Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:40 am BST

PDB ID	:	6HSC
Title	:	Structure of Human Serum Albumin in complex with Aristolochic Acid at 1.9 A resolution
Authors	:	Pomyalov, S.; Sidorenko, V.S.; Grollman, A.P.; Shoham, G.
Deposited on	:	2018-09-29
Resolution	:	1.90 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:

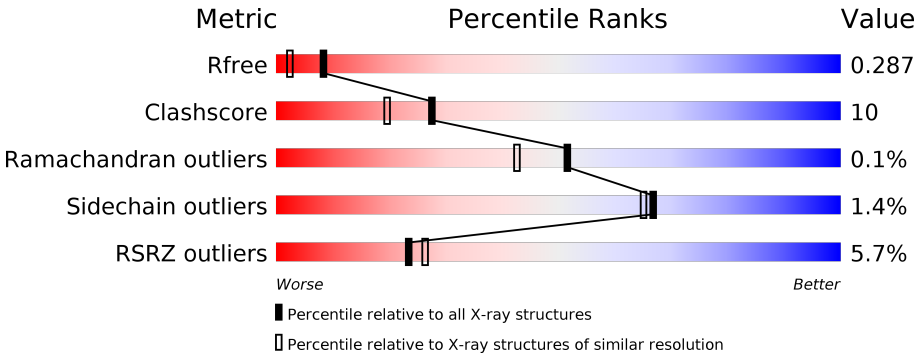
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	609	7% 79% 16%
1	B	609	4% 78% 18%

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
2	MYR	A	606	-	-	X	-
2	MYR	B	605	-	-	X	-

2 Entry composition

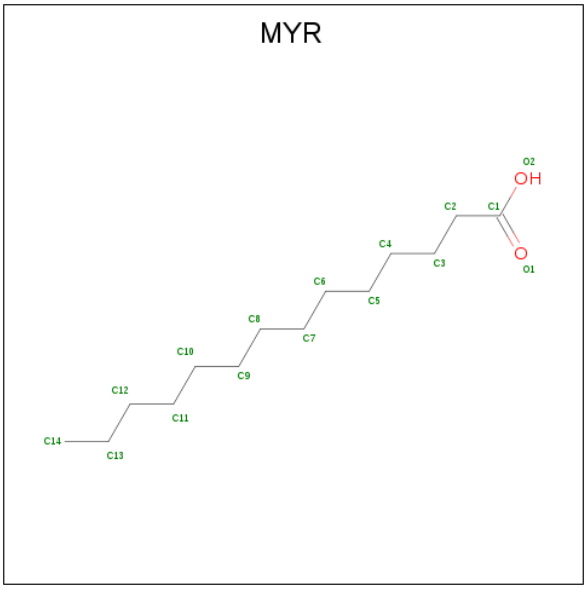
There are 5 unique types of molecules in this entry. The entry contains 9977 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	3	0
			4579	2893	781	864	41			
1	B	582	Total	C	N	O	S	0	2	0
			4598	2903	783	871	41			

- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		

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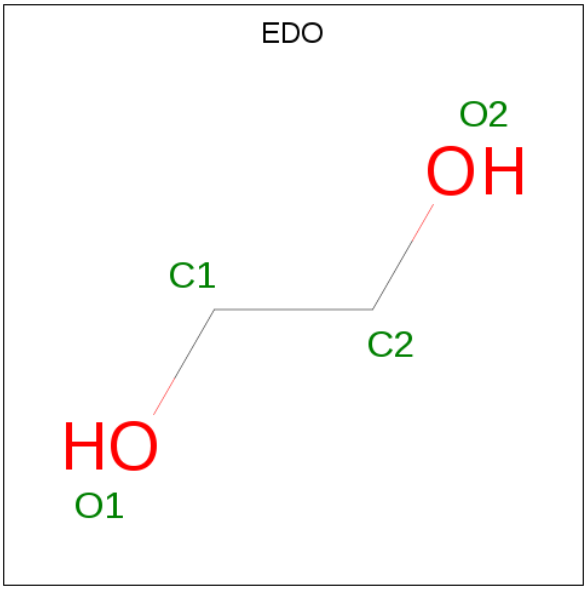
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 16 14 2	0	0
2	A	1	Total C O 16 14 2	0	0
2	A	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

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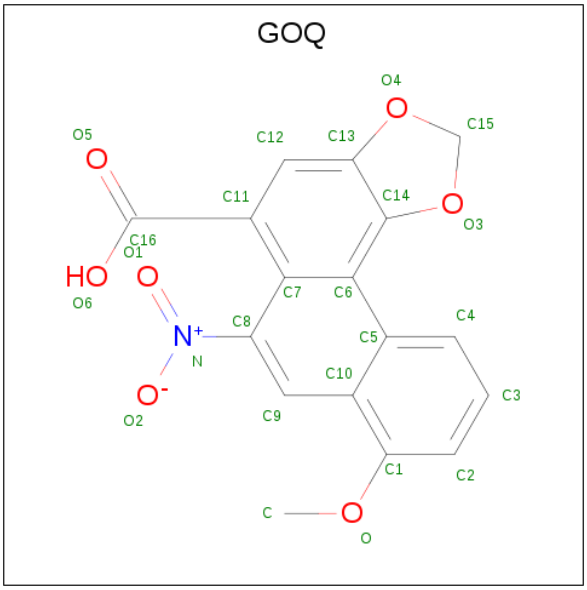
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is 8-methoxy-6-nitro-naphtho[1,2-e][1,3]benzodioxole-5-carboxylic acid (three-letter code: GOQ) (formula: $C_{17}H_{11}NO_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 25 17 1 7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	183	Total O 183 183	0	0

