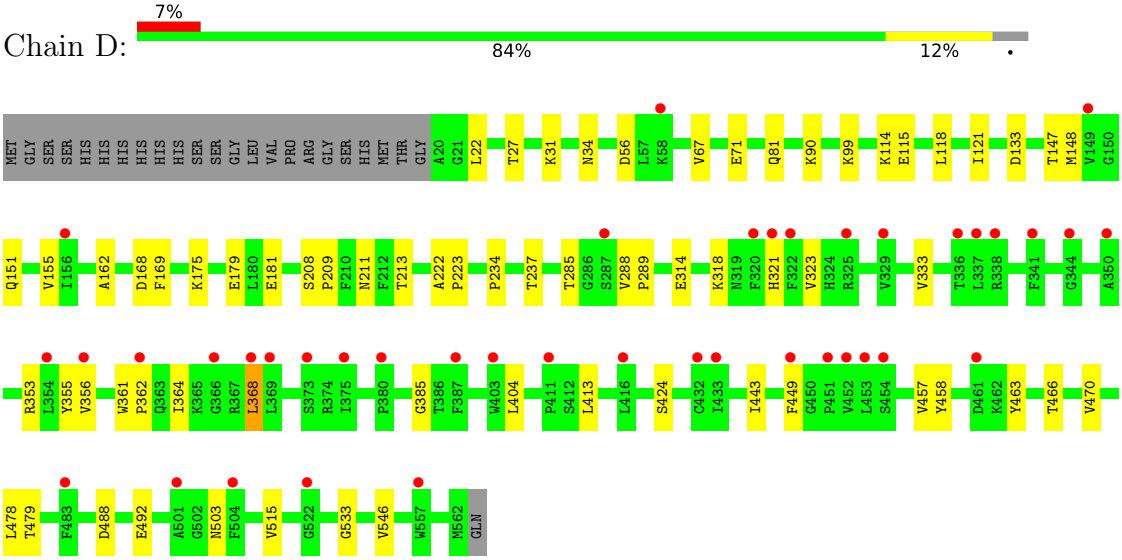
• Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial

Chain C:



• Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	148.75Å 148.75Å 189.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.69 – 2.60 48.69 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.69-2.60) 99.5 (48.69-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.231 , 0.277 0.228 , 0.270	Depositor DCC
R_{free} test set	2101 reflections (2.89%)	wwPDB-VP
Wilson B-factor (Å^2)	79.1	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.042 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16936	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 9SZ

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	0.65	0/4336	0.71	0/5883
1	B	0.65	0/4310	0.71	0/5848
1	C	0.66	0/4306	0.73	0/5843
1	D	0.66	0/4306	0.72	0/5843
All	All	0.65	0/17258	0.72	0/23417

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4228	0	4177	24	0
1	B	4203	0	4154	23	0
1	C	4199	0	4151	30	0
1	D	4199	0	4151	31	0
2	A	52	0	0	3	0
3	A	24	0	0	0	0
3	B	21	0	0	0	0
3	C	3	0	0	0	0
3	D	7	0	0	0	0
All	All	16936	0	16633	103	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 3.

