Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 10:12 PM BST

PDB ID	:	6HIL
Title	:	X-ray structure of TEAD1(Y421H mutant) complexed with YAP(wildtype): Molecular and structural characterization of a TEAD mutation at the origin of Sveinsson's chorioretinal atrophy
Authors	:	Kallen, J.
Deposited on	:	2018-08-30
Resolution	:	2.30 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:

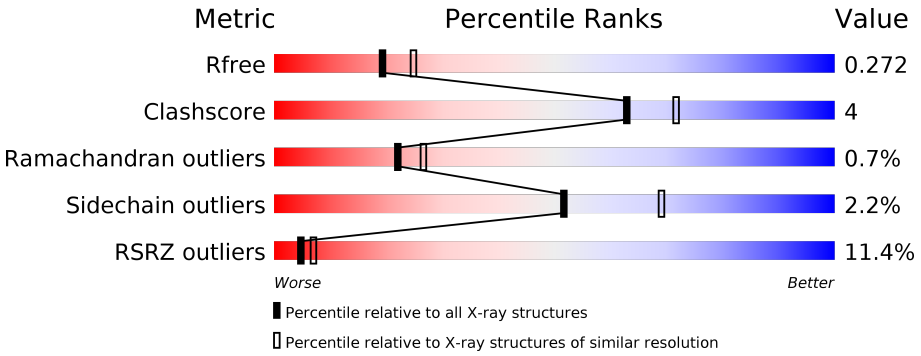
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.30 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.



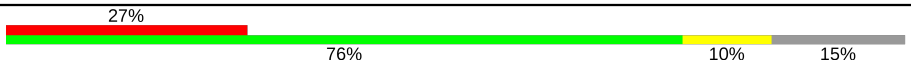
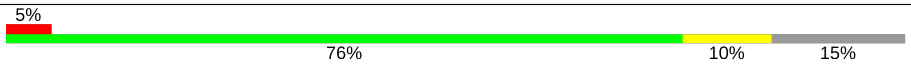
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	218	11% 77% 16% 7%
1	B	218	7% 83% 11% 7%
1	C	218	8% 79% 14% 7%
1	D	218	6% 80% 12% 7%
2	L	41	22% 83% . 15%
2	M	41	32% 73% 12% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	N	41	
2	O	41	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8002 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 Transcriptional enhancer factor TEF-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	3	0
			1657	1061	282	301	13			
1	D	203	Total	C	N	O	S	0	4	0
			1670	1072	283	302	13			
1	B	203	Total	C	N	O	S	0	3	0
			1665	1067	283	302	13			
1	C	203	Total	C	N	O	S	0	4	0
			1670	1072	283	302	13			

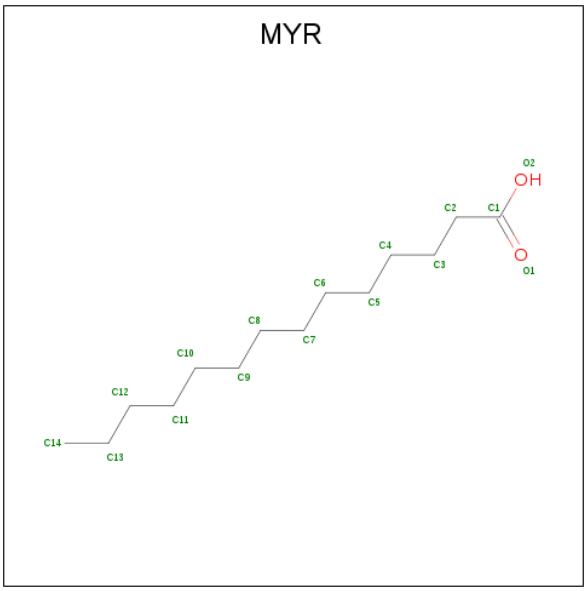
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	HIS	TYR	engineered mutation	UNP P28347
D	406	HIS	TYR	engineered mutation	UNP P28347
B	406	HIS	TYR	engineered mutation	UNP P28347
C	406	HIS	TYR	engineered mutation	UNP P28347

- Molecule 2 is a protein called Transcriptional coactivator YAP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	35	Total	C	N	O	S	0	1	0
			284	185	48	48	3			
2	O	35	Total	C	N	O	S	0	1	0
			284	185	48	48	3			
2	M	35	Total	C	N	O	S	0	1	0
			284	185	48	48	3			
2	N	35	Total	C	N	O	S	0	1	0
			284	185	48	48	3			

- Molecule 3 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



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

- Molecule 4 is water.