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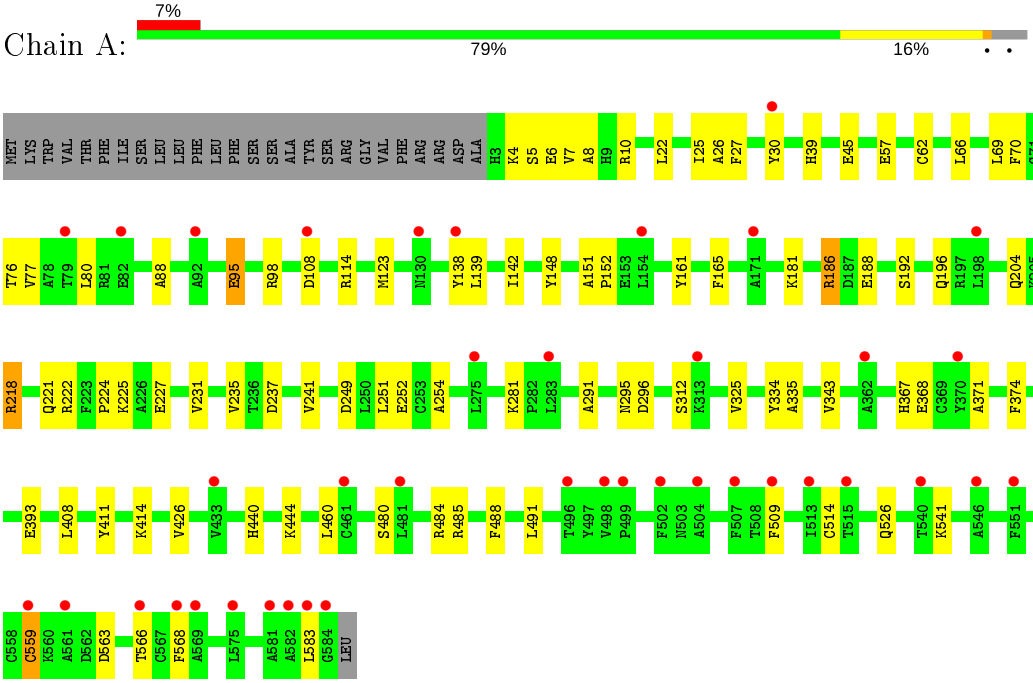
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	348	Total	O	0	0
			348	348		

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.

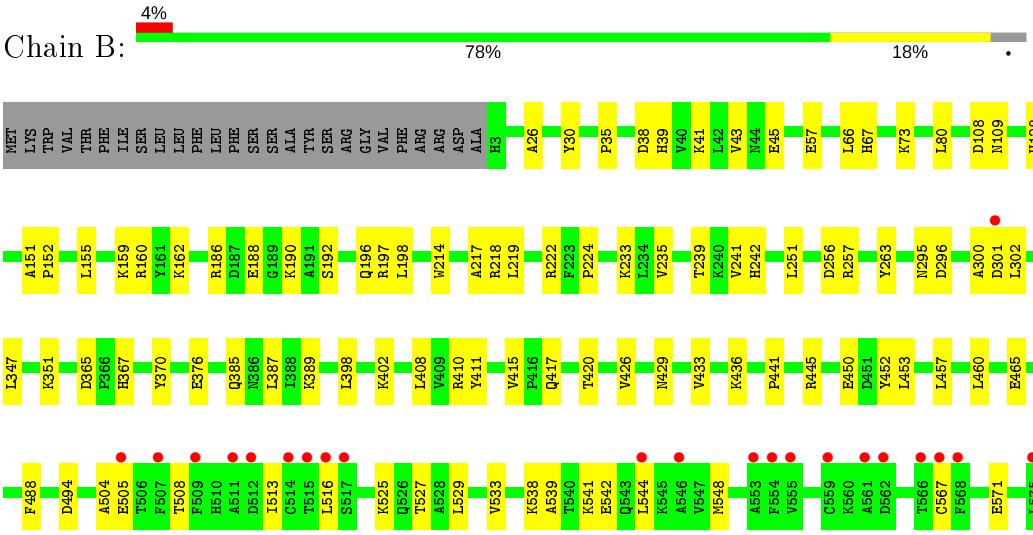
- Molecule 1: Serum albumin

Chain A:



- Molecule 1: Serum albumin

Chain B:




L583
G584
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.40Å 37.87Å 180.25Å 90.00° 105.12° 90.00°	Depositor
Resolution (Å)	47.20 – 1.90 47.20 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.20-1.90) 98.8 (47.20-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.14_3228	Depositor
R, R_{free}	0.238 , 0.286 0.238 , 0.287	Depositor DCC
R_{free} test set	4931 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9977	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2001e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: MYR, GOQ, EDO

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	0.37	0/4670	0.51	0/6311
1	B	0.53	0/4688	0.65	0/6332
All	All	0.45	0/9358	0.58	0/12643

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	4579	0	4450	96	0
1	B	4598	0	4482	80	0
2	A	112	0	186	25	0
2	B	96	0	162	30	0
3	A	8	0	12	0	0
3	B	28	0	42	5	0
4	B	25	0	0	1	0
5	A	183	0	0	8	0
5	B	348	0	0	7	0
All	All	9977	0	9334	186	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 10.