All (103) 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:22:LEU:CD1	2:A:601:9SZ:CBV	2.71	0.68
1:C:64:ILE:HD11	1:C:239:MET:HG3	1.77	0.67
1:C:559:TYR:H	1:C:562:MET:HE1	1.61	0.64
1:B:470:VAL:HG13	1:B:497:LEU:HD21	1.84	0.60
1:C:562:MET:HB3	1:D:385:GLY:HA2	1.83	0.60
1:D:479:THR:HG22	1:D:503:ASN:HB2	1.85	0.59
1:C:518:GLN:HA	1:D:546:VAL:HG11	1.87	0.57
1:C:222:ALA:HB3	1:C:223:PRO:HD3	1.88	0.56
1:D:147:THR:HG21	1:D:162:ALA:HB2	1.88	0.56
1:D:147:THR:HG22	1:D:213:THR:HG21	1.88	0.55
1:D:458:TYR:HB2	1:D:466:THR:HG21	1.88	0.55
1:A:22:LEU:HD13	2:A:601:9SZ:CBV	2.37	0.54
1:B:222:ALA:HB3	1:B:223:PRO:HD3	1.90	0.54
1:B:54:LEU:HD21	1:B:148:MET:HE2	1.89	0.54
1:C:220:ALA:HA	1:C:230:VAL:HG11	1.90	0.54
1:D:222:ALA:HB3	1:D:223:PRO:HD3	1.90	0.54
1:B:339:SER:HB2	1:B:509:LYS:HB2	1.90	0.53
1:C:408:ARG:HG2	1:C:415:ILE:HD12	1.90	0.53
1:D:355:TYR:CZ	1:D:470:VAL:HG12	2.44	0.52
1:B:163:ALA:O	1:B:167:ILE:HG12	2.10	0.52
1:B:244:ALA:O	1:B:248:ILE:HG12	2.10	0.52
1:B:413:LEU:HD21	1:B:441:GLU:HG2	1.92	0.51
1:A:155:VAL:HG22	1:B:561:TYR:CE2	2.46	0.51
1:A:135:LEU:HD13	1:A:248:ILE:HD13	1.93	0.51
1:D:151:GLN:HE22	1:D:213:THR:HG22	1.76	0.50
1:A:130:LYS:HE2	1:A:252:ALA:HA	1.92	0.50
1:C:66:CYS:HG	1:C:95:CYS:HG	1.59	0.50
1:C:288:VAL:N	1:C:289:PRO:HD2	2.27	0.49
1:D:175:LYS:O	1:D:179:GLU:HG2	2.12	0.49
1:A:222:ALA:HB3	1:A:223:PRO:HD3	1.94	0.48
1:C:372:HIS:NE2	1:C:431:PRO:O	2.39	0.48
1:D:121:ILE:HG21	1:D:181:GLU:HG3	1.95	0.47
1:D:333:VAL:HG23	1:D:368:LEU:HB3	1.96	0.47
1:D:318:LYS:O	1:D:353:ARG:NH1	2.45	0.47
1:D:361:TRP:HB3	1:D:362:PRO:HD3	1.95	0.47
1:C:81:GLN:HB3	1:C:92:ALA:HB3	1.96	0.47
1:D:288:VAL:HG13	1:D:289:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:ARG:NH2	1:C:371:GLU:OE2	2.48	0.47
1:B:333:VAL:HG23	1:B:368:LEU:HD23	1.97	0.47
1:D:285:THR:HG23	1:D:314:GLU:HG3	1.98	0.46
1:A:19:GLY:N	1:D:133:ASP:OD2	2.48	0.46
1:C:75:THR:HG22	1:C:95:CYS:HB2	1.97	0.46
1:C:288:VAL:HG12	1:C:289:PRO:HD3	1.97	0.46
1:B:478:LEU:O	1:B:502:GLY:N	2.48	0.46
1:A:288:VAL:HG22	1:A:289:PRO:HD3	1.98	0.46
1:C:487:LYS:HD3	1:C:487:LYS:O	2.16	0.46
1:A:131:ALA:O	1:A:135:LEU:HB2	2.15	0.46
1:A:288:VAL:N	1:A:289:PRO:HD2	2.31	0.46
1:D:148:MET:CE	1:D:155:VAL:HA	2.45	0.45
1:C:458:TYR:HB2	1:C:466:THR:HG21	1.97	0.45
1:D:208:SER:HB2	1:D:234:PRO:HA	1.97	0.45
1:A:139:ARG:HE	1:A:248:ILE:HG12	1.81	0.45
1:C:169:PHE:CD2	1:C:218:ASN:HB2	2.51	0.45
1:C:244:ALA:O	1:C:248:ILE:HG13	2.16	0.45
1:D:34:ASN:ND2	1:D:515:VAL:O	2.45	0.45
1:B:132:ALA:O	1:B:167:ILE:HD12	2.17	0.44
1:B:320:PHE:CZ	1:B:480:GLY:HA3	2.52	0.44
