Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:26 pm BST

PDB ID	:	5ER8
Title	:	Crystal structure of cyclization domain of Phomopsis amygdali fusicoccadiene synthase complexed with manganese ions and neridronate
Authors	:	Chen, M.; Christianson, D.W.
Deposited on	:	2015-11-13
Resolution	:	2.50 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 following versions of software and data (see references ⓘ) were used in the production of this report:

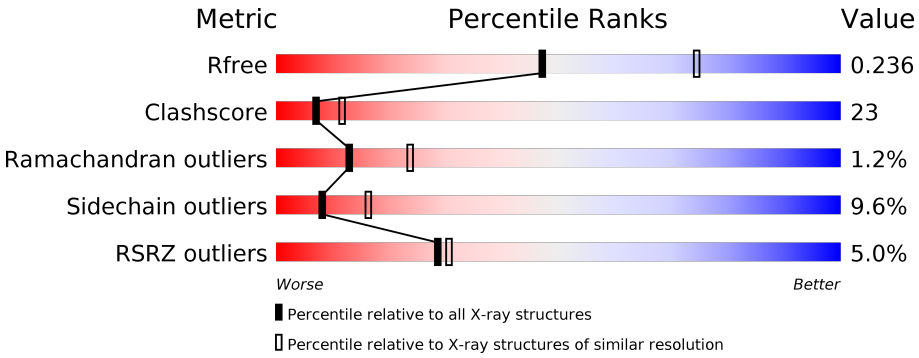
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	363	3% 40% 36% 19%
1	B	363	5% 43% 37% 16%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	B	705	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4972 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 Fusicoccadiene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2388	1531	400	441	16			
1	B	304	Total	C	N	O	S	0	0	0
			2465	1578	413	458	16			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP A2PZA5
A	-17	GLY	-	expression tag	UNP A2PZA5
A	-16	SER	-	expression tag	UNP A2PZA5
A	-15	SER	-	expression tag	UNP A2PZA5
A	-14	HIS	-	expression tag	UNP A2PZA5
A	-13	HIS	-	expression tag	UNP A2PZA5
A	-12	HIS	-	expression tag	UNP A2PZA5
A	-11	HIS	-	expression tag	UNP A2PZA5
A	-10	HIS	-	expression tag	UNP A2PZA5
A	-9	HIS	-	expression tag	UNP A2PZA5
A	-8	SER	-	expression tag	UNP A2PZA5
A	-7	SER	-	expression tag	UNP A2PZA5
A	-6	GLY	-	expression tag	UNP A2PZA5
A	-5	LEU	-	expression tag	UNP A2PZA5
A	-4	VAL	-	expression tag	UNP A2PZA5
A	-3	PRO	-	expression tag	UNP A2PZA5
A	-2	ARG	-	expression tag	UNP A2PZA5
A	-1	GLY	-	expression tag	UNP A2PZA5
A	0	SER	-	expression tag	UNP A2PZA5
A	53	ARG	GLY	conflict	UNP A2PZA5
B	-18	MET	-	initiating methionine	UNP A2PZA5
B	-17	GLY	-	expression tag	UNP A2PZA5
B	-16	SER	-	expression tag	UNP A2PZA5
B	-15	SER	-	expression tag	UNP A2PZA5
B	-14	HIS	-	expression tag	UNP A2PZA5

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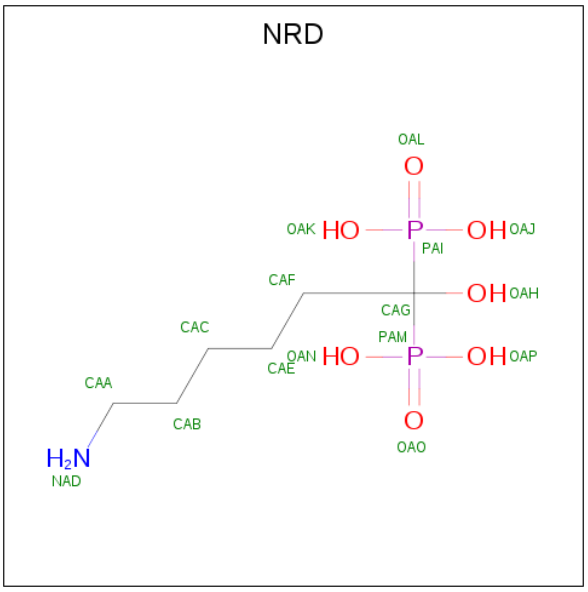
Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP A2PZA5
B	-12	HIS	-	expression tag	UNP A2PZA5
B	-11	HIS	-	expression tag	UNP A2PZA5
B	-10	HIS	-	expression tag	UNP A2PZA5
B	-9	HIS	-	expression tag	UNP A2PZA5
B	-8	SER	-	expression tag	UNP A2PZA5
B	-7	SER	-	expression tag	UNP A2PZA5
B	-6	GLY	-	expression tag	UNP A2PZA5
B	-5	LEU	-	expression tag	UNP A2PZA5
B	-4	VAL	-	expression tag	UNP A2PZA5
B	-3	PRO	-	expression tag	UNP A2PZA5
B	-2	ARG	-	expression tag	UNP A2PZA5
B	-1	GLY	-	expression tag	UNP A2PZA5
B	0	SER	-	expression tag	UNP A2PZA5
B	53	ARG	GLY	conflict	UNP A2PZA5

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	5	Total Mn 5 5	0	0
2	A	4	Total Mn 4 4	0	0

- Molecule 3 is (6-azanyl-1-oxidanyl-1-phosphono-hexyl)phosphonic acid (three-letter code: NRD) (formula: $C_6H_{17}NO_7P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	6	1	7	2		
3	B	1	Total	C	N	O	P	0	0
			16	6	1	7	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is water.