All (186) 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:218:ARG:NH1	1:A:222:ARG:HH21	1.74	0.84
1:A:514:CYS:SG	1:A:559:CYS:HB3	2.21	0.80
1:A:514:CYS:SG	1:A:559:CYS:CB	2.73	0.76
1:B:66:LEU:HD21	2:B:602:MYR:H132	1.68	0.76
2:A:606:MYR:H21	2:A:606:MYR:H92	1.66	0.76
1:B:45:GLU:OE1	1:B:73:LYS:NZ	2.23	0.71
1:B:376:GLU:HB3	3:B:608:EDO:H11	1.73	0.71
2:B:604:MYR:C1	2:B:604:MYR:H52	2.21	0.70
1:A:514:CYS:HG	1:A:559:CYS:CB	2.02	0.70
1:B:389:LYS:NZ	5:B:703:HOH:O	2.22	0.69
1:A:218:ARG:HH12	1:A:222:ARG:HH21	1.43	0.67
1:B:128:HIS:HB2	3:B:612:EDO:H22	1.77	0.66
1:B:460:LEU:HD13	2:B:605:MYR:H142	1.79	0.65
1:B:152:PRO:HG3	2:B:602:MYR:H51	1.80	0.64
1:B:450:GLU:HA	2:B:604:MYR:H31	1.78	0.64
1:A:514:CYS:HG	1:A:559:CYS:HG	0.64	0.63
1:A:27:PHE:HB3	1:A:39:HIS:CD2	2.33	0.62
2:B:604:MYR:H91	2:B:605:MYR:H21	1.80	0.62
1:A:95[A]:GLU:OE2	1:A:98:ARG:NE	2.27	0.62
1:A:325:VAL:HG22	2:A:605:MYR:H101	1.83	0.61
1:A:408:LEU:HD21	1:A:526:GLN:HB3	1.81	0.61
1:A:218:ARG:NH1	1:A:222:ARG:NH2	2.49	0.61
1:A:80:LEU:HD23	1:A:88:ALA:HA	1.83	0.59
1:B:504:ALA:O	1:B:508:THR:HG23	2.02	0.59
1:A:181:LYS:NZ	5:A:715:HOH:O	2.35	0.58
1:A:218:ARG:HH12	1:A:222:ARG:HE	1.50	0.58
1:B:429:ASN:ND2	5:B:715:HOH:O	2.36	0.58
1:B:426:VAL:HG21	2:B:605:MYR:H141	1.86	0.57
1:A:142:ILE:HG13	2:A:606:MYR:H112	1.86	0.57
1:A:218:ARG:NH1	1:A:222:ARG:HE	2.01	0.57
1:B:218[B]:ARG:NH1	1:B:222:ARG:HE	2.03	0.57
1:B:160:ARG:NH1	1:B:188:GLU:OE2	2.21	0.57
1:A:165:PHE:CE2	2:A:606:MYR:H62	2.40	0.56
1:A:77:VAL:HB	1:A:80:LEU:HD13	1.88	0.55
1:A:563:ASP:OD2	1:A:566:THR:HG22	2.05	0.55
1:A:411:TYR:HB3	2:A:602:MYR:H122	1.88	0.55
1:A:26:ALA:O	1:A:30:TYR:HD2	1.90	0.55
1:B:57:GLU:HG2	5:B:869:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:TYR:CG	2:A:606:MYR:H71	2.42	0.54
1:A:368:GLU:OE2	1:B:410:ARG:NH1	2.29	0.54
1:B:465:GLU:O	1:B:468:PRO:HD3	2.07	0.54
1:A:374:PHE:HB2	5:A:785:HOH:O	2.09	0.53
1:B:548:MET:HG2	2:B:601:MYR:H41	1.90	0.53
1:B:417:GLN:O	1:B:469:VAL:HG11	2.08	0.53
1:B:488:PHE:HB3	2:B:605:MYR:H71	1.91	0.53
1:A:10:ARG:HE	1:A:66:LEU:CD1	2.22	0.53
1:B:387:LEU:HD13	2:B:604:MYR:H92	1.90	0.53
1:A:225:LYS:NZ	5:A:720:HOH:O	2.41	0.52
1:A:5:SER:HB3	1:A:8:ALA:HB3	1.92	0.52
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.92	0.52
1:B:242:HIS:CE1	2:B:606:MYR:H141	2.44	0.52
1:A:218:ARG:HH12	1:A:222:ARG:NH2	2.07	0.51
1:B:417:GLN:NE2	1:B:494:ASP:OD1	2.33	0.51
1:A:72:ASP:O	1:A:76:THR:HG23	2.10	0.51
1:A:389:LYS:HD2	1:A:393:GLU:HG3	1.93	0.51
1:A:10:ARG:HE	1:A:66:LEU:HD13	1.75	0.51
1:A:414:LYS:NZ	1:A:491:LEU:O	2.28	0.51
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.92	0.51
1:B:241:VAL:HG22	1:B:256:ASP:HB3	1.92	0.51
1:B:542:GLU:N	1:B:542:GLU:OE1	2.44	0.51
1:B:533:VAL:HG22	1:B:544:LEU:HD21	1.92	0.50
1:A:222:ARG:HD3	1:A:295:ASN:OD1	2.12	0.50
2:B:604:MYR:O2	2:B:604:MYR:H52	2.12	0.50
1:A:227[B]:GLU:O	1:A:231:VAL:HG23	2.12	0.50
1:B:218[A]:ARG:NH2	2:B:606:MYR:H22	2.27	0.50
1:A:27:PHE:HB3	1:A:39:HIS:HD2	1.76	0.50
1:A:7:VAL:HG22	1:A:66:LEU:HD23	1.93	0.49
4:B:614:GOQ:O6	5:B:702:HOH:O	2.20	0.49
1:A:206:PHE:CZ	1:A:480:SER:HA	2.47	0.49
1:A:4:LYS:HD2	1:A:57:GLU:CB	2.42	0.49
1:B:376:GLU:CB	3:B:608:EDO:H11	2.43	0.48
1:B:41:LYS:HE2	1:B:45:GLU:OE2	2.13	0.48
1:A:22:LEU:HD13	2:A:603:MYR:H81	1.95	0.48
1:A:388:ILE:HG13	2:A:601:MYR:H72	1.95	0.48
2:B:605:MYR:H132	2:B:605:MYR:H102	1.51	0.48
1:A:555:VAL:O	1:A:559:CYS:SG	2.72	0.48
1:A:251:LEU:HD11	2:A:603:MYR:H141	1.96	0.48
1:B:222:ARG:HD3	1:B:295:ASN:OD1	2.13	0.48
1:B:457:LEU:HD12	3:B:607:EDO:H22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:NH2	1:A:222:ARG:HE	2.12	0.48
1:B:198:LEU:HD11	1:B:481:LEU:HD11	1.96	0.48
1:B:408:LEU:HD23	1:B:529:LEU:HD23	1.96	0.48
1:A:440:HIS:HB3	1:A:444:LYS:HB2	1.95	0.47
1:A:325:VAL:HG13	2:A:605:MYR:H121	1.96	0.47
1:B:417:GLN:HB3	1:B:469:VAL:HG12	1.96	0.47
2:A:603:MYR:H82	2:A:603:MYR:H51	1.42	0.47
1:B:300:ALA:O	1:B:301:ASP:CB	2.61	0.47
1:A:25:ILE:HD11	1:A:139:LEU:HD11	1.97	0.47
1:B:109:ASN:HB3	5:B:955:HOH:O	2.14	0.47
1:A:249:ASP:OD2	1:A:252:GLU:HG2	2.14	0.47
1:B:233:LYS:HE3	1:B:263:TYR:CZ	2.50	0.47
1:A:138:TYR:CZ	2:A:606:MYR:H31	2.50	0.47
2:B:604:MYR:H102	2:B:604:MYR:H71	1.69	0.47
1:B:347:LEU:HD22	2:B:603:MYR:H31	1.96	0.46
1:A:161:TYR:CZ	2:A:606:MYR:H91	2.50	0.46
1:B:26:ALA:O	1:B:30:TYR:HD2	1.99	0.46