1:A:357:PRO:HG2	1:A:360:LEU:HB2	1.99	0.44
1:C:493:ALA:O	1:C:497:LEU:HB2	2.17	0.44
1:D:168:ASP:HB3	1:D:515:VAL:HB	1.99	0.44
1:C:146:LYS:HD3	1:C:244:ALA:HB2	2.00	0.44
1:D:81:GLN:HG3	1:D:237:THR:HA	2.00	0.44
1:A:27:THR:HG23	1:D:27:THR:HG23	1.99	0.44
1:A:17:MET:SD	2:A:601:9SZ:CBV	3.06	0.44
1:A:288:VAL:N	1:A:289:PRO:CD	2.81	0.43
1:D:288:VAL:CG1	1:D:289:PRO:HD3	2.49	0.43
1:C:144:LEU:HD21	1:C:159:GLU:HA	2.00	0.43
1:B:175:LYS:O	1:B:179:GLU:HG2	2.18	0.43
1:D:515:VAL:HG13	1:D:533:GLY:HA2	2.01	0.43
1:D:364:ILE:O	1:D:368:LEU:HD23	2.18	0.43
1:D:413:LEU:HD21	1:D:443:ILE:HG21	2.01	0.43
1:D:488:ASP:O	1:D:492:GLU:HG2	2.19	0.42
1:A:69:GLY:O	1:A:250:ARG:NH1	2.48	0.42
1:A:423:ASP:HA	1:A:426:GLY:O	2.19	0.42
1:C:539:LEU:HA	1:C:542:THR:HG22	2.01	0.42
1:B:288:VAL:N	1:B:289:PRO:CD	2.82	0.42
1:C:106:ILE:O	1:C:110:LEU:HD12	2.19	0.42
1:C:496:VAL:HG23	1:C:497:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LEU:HG	1:B:248:ILE:HG21	2.00	0.42
1:C:64:ILE:O	1:C:64:ILE:HG13	2.20	0.42
1:A:159:GLU:O	1:A:163:ALA:HB3	2.19	0.42
1:B:520:PHE:O	1:B:532:PRO:HD2	2.19	0.42
1:D:288:VAL:N	1:D:289:PRO:CD	2.83	0.42
1:A:369:LEU:HD22	1:A:417:ALA:HB2	2.02	0.42
1:A:22:LEU:H	1:A:22:LEU:HG	1.57	0.42
1:B:369:LEU:HD22	1:B:417:ALA:HB2	2.01	0.42
1:C:462:LYS:HE2	1:C:462:LYS:HB3	1.95	0.42
1:C:463:TYR:O	1:C:467:LEU:HB2	2.20	0.42
1:C:254:LEU:HG	1:C:258:ILE:HD11	2.00	0.41
1:A:234:PRO:HG2	1:A:261:PHE:CZ	2.55	0.41
1:C:515:VAL:HG13	1:C:533:GLY:HA2	2.01	0.41
1:A:215:ILE:O	1:A:219:LEU:HG	2.20	0.41
1:B:53:ALA:O	1:B:57:LEU:HD22	2.20	0.41
1:D:478:LEU:HD13	1:D:479:THR:HG23	2.02	0.41
1:A:288:VAL:CG2	1:A:289:PRO:HD3	2.50	0.41
1:A:520:PHE:O	1:A:531:LYS:HA	2.20	0.41
1:D:209:PRO:HB2	1:D:211:ASN:OD1	2.21	0.41
1:B:416:LEU:HD11	1:B:435:GLU:HB2	2.03	0.40
1:C:56:ASP:O	1:C:60:ARG:HG2	2.20	0.40
1:B:400:ILE:HG21	1:B:429:VAL:HG11	2.02	0.40
1:B:288:VAL:CG1	1:B:289:PRO:HD3	2.52	0.40
1:B:406:HIS:NE2	1:B:441:GLU:OE2	2.46	0.40
1:B:479:THR:HG22	1:B:503:ASN:HB2	2.04	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	545/567 (96%)	526 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	541/567 (95%)	513 (95%)	28 (5%)	0	100	100
1	C	541/567 (95%)	506 (94%)	35 (6%)	0	100	100
1	D	541/567 (95%)	504 (93%)	37 (7%)	0	100	100
All	All	2168/2268 (96%)	2049 (94%)	119 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	448/465 (96%)	436 (97%)	12 (3%)	44	71
1	B	446/465 (96%)	435 (98%)	11 (2%)	47	73
1	C	445/465 (96%)	428 (96%)	17 (4%)	33	59
1	D	445/465 (96%)	425 (96%)	20 (4%)	27	52
All	All	1784/1860 (96%)	1724 (97%)	60 (3%)	37	63