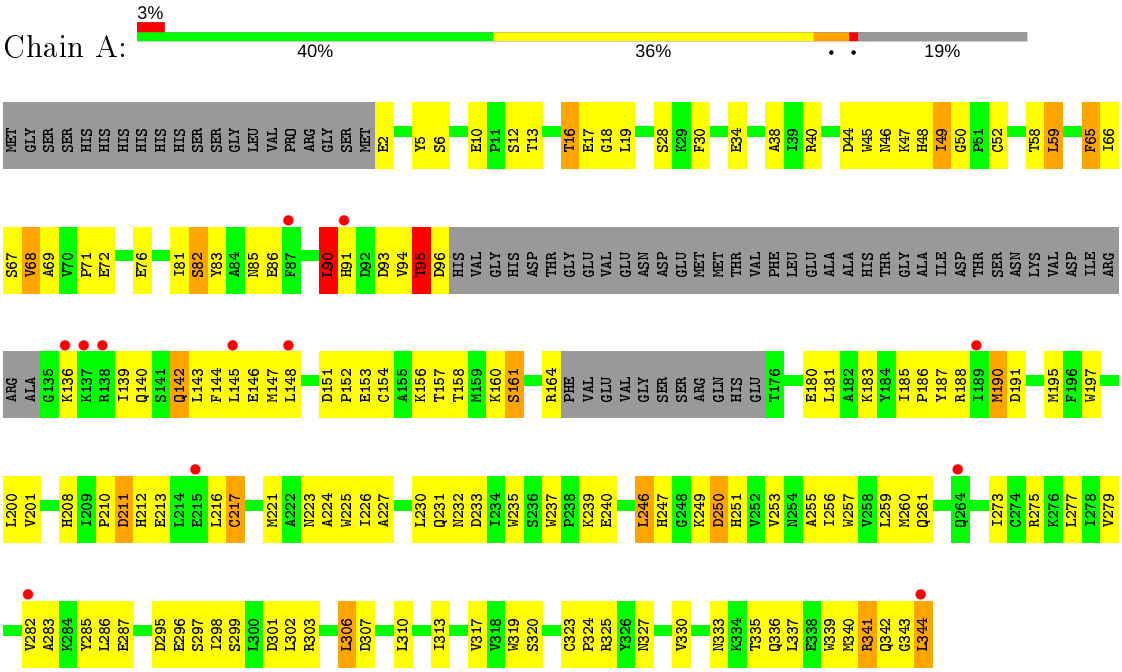
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	33	Total	O	0	0
			33	33		
5	B	43	Total	O	0	0
			43	43		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

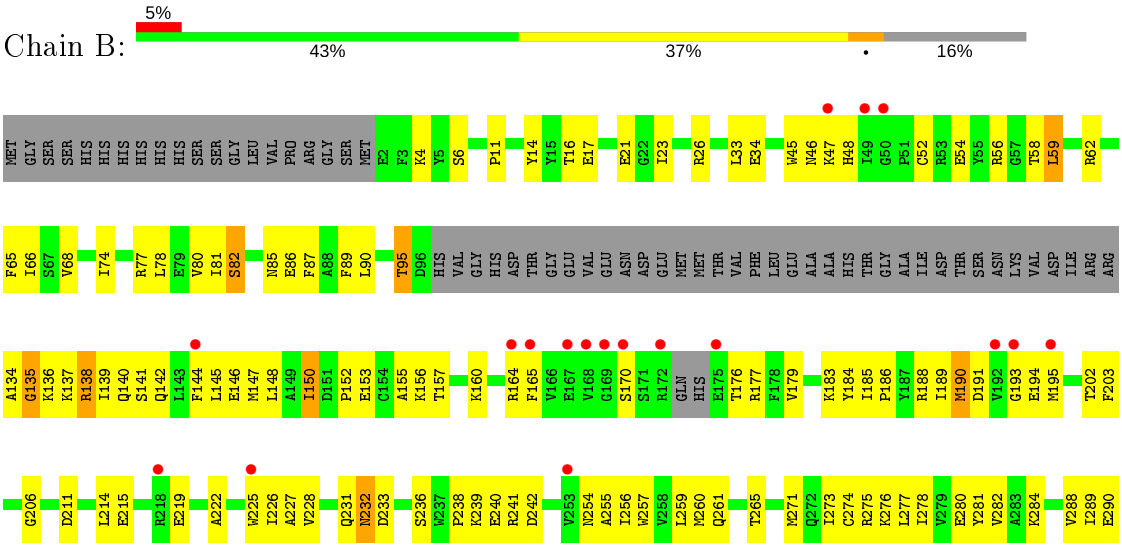
- Molecule 1: Fusicoccadiene synthase

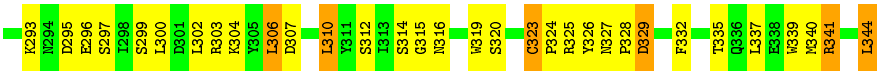
Chain A:



- Molecule 1: Fusicoccadiene synthase

Chain B:




K293
N294
D295
E296
S297
I298
S299
L300
D301
L302
R303
K304
Y305
L306
D307
L310
Y311
S312
I313
S314
G315
N316
W319
S320
C323
P324
R325
Y326
N327
P328
D329
F332
T335
Q336
L337
E338
W339
M340
R341
L344

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.60Å 142.60Å 117.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.39 – 2.50 43.39 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.39-2.50) 93.5 (43.39-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.51Å)	Xtriage
Refinement program	PHENIX dev_1839	Depositor
R, R_{free}	0.207 , 0.238 0.205 , 0.236	Depositor DCC
R_{free} test set	2383 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	63.6	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 63.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.210 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4972	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: CL, MN, NRD

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	0.57	2/2446 (0.1%)	0.63	3/3312 (0.1%)
1	B	0.56	0/2524	0.61	2/3417 (0.1%)
All	All	0.57	2/4970 (0.0%)	0.62	5/6729 (0.1%)

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	2
1	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	THR	C-N	8.20	1.52	1.34
1	A	90	LEU	C-N	5.36	1.46	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	LEU	O-C-N	-11.08	104.97	122.70
1	B	135	GLY	N-CA-C	-6.80	96.09	113.10
1	A	90	LEU	C-N-CA	6.45	137.81	121.70
1	B	95	THR	CB-CA-C	-5.86	95.79	111.60
1	A	90	LEU	CB-CA-C	5.80	121.23	110.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	90	LEU	Mainchain
1	A	95	THR	Mainchain
1	B	170	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2325	108	0
1	B	2465	0	2401	109	0
2	A	4	0	0	0	0
2	B	5	0	0	0	0
3	A	16	0	15	6	0
3	B	16	0	15	6	0
4	A	1	0	0	1	0
4	B	1	0	0	3	0
5	A	33	0	0	8	0
5	B	43	0	0	5	0
All	All	4972	0	4756	220	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 23.