1:B:436:LYS:HG2	1:B:452:TYR:CE2	2.51	0.46
1:B:460:LEU:HD12	1:B:460:LEU:O	2.15	0.46
1:B:567:CYS:O	1:B:571:GLU:HB2	2.16	0.46
1:A:237:ASP:O	1:A:241:VAL:HG23	2.15	0.46
1:A:541:LYS:HA	1:A:541:LYS:HD2	1.54	0.46
1:B:460:LEU:HD13	2:B:605:MYR:C14	2.43	0.46
1:B:433:VAL:HG22	1:B:452:TYR:HB3	1.97	0.45
1:A:227[A]:GLU:O	1:A:231:VAL:HG23	2.16	0.45
1:A:218:ARG:HH12	1:A:222:ARG:NE	2.14	0.45
1:A:123:MET:HB3	1:A:165:PHE:HE1	1.81	0.45
1:B:426:VAL:CG2	2:B:605:MYR:H141	2.47	0.45
1:A:7:VAL:HG21	1:A:69:LEU:HD13	1.98	0.45
1:A:389:LYS:HA	1:A:389:LYS:HD3	1.69	0.45
1:A:583:LEU:HA	1:A:583:LEU:HD13	1.72	0.45
1:A:138:TYR:CE1	2:A:606:MYR:H51	2.51	0.45
1:A:251:LEU:HD21	2:A:603:MYR:H132	1.98	0.45
1:A:218:ARG:HH22	1:A:222:ARG:HE	1.64	0.44
1:B:385:GLN:O	1:B:389:LYS:HG2	2.18	0.44
1:B:420:THR:HG21	1:B:527:THR:HG23	1.99	0.44
1:B:257:ARG:HG2	2:B:606:MYR:H122	1.98	0.44
1:A:254:ALA:HB1	2:A:603:MYR:H31	1.99	0.44
1:B:151:ALA:HB3	1:B:152:PRO:HD3	2.00	0.44
1:A:192:SER:O	1:A:196:GLN:HG2	2.18	0.44
1:A:488:PHE:HB3	2:A:602:MYR:H81	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:SER:OG	1:A:62:CYS:O	2.32	0.44
1:B:214:TRP:HH2	2:B:606:MYR:O1	2.01	0.44
1:A:426:VAL:HG21	1:A:460:LEU:HD13	1.99	0.43
1:A:221:GLN:HG3	1:A:335:ALA:HB1	1.99	0.43
1:A:281:LYS:NZ	5:A:738:HOH:O	2.51	0.43
2:A:602:MYR:H31	2:A:602:MYR:H61	1.65	0.43
1:B:155:LEU:HG	1:B:159:LYS:HE3	2.00	0.43
1:B:186:ARG:CZ	1:B:190:LYS:HE2	2.49	0.43
1:B:39:HIS:O	1:B:43:VAL:HG23	2.17	0.43
1:B:441:PRO:O	1:B:445:ARG:HG3	2.18	0.43
1:A:218:ARG:NH2	1:A:295:ASN:OD1	2.51	0.43
1:A:218:ARG:CZ	1:A:222:ARG:HE	2.30	0.43
1:B:411:TYR:HB3	2:B:605:MYR:H101	1.99	0.43
1:A:161:TYR:CE1	2:A:606:MYR:H91	2.54	0.43
1:B:398:LEU:HB3	1:B:402:LYS:CB	2.49	0.43
1:B:367:HIS:HA	1:B:370:TYR:CE1	2.54	0.43
1:B:538:LYS:HB3	1:B:538:LYS:HE3	1.95	0.43
1:A:541:LYS:HE3	1:B:365:ASP:HB2	2.00	0.42
1:B:582:ALA:O	1:B:583:LEU:HD23	2.19	0.42
1:B:80:LEU:HD12	1:B:80:LEU:HA	1.90	0.42
1:B:579:SER:HB2	2:B:601:MYR:H132	2.02	0.42
1:A:186:ARG:HA	1:A:186:ARG:HE	1.84	0.42
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.54	0.42
1:B:108:ASP:CG	1:B:197:ARG:HH12	2.22	0.42
1:B:539:ALA:HB3	1:B:544:LEU:HD11	2.02	0.42
1:A:251:LEU:HA	1:A:251:LEU:HD23	1.88	0.42
1:A:312:SER:O	5:A:702:HOH:O	2.22	0.42
1:A:411:TYR:CD1	2:A:602:MYR:H101	2.55	0.42
1:B:453:LEU:CD1	2:B:604:MYR:H81	2.50	0.42
1:A:151:ALA:HB3	1:A:152:PRO:HD3	2.02	0.42
1:B:192:SER:O	1:B:196:GLN:HG2	2.20	0.41
1:A:231:VAL:O	1:A:235:VAL:HG23	2.20	0.41
1:A:367:HIS:HD2	5:A:702:HOH:O	2.03	0.41
1:B:426:VAL:CB	2:B:605:MYR:H141	2.50	0.41
1:B:415:VAL:O	1:B:415:VAL:HG23	2.20	0.41
2:B:606:MYR:H32	2:B:606:MYR:H62	1.55	0.41
1:A:204:GLN:HA	1:A:204:GLN:OE1	2.20	0.41
1:A:27:PHE:HE1	1:A:74:LEU:HD12	1.84	0.41
1:B:251:LEU:HD21	2:B:602:MYR:H102	2.02	0.41
1:A:291:ALA:HA	2:A:607:MYR:H52	2.03	0.41
1:B:239:THR:HG22	3:B:609:EDO:O1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLU:HB3	1:A:73:LYS:NZ	2.36	0.41
1:A:70:PHE:CZ	1:A:74:LEU:HD11	2.56	0.41
2:B:604:MYR:H51	2:B:604:MYR:H82	1.39	0.41
1:B:146:HIS:ND1	5:B:710:HOH:O	2.27	0.41
1:B:35:PRO:HD2	1:B:38:ASP:OD2	2.21	0.41
1:A:45:GLU:OE1	1:A:73:LYS:HE2	2.21	0.40
1:B:219:LEU:HD12	1:B:235:VAL:CG2	2.51	0.40
1:B:217:ALA:HB3	1:B:343:VAL:HG13	2.03	0.40
1:B:66:LEU:CD2	2:B:602:MYR:H132	2.45	0.40
1:A:371:ALA:O	5:A:701:HOH:O	2.21	0.40
1:A:108:ASP:HB2	1:A:148:TYR:HE2	1.86	0.40
1:A:188:GLU:OE2	5:A:703:HOH:O	2.22	0.40
1:A:509:PHE:O	1:A:568:PHE:HB3	2.20	0.40
1:B:347:LEU:HD23	1:B:347:LEU:HA	1.86	0.40
1:B:525:LYS:HB3	2:B:601:MYR:H31	2.03	0.40
1:B:66:LEU:HD12	1:B:66:LEU:HA	1.89	0.40
1:A:152:PRO:HG3	2:A:603:MYR:H62	2.04	0.40
1:A:161:TYR:CD1	2:A:606:MYR:H82	2.56	0.40
1:A:6:GLU:HB3	1:A:66:LEU:CD1	2.52	0.40
1:B:513:ILE:HA	1:B:516:LEU:HD12	2.03	0.40
1:B:67:HIS:CD2	5:B:910:HOH:O	2.74	0.40
1:A:378:LYS:HA	1:A:378:LYS:HE2	2.04	0.40
1:A:485:ARG:NE	2:A:601:MYR:H51	2.37	0.40
1:A:161:TYR:CE2	2:A:606:MYR:H111	2.56	0.40
2:B:606:MYR:H62	2:B:606:MYR:H91	1.66	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	583/609 (96%)	569 (98%)	12 (2%)	2 (0%)	41 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	582/609 (96%)	571 (98%)	11 (2%)	0	100 100
All	All	1165/1218 (96%)	1140 (98%)	23 (2%)	2 (0%)	51 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95[A]	GLU
1	A	95[B]	GLU