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	130	LYS
1	A	169	PHE
1	A	191	SER
1	A	315	CYS
1	A	334	SER
1	A	348	CYS
1	A	449	PHE
1	A	460	ASP
1	A	461	ASP
1	A	478	LEU
1	A	513	SER
1	B	25	LYS

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Mol	Chain	Res	Type
1	B	57	LEU
1	B	58	LYS
1	B	382	GLU
1	B	414	THR
1	B	420	LYS
1	B	449	PHE
1	B	460	ASP
1	B	463	TYR
1	B	478	LEU
1	B	552	LYS
1	C	47	ARG
1	C	55	LYS
1	C	123	ASP
1	C	169	PHE
1	C	231	LEU
1	C	247	ARG
1	C	262	VAL
1	C	298	VAL
1	C	331	SER
1	C	367	ARG
1	C	449	PHE
1	C	452	VAL
1	C	460	ASP
1	C	462	LYS
1	C	463	TYR
1	C	558	SER
1	C	562	MET
1	D	22	LEU
1	D	31	LYS
1	D	56	ASP
1	D	67	VAL
1	D	71	GLU
1	D	90	LYS
1	D	99	LYS
1	D	114	LYS
1	D	115	GLU
1	D	118	LEU
1	D	169	PHE
1	D	321	HIS
1	D	323	VAL
1	D	356	VAL
1	D	368	LEU