All (220) 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)
4:B:705:CL:CL	5:B:814:HOH:O	2.17	0.98
1:B:188:ARG:NH2	1:B:232:ASN:OD1	2.07	0.86
1:B:295:ASP:O	1:B:303:ARG:NH2	2.08	0.86
1:A:240:GLU:OE2	5:A:803:HOH:O	1.95	0.84
4:A:705:CL:CL	5:A:822:HOH:O	2.37	0.79
1:B:56:ARG:NH1	1:B:324:PRO:O	2.16	0.77
1:B:339:TRP:O	5:B:801:HOH:O	2.02	0.77
1:A:239:LYS:NZ	5:A:806:HOH:O	2.15	0.77
1:B:6:SER:OG	1:B:26:ARG:NH1	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LYS:HA	1:B:138:ARG:CZ	2.18	0.73
1:B:188:ARG:NH2	3:B:704:NRD:OAP	2.19	0.72
1:A:191:ASP:O	5:A:804:HOH:O	2.05	0.72
1:B:239:LYS:NZ	3:B:704:NRD:OAL	2.22	0.72
1:A:333:ASN:HB2	1:A:336:GLN:H	1.54	0.71
1:B:323:CYS:O	1:B:327:ASN:ND2	2.17	0.70
1:B:62:ARG:NH1	5:B:807:HOH:O	2.24	0.70
1:A:66:ILE:HD13	1:A:81:ILE:HG22	1.73	0.70
1:B:329:ASP:OD2	1:B:329:ASP:N	2.20	0.69
1:A:295:ASP:OD1	1:A:297:SER:OG	2.07	0.69
1:B:95:THR:O	1:B:95:THR:HG22	1.91	0.69
1:B:233:ASP:OD1	5:B:802:HOH:O	2.11	0.67
1:A:191:ASP:OD2	5:A:804:HOH:O	2.12	0.67
1:A:58:THR:HG23	1:A:59:LEU:HD13	1.75	0.67
1:B:231:GLN:OE1	1:B:316:ASN:ND2	2.26	0.66
1:B:241:ARG:NH1	1:B:242:ASP:OD1	2.29	0.66
1:B:66:ILE:HD12	1:B:82:SER:HA	1.77	0.66
1:B:134:ALA:O	1:B:135:GLY:C	2.33	0.66
1:A:232:ASN:ND2	3:A:704:NRD:H7	2.11	0.65
1:B:66:ILE:HD13	1:B:81:ILE:HG22	1.79	0.65
1:A:2:GLU:OE1	5:A:805:HOH:O	2.14	0.64
1:B:140:GLN:OE1	1:B:140:GLN:N	2.30	0.64
1:B:33:LEU:HB2	1:B:78:LEU:HD23	1.79	0.64
1:A:325:ARG:NH2	3:A:704:NRD:OAJ	2.30	0.63
1:B:34:GLU:HG3	1:B:82:SER:HB3	1.80	0.63
1:B:153:GLU:HA	1:B:156:LYS:HE3	1.81	0.63
1:A:93:ASP:OD1	1:A:325:ARG:NH1	2.31	0.62
1:B:144:PHE:O	1:B:148:LEU:N	2.28	0.62
1:B:54:GLU:OE2	1:B:341:ARG:NH1	2.32	0.61
1:B:87:PHE:HA	1:B:90:LEU:HD12	1.80	0.61
1:B:295:ASP:OD1	1:B:297:SER:OG	2.17	0.61
1:A:40:ARG:HG2	1:A:83:TYR:HE2	1.67	0.60
1:B:134:ALA:O	1:B:136:LYS:N	2.35	0.60
1:A:17:GLU:OE1	1:A:275:ARG:NH2	2.33	0.60
1:A:157:THR:O	1:A:161:SER:N	2.24	0.59
1:A:275:ARG:O	1:A:279:VAL:HG23	2.01	0.59
1:A:28:SER:OG	1:A:28:SER:O	2.19	0.59
1:B:188:ARG:NH1	3:B:704:NRD:OAN	2.35	0.59
1:A:310:LEU:HA	1:A:313:ILE:HD12	1.83	0.58
1:A:239:LYS:NZ	3:A:704:NRD:OAK	2.32	0.58
1:B:153:GLU:N	1:B:153:GLU:OE2	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ARG:NH1	1:A:191:ASP:OD2	2.37	0.58
1:B:77:ARG:NH1	1:B:203:PHE:O	2.36	0.58
1:B:78:LEU:O	1:B:82:SER:OG	2.21	0.57
1:A:10:GLU:HG3	1:A:13:THR:HG23	1.86	0.56
1:A:187:TYR:O	1:A:190:MET:HG2	2.06	0.56
1:A:210:PRO:HB2	1:A:212:HIS:CD2	2.40	0.56
1:B:48:HIS:HD2	1:B:139:ILE:HD12	1.71	0.55
1:B:319:TRP:O	1:B:323:CYS:N	2.36	0.55
1:A:34:GLU:HG3	1:A:82:SER:HB3	1.89	0.55
1:B:68:VAL:HG22	1:B:315:GLY:HA2	1.87	0.55
1:B:274:CYS:O	1:B:278:ILE:HG13	2.08	0.54
1:A:16:THR:HG22	1:A:18:GLY:H	1.73	0.54
1:A:324:PRO:HA	1:A:327:ASN:O	2.07	0.54
1:B:16:THR:N	4:B:705:CL:CL	2.76	0.54
1:B:136:LYS:HG3	1:B:138:ARG:HD2	1.88	0.53
1:B:188:ARG:HA	1:B:191:ASP:HB3	1.89	0.53
1:A:148:LEU:HD12	1:A:152:PRO:HA	1.90	0.53
1:B:184:TYR:OH	1:B:233:ASP:OD2	2.16	0.52
1:A:46:ASN:HA	1:A:50:GLY:O	2.09	0.52
1:B:164:ARG:HB3	1:B:195:MET:SD	2.48	0.52
1:B:135:GLY:O	1:B:138:ARG:NH2	2.42	0.52
1:B:188:ARG:HH22	3:B:704:NRD:PAM	2.30	0.52
1:B:17:GLU:N	4:B:705:CL:CL	2.68	0.52
1:B:56:ARG:HB3	1:B:325:ARG:HA	1.91	0.52
1:A:10:GLU:OE2	1:A:12:SER:N	2.27	0.51
1:A:223:ASN:HB2	1:A:285:TYR:HB2	1.92	0.51