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	492/533 (92%)	485 (99%)	7 (1%)	67 65
1	B	498/533 (93%)	491 (99%)	7 (1%)	67 65
All	All	990/1066 (93%)	976 (99%)	14 (1%)	67 65

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ARG
1	A	186	ARG
1	A	218	ARG
1	A	334	TYR
1	A	484	ARG
1	A	557	LYS
1	A	559	CYS
1	B	140	TYR
1	B	162	LYS
1	B	302	LEU
1	B	334	TYR
1	B	351	LYS
1	B	505	GLU
1	B	541	LYS

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

23 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	EDO	B	609	-	3,3,3	0.37	0	2,2,2	0.55	0
3	EDO	B	612	-	3,3,3	0.55	0	2,2,2	0.12	0
3	EDO	B	613	-	3,3,3	0.43	0	2,2,2	0.47	0
2	MYR	A	601	-	12,15,15	0.26	0	11,15,15	1.03	0
2	MYR	A	606	-	12,15,15	0.23	0	11,15,15	0.90	0
2	MYR	B	601	-	12,15,15	0.30	0	11,15,15	0.84	0
2	MYR	A	604	-	12,15,15	0.31	0	11,15,15	0.93	0
3	EDO	B	611	-	3,3,3	0.49	0	2,2,2	0.39	0
2	MYR	A	602	-	12,15,15	0.35	0	11,15,15	0.76	0
2	MYR	B	602	-	12,15,15	0.30	0	11,15,15	1.12	0
3	EDO	A	609	-	3,3,3	0.46	0	2,2,2	0.45	0
2	MYR	B	604	-	12,15,15	0.19	0	11,15,15	1.45	2 (18%)
3	EDO	B	610	-	3,3,3	0.38	0	2,2,2	0.58	0
2	MYR	B	605	-	12,15,15	0.19	0	11,15,15	1.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	B	607	-	3,3,3	0.59	0	2,2,2	0.12	0
3	EDO	B	608	-	3,3,3	0.30	0	2,2,2	0.76	0
4	GOQ	B	614	-	25,28,28	2.87	9 (36%)	30,42,42	2.20	9 (30%)
2	MYR	A	605	-	12,15,15	0.39	0	11,15,15	0.73	0
2	MYR	B	603	-	12,15,15	0.31	0	11,15,15	1.22	0
2	MYR	B	606	-	12,15,15	0.29	0	11,15,15	0.98	0
2	MYR	A	603	-	12,15,15	0.27	0	11,15,15	1.00	0
3	EDO	A	608	-	3,3,3	0.50	0	2,2,2	0.18	0
2	MYR	A	607	-	12,15,15	0.27	0	11,15,15	0.99	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	EDO	B	609	-	-	1/1/1/1	-
3	EDO	B	612	-	-	1/1/1/1	-
3	EDO	B	613	-	-	1/1/1/1	-
2	MYR	A	601	-	-	6/11/13/13	-
2	MYR	A	606	-	-	9/11/13/13	-
2	MYR	B	601	-	-	7/11/13/13	-
2	MYR	A	604	-	-	7/11/13/13	-
3	EDO	B	611	-	-	0/1/1/1	-
2	MYR	A	602	-	-	4/11/13/13	-
2	MYR	B	602	-	-	4/11/13/13	-
3	EDO	A	609	-	-	0/1/1/1	-
2	MYR	B	604	-	-	9/11/13/13	-
3	EDO	B	610	-	-	1/1/1/1	-
2	MYR	B	605	-	-	5/11/13/13	-
3	EDO	B	607	-	-	1/1/1/1	-
3	EDO	B	608	-	-	0/1/1/1	-
4	GOQ	B	614	-	-	3/4/16/16	0/4/4/4
2	MYR	A	605	-	-	5/11/13/13	-
2	MYR	B	603	-	-	8/11/13/13	-
2	MYR	B	606	-	-	6/11/13/13	-
2	MYR	A	603	-	-	6/11/13/13	-
3	EDO	A	608	-	-	0/1/1/1	-
2	MYR	A	607	-	-	8/11/13/13	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	614	GOQ	O1-N	9.80	1.39	1.22
4	B	614	GOQ	C11-C7	5.29	1.52	1.43
4	B	614	GOQ	C8-C7	4.88	1.50	1.43
4	B	614	GOQ	C6-C7	3.66	1.49	1.42
4	B	614	GOQ	C8-N	-2.91	1.40	1.45
4	B	614	GOQ	C10-C5	2.53	1.46	1.42
4	B	614	GOQ	O4-C13	-2.43	1.34	1.38
4	B	614	GOQ	C1-C10	2.20	1.48	1.42
4	B	614	GOQ	O3-C14	-2.05	1.35	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	614	GOQ	C-O-C1	6.11	126.29	117.75
4	B	614	GOQ	O-C1-C10	3.91	118.28	114.46
4	B	614	GOQ	C10-C5-C6	-3.79	115.45	119.48
4	B	614	GOQ	C8-C7-C6	-3.68	116.18	118.69
4	B	614	GOQ	O1-N-C8	-3.51	113.03	119.03
4	B	614	GOQ	C12-C11-C7	3.13	121.67	117.53
4	B	614	GOQ	C14-C6-C5	-3.12	120.26	124.06
4	B	614	GOQ	O4-C13-C14	-2.76	107.10	109.64
2	B	604	MYR	C5-C4-C3	-2.67	100.88	114.42
2	B	604	MYR	C7-C6-C5	-2.36	102.42	114.42
4	B	614	GOQ	C5-C6-C7	2.33	122.87	117.39