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Mol	Chain	Res	Type
1	D	404	LEU
1	D	424	SER
1	D	449	PHE
1	D	457	VAL
1	D	463	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	440	GLN
1	B	491	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	9SZ	A	601	-	64,64,64	5.30	52 (81%)	108,108,108	2.77	32 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9SZ	A	601	-	-	0/10/90/90	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	9SZ	CAG-CBK	-12.27	1.38	1.52
2	A	601	9SZ	CAO-CAS	-10.75	1.40	1.52
2	A	601	9SZ	CAP-CAQ	-10.44	1.40	1.52
2	A	601	9SZ	CBN-CBT	-9.47	1.37	1.52
2	A	601	9SZ	CAH-CBI	-9.42	1.41	1.52
2	A	601	9SZ	CBZ-CBR	-8.77	1.38	1.52
2	A	601	9SZ	CAY-CAQ	-8.38	1.39	1.52
2	A	601	9SZ	CBQ-CBI	-8.24	1.39	1.52
2	A	601	9SZ	CAW-CAZ	-8.01	1.39	1.52
2	A	601	9SZ	CBH-CAZ	-7.89	1.40	1.52
2	A	601	9SZ	CBL-CBK	-7.70	1.40	1.52
2	A	601	9SZ	CBC-CBB	-7.34	1.40	1.52
2	A	601	9SZ	CAV-CBB	-7.27	1.41	1.52
2	A	601	9SZ	CBJ-CBI	-7.15	1.47	1.55
2	A	601	9SZ	CAT-CAS	-7.03	1.41	1.52
2	A	601	9SZ	CBU-CBT	-6.94	1.41	1.52
2	A	601	9SZ	CBO-CBR	-6.77	1.41	1.52
2	A	601	9SZ	CBS-CBR	-6.27	1.48	1.55
2	A	601	9SZ	CBS-CBT	-5.78	1.49	1.55
2	A	601	9SZ	CBA-CBB	-5.78	1.49	1.55
2	A	601	9SZ	CBJ-CBK	-5.73	1.49	1.55
2	A	601	9SZ	CAR-CAQ	-5.51	1.49	1.55
2	A	601	9SZ	CBA-CAZ	-5.24	1.49	1.55
2	A	601	9SZ	CBV-CBU	-4.92	1.33	1.39
2	A	601	9SZ	CBY-CBZ	-4.57	1.33	1.39
2	A	601	9SZ	CBG-CBH	-4.30	1.34	1.39
2	A	601	9SZ	CBD-CBC	-4.28	1.34	1.39
2	A	601	9SZ	CBM-CBL	-3.97	1.33	1.39
2	A	601	9SZ	CBM-CBN	-3.77	1.33	1.39
2	A	601	9SZ	CAX-CAW	-3.67	1.33	1.39
2	A	601	9SZ	CAX-CAY	-3.64	1.33	1.39
2	A	601	9SZ	PAB-OAD	3.59	1.62	1.50
2	A	601	9SZ	CAP-CAO	-3.57	1.34	1.40
2	A	601	9SZ	CBP-CBO	-3.51	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	9SZ	CBP-CBQ	-3.31	1.34	1.39
2	A	601	9SZ	CAF-CAP	-3.30	1.33	1.39
2	A	601	9SZ	CAU-CAT	-3.24	1.34	1.39
2	A	601	9SZ	CAF-CAG	-3.23	1.33	1.39
2	A	601	9SZ	CAR-CAS	-3.23	1.51	1.55
2	A	601	9SZ	CAU-CAV	-3.20	1.34	1.39
2	A	601	9SZ	CBZ-CBU	-3.17	1.34	1.40
2	A	601	9SZ	CAY-CAT	-3.12	1.34	1.40
2	A	601	9SZ	CAH-CAG	-3.09	1.35	1.40
2	A	601	9SZ	CAI-CAH	-2.97	1.34	1.39
2	A	601	9SZ	CBO-CBN	-2.93	1.35	1.40
2	A	601	9SZ	CBQ-CBL	-2.84	1.35	1.40
2	A	601	9SZ	CAV-CAW	-2.80	1.35	1.40
2	A	601	9SZ	CBC-CBH	-2.70	1.35	1.40
2	A	601	9SZ	CAI-CAO	-2.56	1.34	1.39
2	A	601	9SZ	OAE-CAF	-2.39	1.36	1.40
2	A	601	9SZ	OAJ-CAI	-2.02	1.37	1.40
2	A	601	9SZ	PAB-OAE	2.01	1.62	1.59

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	9SZ	CAS-CAR-CAQ	-14.81	86.81	94.43
2	A	601	9SZ	CBR-CBS-CBT	-9.62	89.48	94.43
2	A	601	9SZ	CBB-CBA-CAZ	-9.51	89.53	94.43
2	A	601	9SZ	CBI-CBJ-CBK	-7.75	90.44	94.43
2	A	601	9SZ	CAO-CAS-CAT	5.88	109.32	104.53
2	A	601	9SZ	CAP-CAQ-CAY	5.63	109.11	104.53
2	A	601	9SZ	CBH-CAZ-CAW	4.21	109.96	105.39
2	A	601	9SZ	CAV-CBB-CBC	4.16	109.91	105.39
2	A	601	9SZ	CAR-CAS-CAO	3.60	101.98	99.24
2	A	601	9SZ	OAA-PAB-OAE	3.24	115.36	105.24
2	A	601	9SZ	CAR-CAQ-CAP	3.14	101.63	99.24
2	A	601	9SZ	CBS-CBR-CBZ	3.03	101.93	99.28
2	A	601	9SZ	CBY-CBZ-CBR	2.89	133.63	129.37
2	A	601	9SZ	CBN-CBM-CBL	-2.84	118.40	123.20
2	A	601	9SZ	CBD-CBC-CBB	2.80	133.50	129.37
2	A	601	9SZ	CAP-CAO-CAS	-2.80	104.09	106.69
2	A	601	9SZ	CBV-CBU-CBT	2.79	133.48	129.37
2	A	601	9SZ	CAR-CAQ-CAY	2.77	101.70	99.28
2	A	601	9SZ	CAU-CAT-CAS	2.76	135.37	130.88
2	A	601	9SZ	CAW-CAX-CAY	-2.63	118.76	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	9SZ	CBQ-CBP-CBO	-2.56	118.88	123.20
2	A	601	9SZ	CBJ-CBI-CBQ	2.53	101.49	99.28
2	A	601	9SZ	CBS-CBT-CBN	2.48	101.45	99.28
2	A	601	9SZ	CAV-CAU-CAT	-2.40	119.15	123.20
2	A	601	9SZ	CBP-CBO-CBR	2.37	134.74	130.88
2	A	601	9SZ	CAH-CBI-CBQ	2.35	106.45	104.53
2	A	601	9SZ	CAG-CBK-CBL	2.34	106.44	104.53
2	A	601	9SZ	CBJ-CBK-CAG	2.34	101.02	99.24
2	A	601	9SZ	CBG-CBH-CAZ	2.30	132.75	129.37
2	A	601	9SZ	CAU-CAV-CBB	2.25	134.53	130.88
2	A	601	9SZ	CAI-CAO-CAS	2.03	136.00	131.67
2	A	601	9SZ	CBU-CBZ-CBR	-2.01	104.50	106.58