1:A:142:GLN:HG3	1:A:143:LEU:N	2.25	0.51
1:A:257:TRP:O	1:A:261:GLN:HG2	2.10	0.51
1:A:76:GLU:OE1	1:A:76:GLU:N	2.40	0.51
1:A:283:ALA:O	1:A:287:GLU:HG2	2.11	0.51
1:B:11:PRO:HA	1:B:14:TYR:CE2	2.45	0.51
1:A:221:MET:HE3	1:A:225:TRP:HE1	1.76	0.51
1:A:91:HIS:O	1:A:95:THR:OG1	2.29	0.50
1:B:188:ARG:HH12	3:B:704:NRD:PAM	2.33	0.50
1:B:66:ILE:HD11	1:B:85:ASN:HB2	1.92	0.50
1:A:28:SER:HB2	1:A:71:PRO:HA	1.93	0.50
1:B:326:TYR:HH	3:B:704:NRD:H2	0.80	0.50
1:A:28:SER:N	1:A:67:SER:O	2.44	0.50
1:B:227:ALA:O	1:B:231:GLN:HG3	2.11	0.50
1:B:314:SER:OG	5:B:805:HOH:O	2.20	0.50
1:B:56:ARG:NH1	1:B:328:PRO:HA	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ARG:HH12	3:A:704:NRD:PAM	2.35	0.50
1:A:208:HIS:N	1:A:301:ASP:OD2	2.35	0.50
1:A:44:ASP:OD2	1:A:83:TYR:OH	2.13	0.50
1:A:231:GLN:HB3	1:A:235:TRP:CZ3	2.46	0.49
1:A:247:HIS:HB2	1:A:249:LYS:HG2	1.94	0.49
3:A:704:NRD:OAP	5:A:804:HOH:O	2.18	0.49
1:B:290:GLU:OE2	1:B:293:LYS:NZ	2.40	0.49
1:B:302:LEU:O	1:B:306:LEU:HD22	2.12	0.49
1:B:144:PHE:HA	1:B:147:MET:HB3	1.95	0.49
1:A:142:GLN:HG3	1:A:143:LEU:H	1.77	0.49
1:A:16:THR:HG22	1:A:18:GLY:N	2.27	0.49
1:A:226:ILE:O	1:A:230:LEU:HG	2.13	0.49
1:B:232:ASN:ND2	1:B:236:SER:HB3	2.27	0.49
1:A:296:GLU:N	1:A:296:GLU:OE1	2.46	0.49
1:B:232:ASN:O	1:B:236:SER:OG	2.31	0.48
1:B:211:ASP:HA	1:B:214:LEU:HG	1.95	0.48
1:B:185:ILE:HB	1:B:186:PRO:HD3	1.96	0.48
1:B:307:ASP:O	1:B:310:LEU:HB2	2.11	0.48
1:A:227:ALA:O	1:A:231:GLN:HG3	2.13	0.48
1:A:279:VAL:O	1:A:282:VAL:HB	2.14	0.48
1:B:45:TRP:HD1	1:B:52:CYS:HB2	1.78	0.48
1:A:181:LEU:HD12	1:A:181:LEU:HA	1.68	0.48
1:B:284:LYS:O	1:B:288:VAL:HG23	2.14	0.48
1:B:45:TRP:CD1	1:B:52:CYS:HB2	2.49	0.48
1:A:233:ASP:O	1:A:237:TRP:HB2	2.13	0.47
1:B:271:MET:O	1:B:275:ARG:HG3	2.14	0.47
1:B:337:LEU:O	1:B:341:ARG:HG2	2.14	0.47
1:B:183:LYS:O	1:B:186:PRO:HD2	2.14	0.47
1:B:273:ILE:O	1:B:277:LEU:HG	2.15	0.47
1:B:58:THR:HG23	1:B:59:LEU:HD13	1.97	0.47
1:B:337:LEU:O	1:B:340:MET:N	2.48	0.47
1:A:47:LYS:HG2	1:A:48:HIS:CE1	2.50	0.47
1:B:300:LEU:HG	1:B:304:LYS:HD2	1.97	0.47
1:A:211:ASP:N	1:A:211:ASP:OD1	2.47	0.46
1:A:45:TRP:CD1	1:A:52:CYS:HB2	2.50	0.46
1:A:213:GLU:OE2	1:A:299:SER:OG	2.18	0.46
1:A:183:LYS:O	1:A:186:PRO:HD2	2.16	0.46
1:B:139:ILE:C	1:B:141:SER:H	2.18	0.46
1:A:66:ILE:HD11	1:A:85:ASN:HB2	1.97	0.46
1:B:17:GLU:OE1	1:B:275:ARG:NH2	2.48	0.46
1:A:65:PHE:O	1:A:69:ALA:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:GLU:O	1:B:150:ILE:HG13	2.16	0.46
1:A:140:GLN:O	1:A:143:LEU:HB3	2.16	0.46
1:A:28:SER:O	1:A:30:PHE:N	2.49	0.46
1:A:65:PHE:O	1:A:68:VAL:HG12	2.16	0.45
1:A:153:GLU:HG3	1:A:208:HIS:NE2	2.31	0.45
1:A:136:LYS:HB3	1:A:139:ILE:HD11	1.99	0.45
1:A:239:LYS:HE3	1:A:240:GLU:HG3	1.98	0.45
1:A:302:LEU:O	1:A:306:LEU:HD22	2.16	0.45
1:B:148:LEU:HD13	1:B:155:ALA:HB3	1.98	0.45
1:B:142:GLN:O	1:B:145:LEU:HB2	2.16	0.45
1:B:299:SER:O	1:B:303:ARG:HG3	2.16	0.45
1:A:255:ALA:O	1:A:259:LEU:HG	2.16	0.45
1:B:194:GLU:HA	1:B:225:TRP:CZ2	2.52	0.45
1:B:242:ASP:N	1:B:242:ASP:OD1	2.49	0.45
1:A:158:THR:HA	1:A:161:SER:HB3	2.00	0.44
1:B:23:ILE:HG21	1:B:310:LEU:O	2.17	0.44
1:A:256:ILE:O	1:A:260:MET:HG3	2.18	0.44
1:B:58:THR:OG1	1:B:65:PHE:HB3	2.18	0.44
1:A:273:ILE:O	1:A:277:LEU:HG	2.18	0.44
1:A:5:TYR:H	1:A:72:GLU:CD	2.20	0.44
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.67	0.43