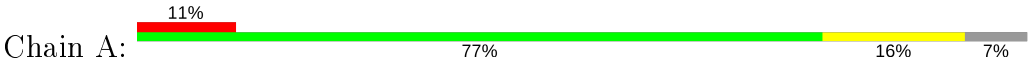
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	30	Total O 30 30	0	0
4	L	4	Total O 4 4	0	0
4	D	43	Total O 43 43	0	0
4	O	4	Total O 4 4	0	0
4	B	30	Total O 30 30	0	0
4	M	4	Total O 4 4	0	0
4	C	22	Total O 22 22	0	0
4	N	3	Total O 3 3	0	0

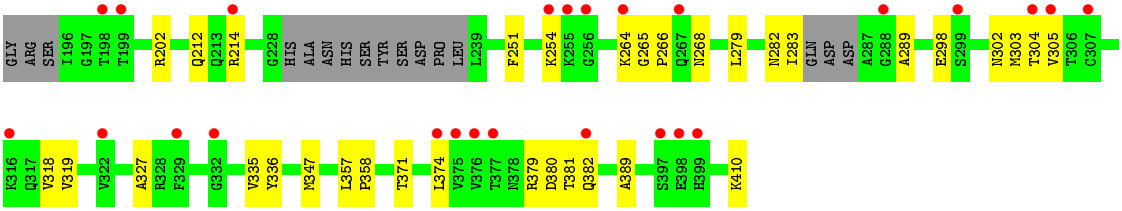
3 Residue-property plots (i)

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

- Molecule 1: Transcriptional enhancer factor TEF-1

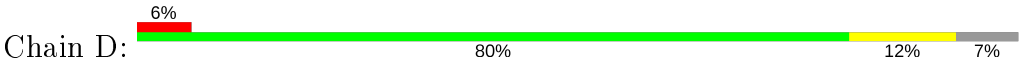
Chain A:

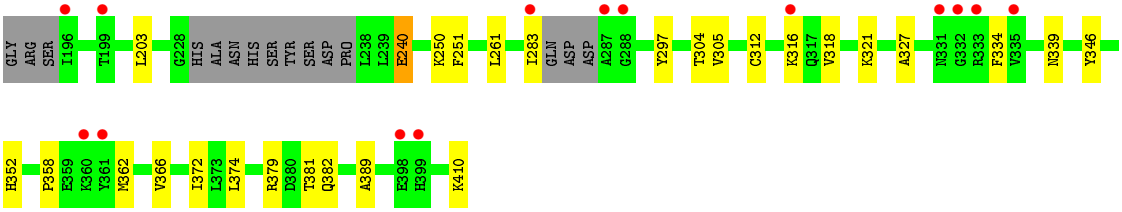




- Molecule 1: Transcriptional enhancer factor TEF-1

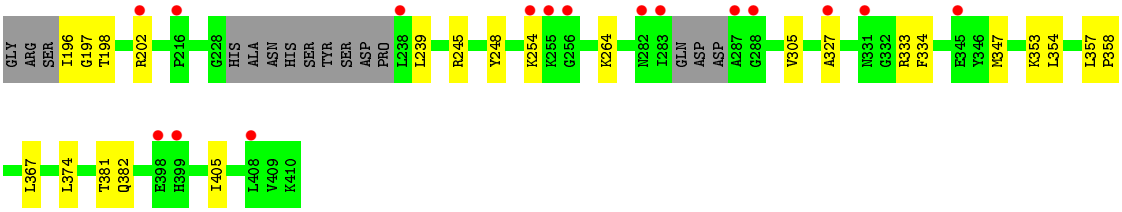
Chain D:





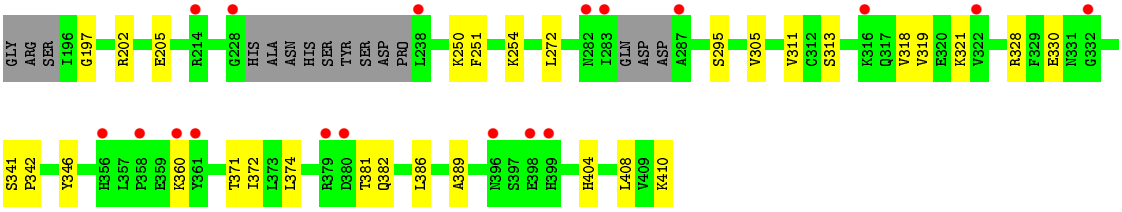
- Molecule 1: Transcriptional enhancer factor TEF-1

Chain B:

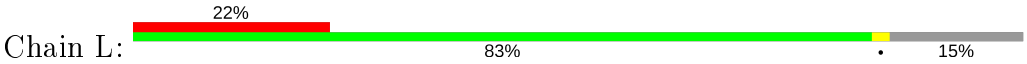


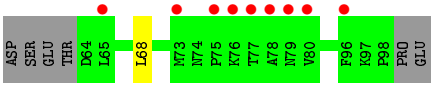
- Molecule 1: Transcriptional enhancer factor TEF-1

Chain C:

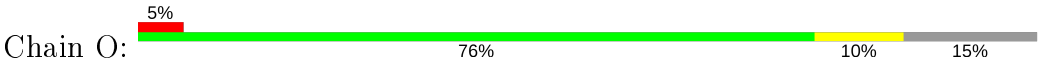


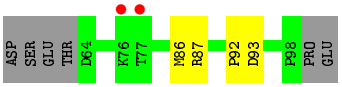
• Molecule 2: Transcriptional coactivator YAP1



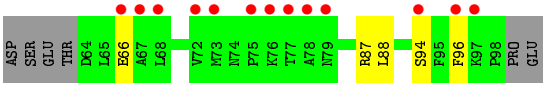


• Molecule 2: Transcriptional coactivator YAP1

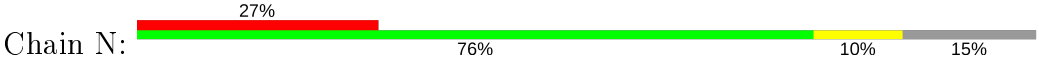


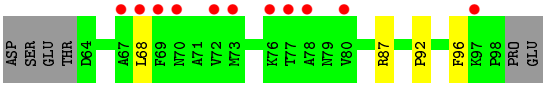


• Molecule 2: Transcriptional coactivator YAP1



• Molecule 2: Transcriptional coactivator YAP1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	40.12Å 46.54Å 144.34Å 98.61° 90.85° 108.14°	Depositor
Resolution (Å)	19.90 – 2.30 19.90 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.5 (19.90-2.30) 95.7 (19.90-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.242 , 0.267 0.245 , 0.272	Depositor DCC
R_{free} test set	2081 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8002	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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: MYR

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	0.39	0/1701	0.52	0/2287
1	B	0.38	0/1709	0.53	0/2298
1	C	0.39	0/1717	0.53	0/2309
1	D	0.42	0/1717	0.54	0/2309
2	L	0.36	0/294	0.47	0/398
2	M	0.38	0/294	0.51	0/398
2	N	0.38	0/294	0.50	0/398
2	O	0.36	0/294	0.54	0/398
All	All	0.39	0/8020	0.53	0/10795

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	1657	0	1641	19	0
1	B	1665	0	1652	12	0
1	C	1670	0	1663	15	0
1	D	1670	0	1663	17	0
2	L	284	0	298	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	284	0	298	4	0
2	N	284	0	298	2	0
2	O	284	0	298	3	0
3	A	16	0	27	1	0
3	B	16	0	27	1	0
3	C	16	0	27	3	0
3	D	16	0	27	3	0
4	A	30	0	0	3	0
4	B	30	0	0	0	0
4	C	22	0	0	2	0
4	D	43	0	0	2	0
4	L	4	0	0	0	0
4	M	4	0	0	0	0
4	N	3	0	0	0	0
4	O	4	0	0	0	0
All	All	8002	0	7919	67	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 4.