There are no chirality outliers.

There are no torsion outliers.

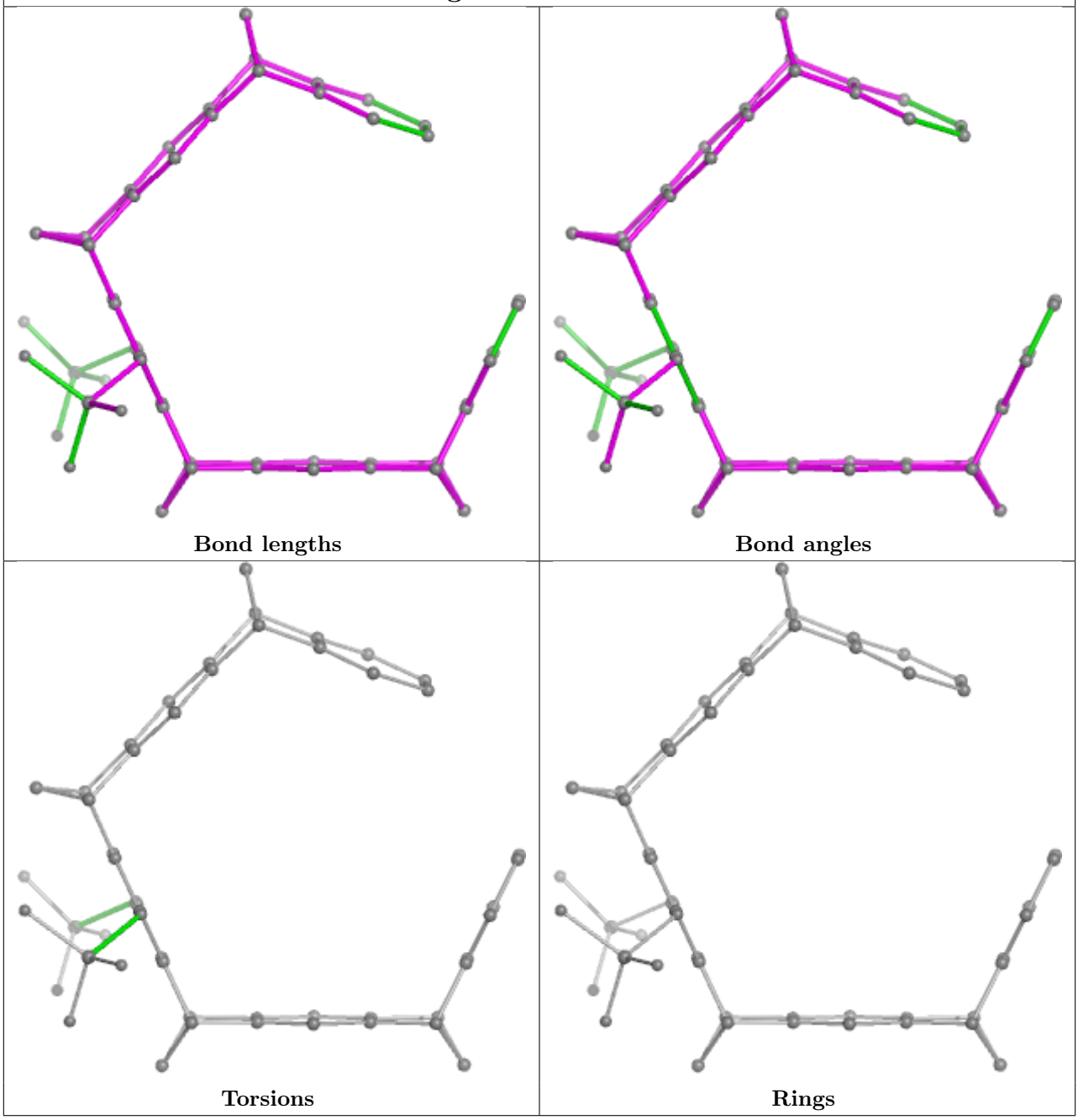
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	9SZ	3	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 then 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 9SZ A 601