1:B:165:PHE:CE1	1:B:193:GLY:HA2	2.53	0.43
1:A:337:LEU:O	1:A:341:ARG:HG2	2.17	0.43
1:A:319:TRP:CE2	1:A:323:CYS:HB3	2.53	0.43
1:B:148:LEU:HD13	1:B:148:LEU:HA	1.73	0.43
1:B:226:ILE:HD13	1:B:281:TYR:CE1	2.54	0.43
1:A:250:ASP:OD1	1:A:251:HIS:ND1	2.36	0.43
1:B:215:GLU:O	1:B:219:GLU:HG3	2.19	0.43
1:B:254:ASN:OD1	1:B:256:ILE:HG12	2.18	0.43
1:B:190:MET:H	1:B:190:MET:HG2	1.62	0.43
1:B:239:LYS:HE3	1:B:240:GLU:HG3	2.01	0.43
1:A:148:LEU:HA	1:A:148:LEU:HD13	1.80	0.43
1:A:153:GLU:HA	1:A:156:LYS:NZ	2.33	0.43
1:A:181:LEU:HD22	1:A:259:LEU:HD21	2.01	0.43
1:A:81:ILE:HG23	1:A:200:LEU:HD11	2.01	0.43
1:A:235:TRP:CE3	1:A:320:SER:HB2	2.54	0.43
1:A:341:ARG:HG2	1:A:341:ARG:H	1.67	0.43
1:A:197:TRP:O	1:A:201:VAL:HG23	2.18	0.43
1:A:216:LEU:HG	1:A:217:CYS:N	2.33	0.43
1:B:296:GLU:OE1	1:B:296:GLU:N	2.52	0.42
1:B:86:GLU:O	1:B:90:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:PRO:HB3	1:B:241:ARG:NH2	2.35	0.42
1:B:47:LYS:HG2	1:B:48:HIS:ND1	2.34	0.42
1:A:320:SER:HA	1:A:323:CYS:SG	2.59	0.42
1:A:344:LEU:HA	1:A:344:LEU:HD22	1.89	0.42
1:B:276:LYS:O	1:B:280:GLU:HG3	2.19	0.42
1:A:181:LEU:O	1:A:185:ILE:HG13	2.19	0.42
1:A:90:LEU:O	1:A:94:VAL:HG23	2.19	0.42
1:B:11:PRO:HA	1:B:14:TYR:CZ	2.54	0.42
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.85	0.42
1:A:324:PRO:HG3	1:A:330:VAL:HG12	2.01	0.42
1:B:280:GLU:O	1:B:284:LYS:HG3	2.20	0.42
1:B:65:PHE:HB2	1:B:319:TRP:NE1	2.35	0.42
1:B:289:ILE:HD13	1:B:289:ILE:HA	1.87	0.42
1:B:332:PHE:HB2	1:B:337:LEU:HD21	2.02	0.42
1:B:74:ILE:HB	1:B:77:ARG:HG3	2.01	0.42
1:A:144:PHE:HD1	1:A:147:MET:HE1	1.84	0.41
1:A:224:ALA:HB2	1:A:285:TYR:CD1	2.55	0.41
1:A:38:ALA:HB1	1:A:86:GLU:HG3	2.03	0.41
1:A:49:ILE:HG13	1:A:50:GLY:N	2.34	0.41
1:A:151:ASP:CG	1:A:154:CYS:HB2	2.41	0.41
1:A:232:ASN:CG	3:A:704:NRD:H7	2.40	0.41
1:B:255:ALA:O	1:B:259:LEU:HG	2.20	0.41
1:B:260:MET:HA	1:B:265:THR:HG22	2.03	0.41
1:A:148:LEU:CD1	1:A:152:PRO:HA	2.50	0.41
1:A:295:ASP:OD1	1:A:298:ILE:HG13	2.20	0.41
1:A:335:THR:HG22	1:A:339:TRP:CZ3	2.55	0.41
1:B:257:TRP:O	1:B:261:GLN:HG2	2.21	0.41
1:A:153:GLU:HG2	1:A:154:CYS:N	2.35	0.41
1:A:164:ARG:NH1	1:A:195:MET:HB2	2.35	0.41
1:A:58:THR:OG1	1:A:65:PHE:HB3	2.20	0.41
1:A:96:ASP:CG	5:A:807:HOH:O	2.58	0.41
1:B:323:CYS:HA	1:B:324:PRO:HD3	1.88	0.41
1:B:319:TRP:O	1:B:323:CYS:HB3	2.21	0.41
1:A:212:HIS:CE1	1:A:213:GLU:HG3	2.56	0.40
1:A:259:LEU:HD23	1:A:259:LEU:HA	1.83	0.40
1:A:337:LEU:O	1:A:340:MET:N	2.54	0.40
1:B:225:TRP:O	1:B:228:VAL:HG22	2.21	0.40
1:B:278:ILE:O	1:B:282:VAL:HG23	2.20	0.40
1:B:341:ARG:H	1:B:341:ARG:HG2	1.50	0.40
1:B:58:THR:HG22	1:B:86:GLU:OE2	2.20	0.40
1:B:228:VAL:O	1:B:231:GLN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:SER:C	1:A:30:PHE:H	2.23	0.40
1:A:295:ASP:HB3	1:A:298:ILE:CD1	2.51	0.40
1:A:6:SER:HB3	1:A:71:PRO:O	2.21	0.40
1:B:339:TRP:HB3	1:B:344:LEU:HD23	2.03	0.40
1:A:299:SER:HB2	1:A:302:LEU:HB2	2.04	0.40
1:B:202:THR:O	1:B:206:GLY:N	2.55	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	288/363 (79%)	253 (88%)	31 (11%)	4 (1%)	11	20
1	B	298/363 (82%)	277 (93%)	18 (6%)	3 (1%)	15	28
All	All	586/726 (81%)	530 (90%)	49 (8%)	7 (1%)	13	24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	222	ALA
1	A	65	PHE
1	B	150	ILE
1	A	253	VAL
1	A	343	GLY
1	A	317	VAL
1	B	152	PRO