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	606	MYR	C1-C2-C3-C4
2	A	605	MYR	C1-C2-C3-C4
2	B	603	MYR	C1-C2-C3-C4
2	A	607	MYR	C1-C2-C3-C4
4	B	614	GOQ	C2-C1-O-C
4	B	614	GOQ	C10-C1-O-C
2	B	606	MYR	C3-C4-C5-C6
2	B	604	MYR	C5-C6-C7-C8
4	B	614	GOQ	C9-C8-N-O1
2	A	603	MYR	C5-C6-C7-C8
2	B	604	MYR	C7-C8-C9-C10
2	A	606	MYR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	B	602	MYR	C6-C7-C8-C9
2	B	603	MYR	C4-C5-C6-C7
2	A	604	MYR	C4-C5-C6-C7
2	A	607	MYR	C5-C6-C7-C8
2	A	601	MYR	C4-C5-C6-C7
2	A	606	MYR	C2-C3-C4-C5
2	A	604	MYR	C3-C4-C5-C6
2	A	604	MYR	C10-C11-C12-C13
2	A	602	MYR	C2-C3-C4-C5
2	A	603	MYR	C11-C10-C9-C8
2	A	606	MYR	C11-C10-C9-C8
2	A	606	MYR	C9-C10-C11-C12
2	B	601	MYR	C7-C8-C9-C10
2	B	603	MYR	C7-C8-C9-C10
2	A	602	MYR	C9-C10-C11-C12
2	A	601	MYR	C2-C3-C4-C5
2	B	602	MYR	C3-C4-C5-C6
2	A	602	MYR	C7-C8-C9-C10
2	A	603	MYR	C9-C10-C11-C12
2	B	604	MYR	C4-C5-C6-C7
2	B	605	MYR	C7-C8-C9-C10
2	B	606	MYR	C10-C11-C12-C13
2	A	606	MYR	C5-C6-C7-C8
2	B	601	MYR	C11-C10-C9-C8
2	B	603	MYR	C5-C6-C7-C8
3	B	609	EDO	O1-C1-C2-O2
2	A	601	MYR	C9-C10-C11-C12
2	B	601	MYR	C5-C6-C7-C8
2	B	603	MYR	C2-C3-C4-C5
2	B	605	MYR	C2-C3-C4-C5
2	A	605	MYR	C6-C7-C8-C9
2	B	605	MYR	C11-C10-C9-C8
2	A	604	MYR	C6-C7-C8-C9
2	A	605	MYR	C5-C6-C7-C8
2	A	607	MYR	C11-C10-C9-C8
2	A	604	MYR	C9-C10-C11-C12
2	B	605	MYR	C11-C12-C13-C14
2	A	603	MYR	C11-C12-C13-C14
2	B	601	MYR	C4-C5-C6-C7
2	B	604	MYR	C9-C10-C11-C12
2	A	607	MYR	C10-C11-C12-C13
2	A	607	MYR	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	A	607	MYR	C9-C10-C11-C12
2	B	604	MYR	C6-C7-C8-C9
2	B	604	MYR	C3-C4-C5-C6
2	B	606	MYR	C9-C10-C11-C12
2	A	607	MYR	C11-C12-C13-C14
2	B	602	MYR	C9-C10-C11-C12
3	B	612	EDO	O1-C1-C2-O2
3	B	610	EDO	O1-C1-C2-O2
2	B	606	MYR	C5-C6-C7-C8
2	B	601	MYR	C6-C7-C8-C9
2	A	605	MYR	C11-C12-C13-C14
2	A	605	MYR	C4-C5-C6-C7
2	B	601	MYR	C1-C2-C3-C4
2	B	604	MYR	C1-C2-C3-C4
2	A	604	MYR	C11-C12-C13-C14
2	B	606	MYR	C11-C10-C9-C8
2	A	603	MYR	C6-C7-C8-C9
3	B	613	EDO	O1-C1-C2-O2
2	A	602	MYR	C3-C4-C5-C6
2	A	606	MYR	C4-C5-C6-C7
2	A	603	MYR	C7-C8-C9-C10
2	A	606	MYR	C11-C12-C13-C14
2	A	601	MYR	C7-C8-C9-C10
2	A	606	MYR	C3-C4-C5-C6
2	B	603	MYR	C3-C4-C5-C6
2	B	602	MYR	C11-C12-C13-C14
2	B	605	MYR	C10-C11-C12-C13
2	B	606	MYR	C2-C3-C4-C5
2	A	601	MYR	C10-C11-C12-C13
2	B	604	MYR	C11-C12-C13-C14
2	B	604	MYR	C2-C3-C4-C5
2	B	601	MYR	C10-C11-C12-C13
2	A	601	MYR	C11-C10-C9-C8
2	B	603	MYR	C6-C7-C8-C9
2	B	603	MYR	C11-C12-C13-C14
2	A	604	MYR	C1-C2-C3-C4
2	A	607	MYR	C4-C5-C6-C7
3	B	607	EDO	O1-C1-C2-O2