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	547/567 (96%)	-0.02	1 (0%)	95	95	58, 77, 97, 135	0
1	B	543/567 (95%)	-0.03	5 (0%)	84	82	59, 81, 111, 121	0
1	C	543/567 (95%)	0.27	25 (4%)	32	26	75, 102, 126, 142	0
1	D	543/567 (95%)	0.37	41 (7%)	13	10	67, 106, 146, 165	0
All	All	2176/2268 (95%)	0.15	72 (3%)	46	39	58, 90, 131, 165	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	403	TRP	5.5
1	C	559	TYR	5.3
1	D	433	ILE	5.1
1	D	449	PHE	4.6
1	D	368	LEU	4.0
1	D	451	PRO	4.0
1	D	337	LEU	3.8
1	D	432	CYS	3.8
1	D	366	GLY	3.8
1	C	413	LEU	3.5
1	D	322	PHE	3.5
1	D	416	LEU	3.5
1	C	558	SER	3.4
1	C	555	GLY	3.4
1	D	356	VAL	3.3
1	D	321	HIS	3.3
1	C	425	VAL	3.2
1	D	350	ALA	3.1
1	D	483	PHE	3.1
1	D	504	PHE	3.0
1	C	444	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	407	ALA	3.0
1	D	336	THR	3.0
1	C	455	VAL	3.0
1	D	362	PRO	3.0
1	D	58	LYS	2.9
1	B	41	THR	2.9
1	D	375	ILE	2.9
1	D	369	LEU	2.8
1	D	387	PHE	2.8
1	D	341	PHE	2.7
1	C	424	SER	2.7
1	D	557	TRP	2.7
1	C	467	LEU	2.6
1	C	85	PHE	2.6
1	D	287	SER	2.6
1	D	325	ARG	2.6
1	D	452	VAL	2.6
1	D	149	VAL	2.6
1	C	90	LYS	2.5
1	D	156	ILE	2.5
1	C	434	VAL	2.5
1	D	320	PHE	2.5
1	D	329	VAL	2.5
1	C	357	PRO	2.5
1	C	384	PHE	2.4
1	C	454	SER	2.4
1	D	380	PRO	2.4
1	B	50	LEU	2.4
1	D	344	GLY	2.4
1	C	337	LEU	2.4
1	C	21	GLY	2.4
1	C	401	LYS	2.4
1	C	368	LEU	2.3
1	D	373	SER	2.3
1	A	557	TRP	2.3
1	D	522	GLY	2.3
1	C	83	SER	2.2
1	D	453	LEU	2.2
1	B	40	PHE	2.2
1	C	84	PRO	2.2
1	D	454	SER	2.2
1	C	101	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	39	ALA	2.2
1	D	338	ARG	2.1
1	C	547	ILE	2.1
1	D	461	ASP	2.1
1	B	52	LYS	2.0
1	D	501	ALA	2.0
1	C	48	ASP	2.0
1	D	411	PRO	2.0
1	D	354	LEU	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)