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	257/317 (81%)	233 (91%)	24 (9%)	9	17
1	B	266/317 (84%)	240 (90%)	26 (10%)	8	15
All	All	523/634 (82%)	473 (90%)	50 (10%)	8	16

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	49	ILE
1	A	59	LEU
1	A	68	VAL
1	A	82	SER
1	A	95	THR
1	A	142	GLN
1	A	145	LEU
1	A	146	GLU
1	A	160	LYS
1	A	161	SER
1	A	180	GLU
1	A	190	MET
1	A	211	ASP
1	A	217	CYS
1	A	246	LEU
1	A	250	ASP
1	A	286	LEU
1	A	303	ARG
1	A	306	LEU
1	A	307	ASP
1	A	341	ARG
1	A	342	GLN
1	A	344	LEU
1	B	4	LYS
1	B	21	GLU
1	B	46	ASN

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Mol	Chain	Res	Type
1	B	59	LEU
1	B	80	VAL
1	B	82	SER
1	B	89	PHE
1	B	137	LYS
1	B	138	ARG
1	B	157	THR
1	B	160	LYS
1	B	176	THR
1	B	177	ARG
1	B	179	VAL
1	B	189	ILE
1	B	190	MET
1	B	232	ASN
1	B	306	LEU
1	B	310	LEU
1	B	312	SER
1	B	320	SER
1	B	323	CYS
1	B	329	ASP
1	B	335	THR
1	B	341	ARG
1	B	344	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NRD	B	704	2	15,15,15	3.91	5 (33%)	21,23,23	2.26	6 (28%)
3	NRD	A	704	1,2	15,15,15	2.87	4 (26%)	21,23,23	2.20	7 (33%)

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	NRD	B	704	2	-	5/25/25/25	-
3	NRD	A	704	1,2	-	4/25/25/25	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	704	NRD	PAI-CAG	-10.76	1.77	1.85
3	B	704	NRD	PAM-CAG	-9.37	1.78	1.85
3	A	704	NRD	PAM-CAG	-7.41	1.80	1.85
3	A	704	NRD	PAI-CAG	-6.79	1.80	1.85
3	B	704	NRD	PAI-OAJ	-2.56	1.50	1.54
3	A	704	NRD	PAI-OAJ	-2.36	1.50	1.54
3	B	704	NRD	CAF-CAG	-2.34	1.50	1.54
3	B	704	NRD	PAM-OAN	-2.20	1.50	1.54
3	A	704	NRD	PAM-OAP	-2.09	1.50	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	704	NRD	PAM-CAG-PAI	-5.68	102.65	112.81
3	A	704	NRD	PAM-CAG-PAI	-5.40	103.15	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	704	NRD	CAE-CAF-CAG	-5.39	106.17	116.07
3	B	704	NRD	CAE-CAF-CAG	-4.46	107.88	116.07
3	B	704	NRD	OAL-PAI-CAG	-3.16	101.60	109.86
3	A	704	NRD	OAJ-PAI-OAK	2.81	115.91	107.99
3	B	704	NRD	OAO-PAM-CAG	-2.77	102.61	109.86
3	B	704	NRD	OAN-PAM-OAP	2.69	115.57	107.99
3	B	704	NRD	OAJ-PAI-OAK	2.55	115.18	107.99
3	A	704	NRD	OAH-CAG-CAF	-2.51	105.13	110.73
3	A	704	NRD	OAK-PAI-CAG	-2.32	100.96	106.17
3	A	704	NRD	OAO-PAM-CAG	-2.11	104.35	109.86
3	A	704	NRD	OAL-PAI-CAG	-2.02	104.59	109.86

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	704	NRD	CAE-CAF-CAG-PAI
3	B	704	NRD	CAE-CAF-CAG-PAM
3	B	704	NRD	CAE-CAF-CAG-OAH
3	A	704	NRD	CAE-CAF-CAG-PAI
3	A	704	NRD	CAE-CAF-CAG-PAM
3	A	704	NRD	CAB-CAC-CAE-CAF
3	A	704	NRD	CAE-CAF-CAG-OAH
3	B	704	NRD	CAF-CAG-PAI-OAL
3	B	704	NRD	CAF-CAG-PAM-OAO

There are no ring outliers.

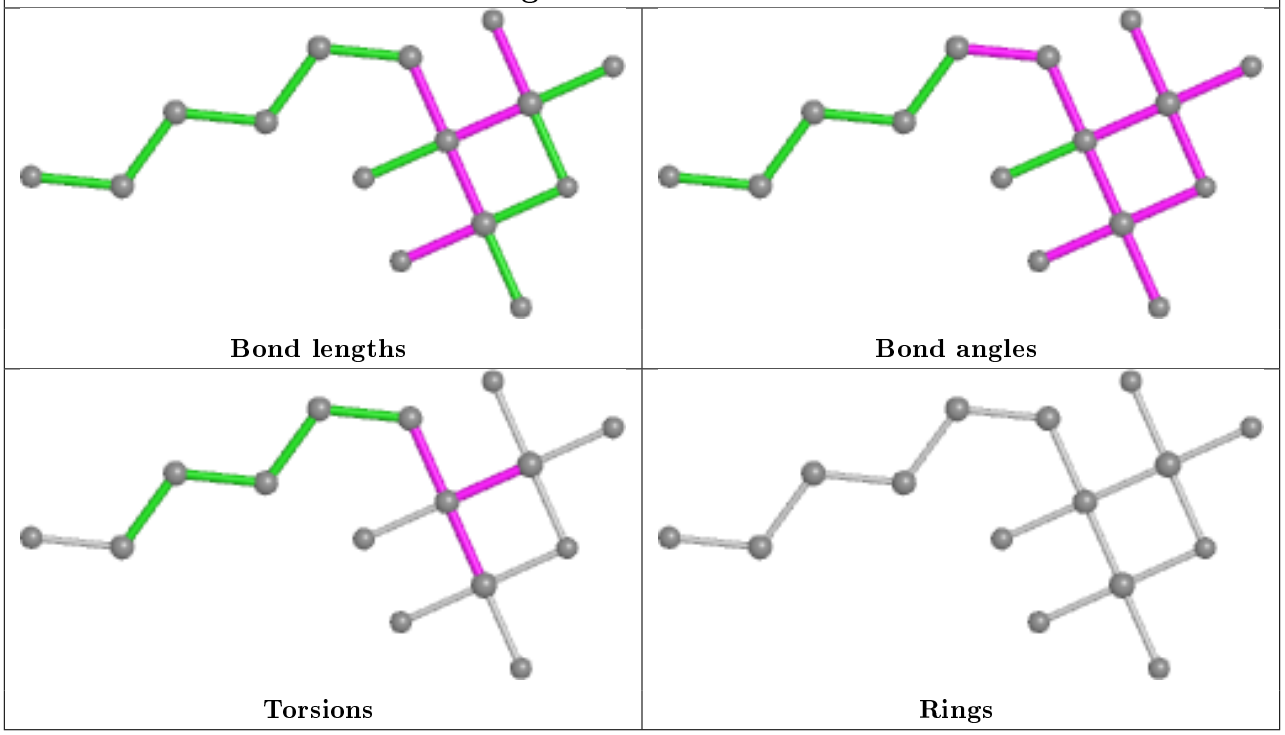
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	704	NRD	6	0
3	A	704	NRD	6	0