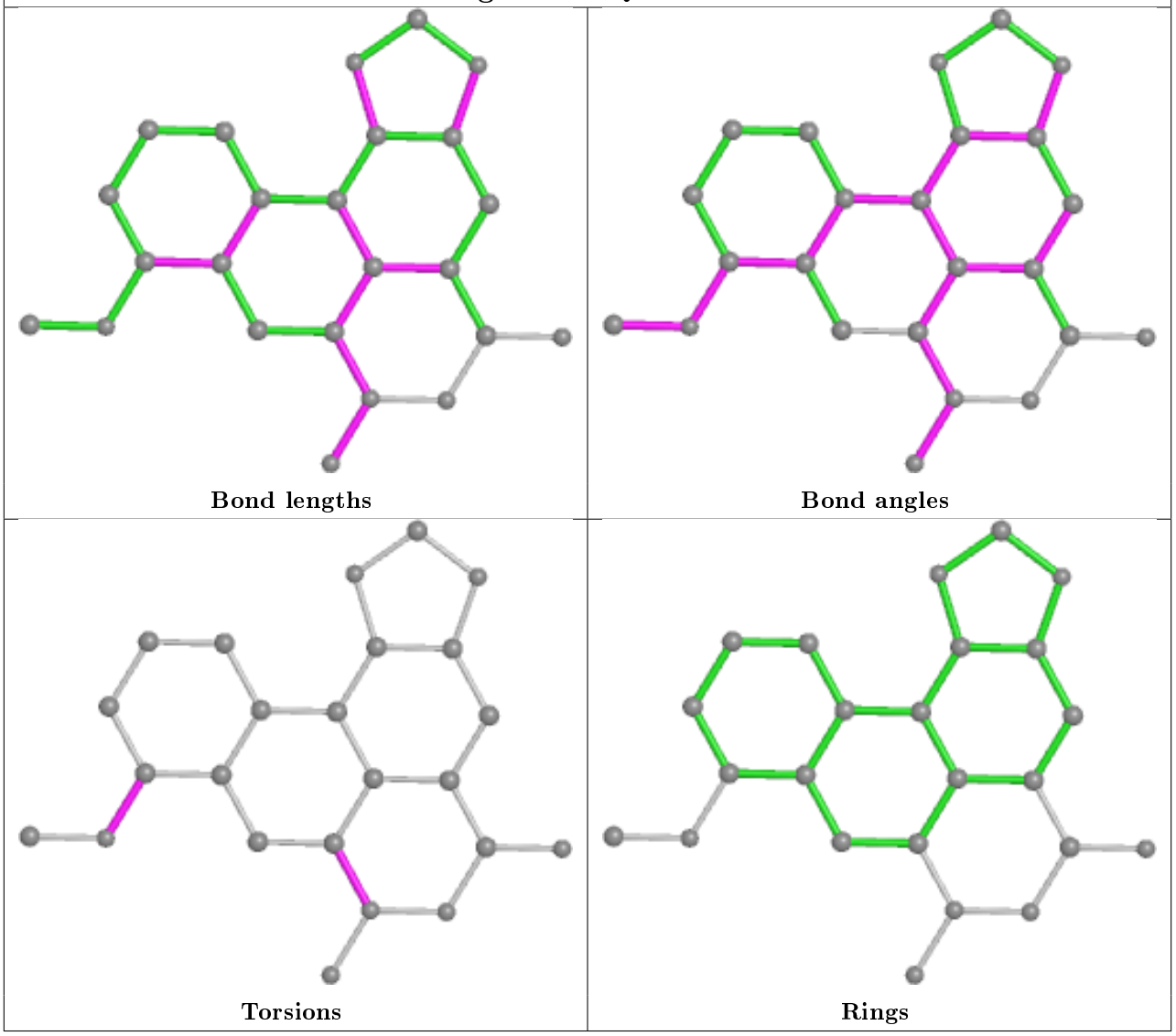
There are no ring outliers.

17 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	609	EDO	1	0
3	B	612	EDO	1	0
2	A	601	MYR	2	0
2	A	606	MYR	10	0
2	B	601	MYR	3	0
2	A	602	MYR	4	0
2	B	602	MYR	4	0
2	B	604	MYR	8	0
2	B	605	MYR	9	0
3	B	607	EDO	1	0
3	B	608	EDO	2	0
4	B	614	GOQ	1	0
2	A	605	MYR	2	0
2	B	603	MYR	1	0
2	B	606	MYR	6	0
2	A	603	MYR	6	0
2	A	607	MYR	1	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 GOQ B 614



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	582/609 (95%)	0.70	42 (7%)	15	17	32, 47, 63, 86	0
1	B	582/609 (95%)	0.43	24 (4%)	37	40	8, 26, 54, 76	0
All	All	1164/1218 (95%)	0.56	66 (5%)	23	26	8, 40, 60, 86	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	546	ALA	4.1
1	A	502	PHE	4.1
1	B	555	VAL	4.0
1	B	509	PHE	4.0
1	A	566	THR	3.9
1	B	511	ALA	3.8
1	A	513	ILE	3.5
1	B	554	PHE	3.5
1	B	561	ALA	3.4
1	A	568	PHE	3.4
1	A	509	PHE	3.3
1	A	555	VAL	3.3
1	B	568	PHE	3.2
1	B	559	CYS	3.2
1	A	559	CYS	3.2
1	A	583	LEU	3.1
1	B	562	ASP	3.1
1	B	516	LEU	3.1
1	A	499	PRO	3.0
1	B	582	ALA	3.0
1	A	79	THR	3.0
1	B	553	ALA	2.9
1	A	198	LEU	2.9
1	A	515	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	313	LYS	2.9
1	A	92	ALA	2.8
1	B	514	CYS	2.7
1	A	569	ALA	2.7
1	B	507	PHE	2.7
1	B	546	ALA	2.7
1	A	575	LEU	2.7
1	A	138	TYR	2.7
1	A	551	PHE	2.6
1	B	515	THR	2.6
1	A	561	ALA	2.5
1	A	275	LEU	2.5
1	A	171	ALA	2.5
1	A	496	THR	2.5
1	B	301	ASP	2.4
1	A	504	ALA	2.4
1	A	30	TYR	2.4
1	A	108	ASP	2.4
1	A	130	ASN	2.4
1	A	507	PHE	2.4
1	A	498	VAL	2.4
1	B	583	LEU	2.4
1	A	461	CYS	2.3
1	A	481	LEU	2.3
1	A	540	THR	2.3
1	B	566	THR	2.3
1	A	154	LEU	2.3
1	A	370	TYR	2.3
1	B	567	CYS	2.2
1	A	283	LEU	2.2
1	B	512	ASP	2.2
1	A	581	ALA	2.2
1	B	505	GLU	2.2
1	B	517	SER	2.2
1	A	554	PHE	2.2
1	B	544	LEU	2.1
1	A	433	VAL	2.1
1	B	575	LEU	2.1
1	A	582	ALA	2.1
1	A	82	GLU	2.0
1	A	362	ALA	2.0
1	A	584	GLY	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)