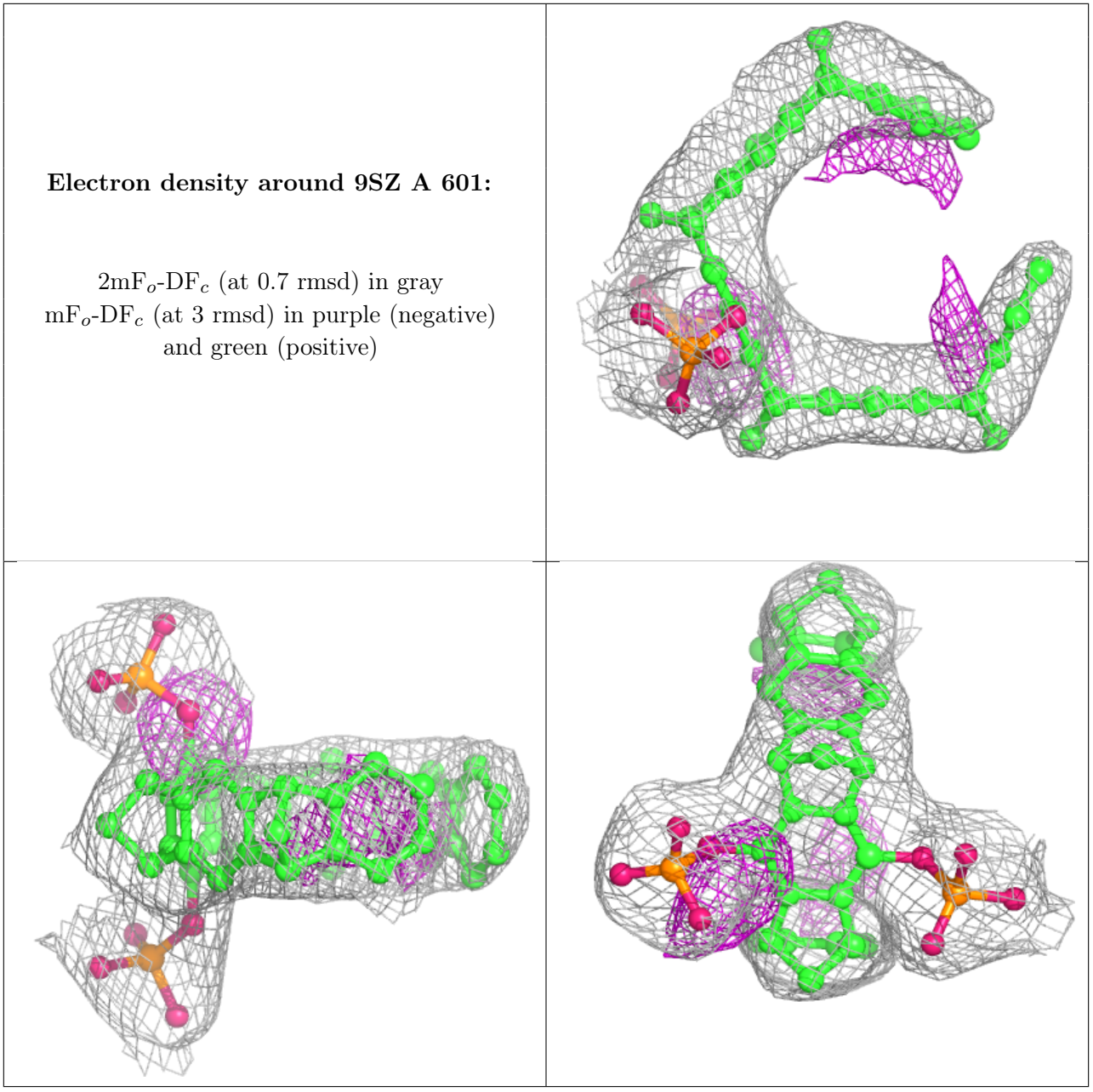
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	9SZ	A	601	52/52	0.92	0.17	91,101,110,110	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 9SZ A 601:

$2mF_o$-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

There are no such residues in this entry.