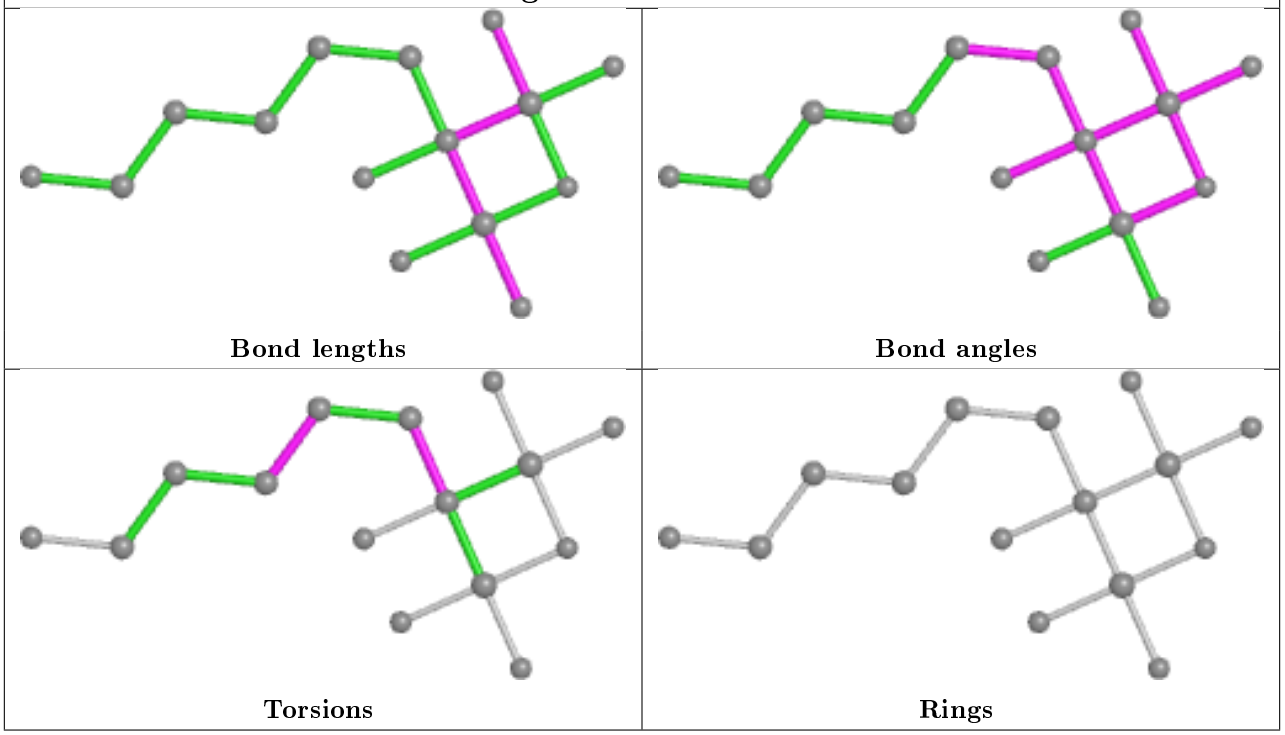
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 NRD B 704



Ligand NRD A 704



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	294/363 (80%)	0.49	12 (4%)	37	40	51, 68, 107, 131	0
1	B	304/363 (83%)	0.50	18 (5%)	22	23	46, 62, 104, 204	0
All	All	598/726 (82%)	0.50	30 (5%)	28	30	46, 65, 107, 204	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170	SER	6.3
1	A	344	LEU	5.0
1	B	253	VAL	4.3
1	A	215	GLU	4.3
1	B	144	PHE	3.5
1	A	136	LYS	3.4
1	B	169	GLY	3.0
1	B	193	GLY	2.9
1	B	167	GLU	2.8
1	B	165	PHE	2.8
1	A	145	LEU	2.7
1	B	225	TRP	2.7
1	B	175	GLU	2.6
1	A	87	PHE	2.6
1	B	218	ARG	2.5
1	B	49	ILE	2.5
1	B	164	ARG	2.4
1	B	172	ARG	2.4
1	B	47	LYS	2.3
1	A	138	ARG	2.3
1	B	195	MET	2.2
1	A	137	LYS	2.2
1	A	282	VAL	2.2
1	B	168	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	192	VAL	2.2
1	A	91	HIS	2.1
1	B	50	GLY	2.1
1	A	148	LEU	2.0
1	A	189	ILE	2.0
1	A	264	GLN	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 carbohydrates in this entry.