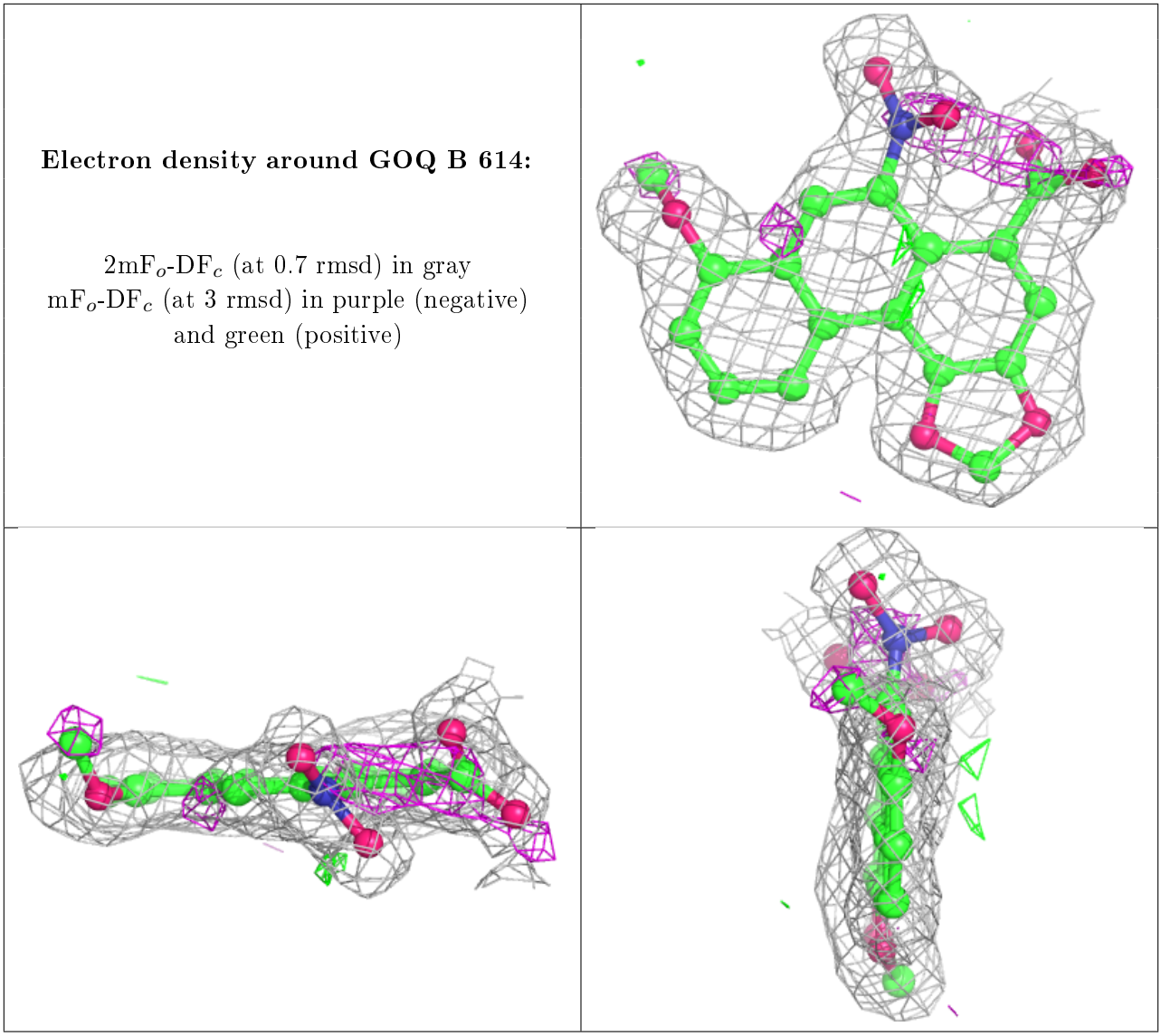
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	MYR	A	607	16/16	0.69	0.23	45,52,60,61	0
2	MYR	A	604	16/16	0.72	0.24	45,54,57,58	0
2	MYR	A	605	16/16	0.74	0.32	44,46,52,53	0
2	MYR	B	601	16/16	0.75	0.15	38,43,48,48	0
2	MYR	B	605	16/16	0.76	0.20	25,35,47,50	0
2	MYR	B	606	16/16	0.78	0.22	23,28,41,46	0
2	MYR	A	606	16/16	0.79	0.22	45,49,52,52	0
3	EDO	A	608	4/4	0.81	0.31	43,44,45,48	0
3	EDO	A	609	4/4	0.83	0.15	50,52,53,55	0
2	MYR	A	602	16/16	0.83	0.18	33,45,49,50	0
3	EDO	B	613	4/4	0.85	0.17	34,40,44,44	0
2	MYR	B	603	16/16	0.86	0.14	21,29,35,36	0
2	MYR	B	602	16/16	0.87	0.15	18,22,30,36	0
4	GOQ	B	614	25/25	0.88	0.14	20,25,31,35	0
3	EDO	B	610	4/4	0.89	0.15	18,24,25,33	0
3	EDO	B	608	4/4	0.89	0.20	31,40,41,44	0
2	MYR	A	603	16/16	0.91	0.13	37,44,49,49	0
3	EDO	B	611	4/4	0.91	0.12	33,35,40,44	0
2	MYR	A	601	16/16	0.91	0.15	37,41,44,45	0
2	MYR	B	604	16/16	0.92	0.20	14,25,34,36	0
3	EDO	B	609	4/4	0.93	0.15	27,30,30,32	0
3	EDO	B	612	4/4	0.93	0.20	22,28,30,37	0
3	EDO	B	607	4/4	0.94	0.13	19,23,25,27	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 GOQ B 614:

$2mF_o$-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.