6.4 Ligands (i)

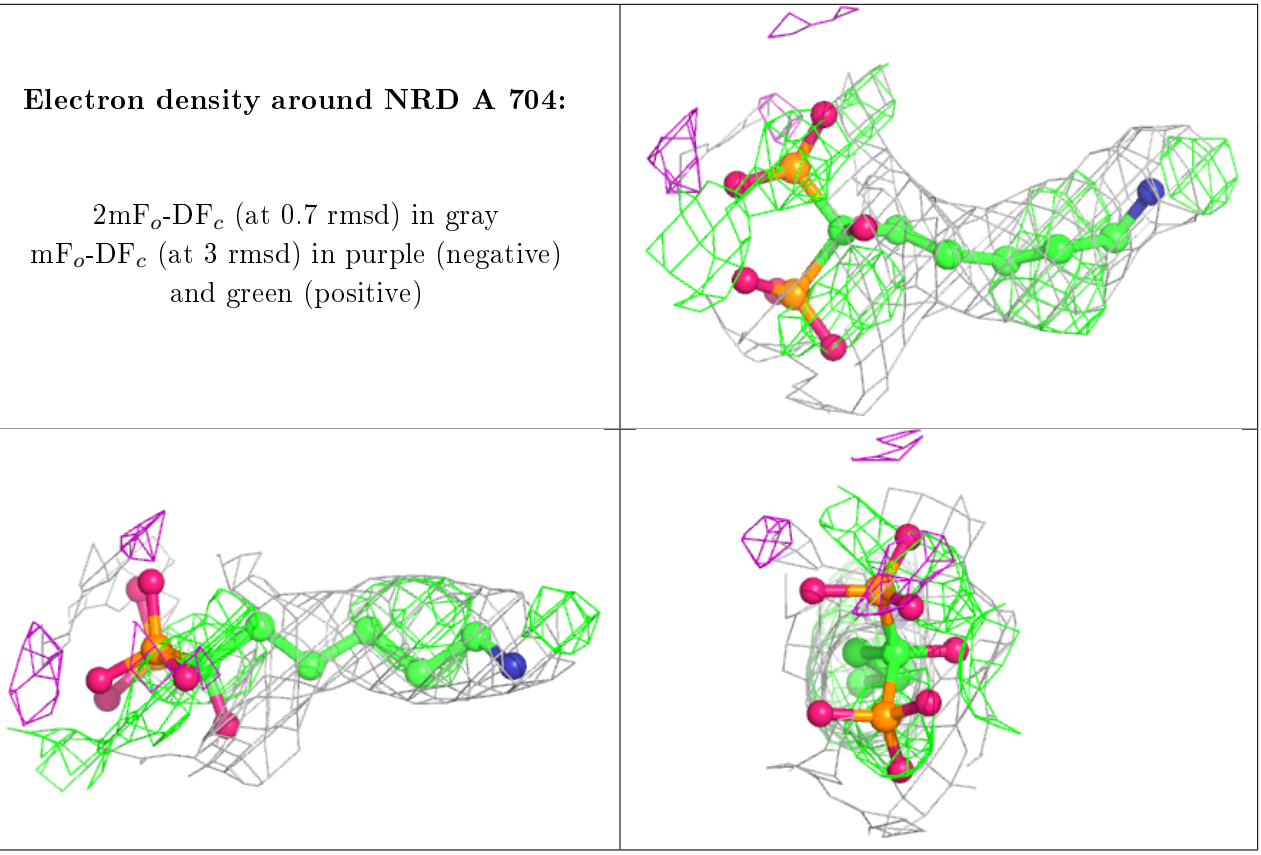
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	MN	B	707	1/1	0.22	0.26	201,201,201,201	0
2	MN	A	701	1/1	0.81	0.26	69,69,69,69	0
4	CL	B	705	1/1	0.90	0.12	70,70,70,70	0
2	MN	A	702	1/1	0.90	0.19	68,68,68,68	0
2	MN	A	706	1/1	0.91	0.03	122,122,122,122	0
2	MN	B	706	1/1	0.95	0.08	94,94,94,94	0
2	MN	B	701	1/1	0.95	0.26	66,66,66,66	0
3	NRD	A	704	16/16	0.95	0.21	58,64,77,83	0
4	CL	A	705	1/1	0.97	0.11	74,74,74,74	0
2	MN	B	702	1/1	0.97	0.23	63,63,63,63	0
3	NRD	B	704	16/16	0.97	0.27	57,65,78,87	0
2	MN	B	703	1/1	0.97	0.25	66,66,66,66	0
2	MN	A	703	1/1	0.98	0.21	55,55,55,55	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.

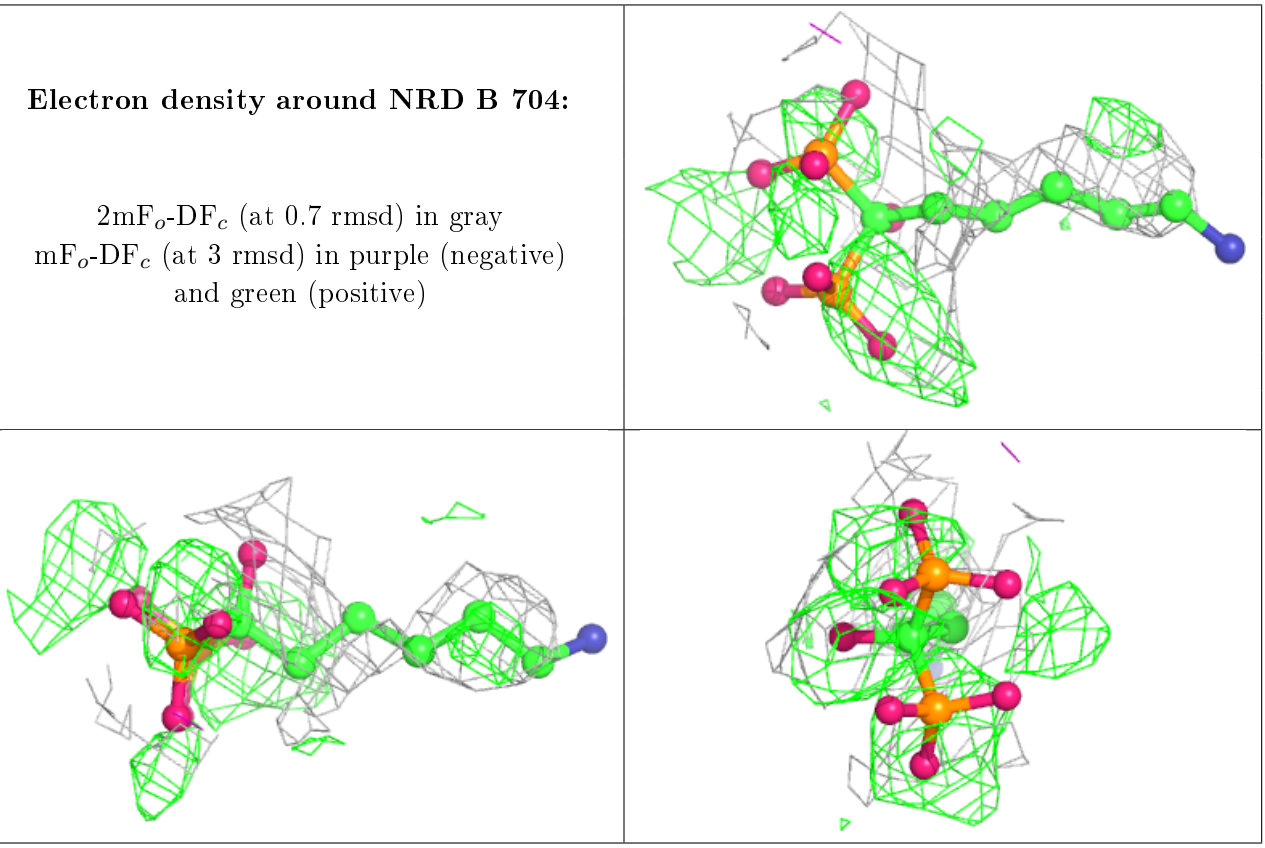
Electron density around NRD A 704:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around NRD B 704:

$2mF_o$-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.