All (67) 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:D:372[A]:ILE:HD13	3:D:501:MYR:H62	1.58	0.86
1:C:386:LEU:HG	4:C:622:HOH:O	1.76	0.84
1:B:353:LYS:HE3	2:M:66:GLU:HG2	1.62	0.79
1:A:265:GLY:HA2	4:A:603:HOH:O	1.88	0.73
1:A:282:ASN:O	1:A:283:ILE:HB	1.91	0.69
1:A:264:LYS:HA	1:B:264:LYS:HA	1.77	0.67
4:D:603:HOH:O	2:O:87:ARG:HG2	1.94	0.66
1:D:250:LYS:HD2	2:O:86:MET:SD	2.38	0.64
1:C:372[A]:ILE:HD13	3:C:501:MYR:H62	1.82	0.61
1:D:240:GLU:HG3	2:O:92:PRO:HB3	1.84	0.59
1:B:347:MET:HG3	3:B:501:MYR:H42	1.87	0.57
1:D:304:THR:HG21	1:D:379:ARG:HH21	1.72	0.55
1:A:381:THR:O	1:A:382:GLN:HB2	2.07	0.55
1:D:372[A]:ILE:CD1	3:D:501:MYR:H62	2.35	0.54
1:C:251:PHE:CZ	1:C:389:ALA:HB1	2.42	0.54
1:B:381:THR:O	1:B:382:GLN:HB2	2.08	0.54
1:D:410:LYS:HA	4:D:642:HOH:O	2.09	0.53
1:C:318:VAL:HG12	1:C:319:VAL:HG23	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:VAL:HG12	1:A:319:VAL:HG23	1.91	0.52
1:D:321:LYS:HD3	3:D:501:MYR:O2	2.10	0.51
1:A:266:PRO:HB2	1:A:268:ASN:OD1	2.11	0.51
1:A:347:MET:HG3	3:A:501:MYR:H42	1.92	0.51
1:A:202:ARG:HB3	4:A:602:HOH:O	2.11	0.51
1:A:298:GLU:HG2	1:A:335:VAL:HG22	1.92	0.50
1:D:358:PRO:HD2	1:D:362:MET:SD	2.50	0.50
1:C:318:VAL:HG11	1:C:346:TYR:CE1	2.47	0.49
1:D:251:PHE:CZ	1:D:389:ALA:HB1	2.48	0.48
1:B:245:ARG:HA	1:B:248:TYR:CD2	2.50	0.47
1:C:372[A]:ILE:CD1	3:C:501:MYR:H62	2.44	0.47
1:C:197:GLY:HA3	1:C:202:ARG:HG2	1.97	0.47
1:C:381:THR:O	1:C:382:GLN:HB2	2.16	0.46
1:A:282:ASN:O	1:A:283:ILE:CB	2.61	0.46
1:B:197:GLY:HA3	1:B:202:ARG:HA	1.97	0.46
1:D:283:ILE:HG21	1:D:352:HIS:NE2	2.31	0.46
2:M:87:ARG:HA	2:M:96:PHE:CE1	2.50	0.45
1:C:328:ARG:HD2	1:C:330:GLU:OE2	2.17	0.45
1:D:312:CYS:HA	1:D:316:LYS:O	2.17	0.45
1:B:333:ARG:HE	1:B:333:ARG:HB2	1.65	0.44
1:D:203:LEU:HD13	1:D:297:TYR:CE2	2.53	0.44
1:D:304:THR:HG21	1:D:379:ARG:NH2	2.33	0.44
1:B:327:ALA:HB1	1:B:334:PHE:HB3	1.98	0.43
1:A:410:LYS:HB2	1:A:410:LYS:HE3	1.80	0.43
1:A:251:PHE:CZ	1:A:389:ALA:HB1	2.54	0.43
1:C:250:LYS:HB3	1:C:371:THR:HG21	2.01	0.43
1:C:205:GLU:O	1:C:295:SER:HA	2.19	0.43
1:B:239:LEU:HD23	2:M:94:SER:HB2	2.01	0.43
2:M:87:ARG:HG3	2:M:88:LEU:HG	2.00	0.42
1:A:212[B]:GLN:HE22	1:A:289:ALA:HB2	1.84	0.42
1:B:357:LEU:HA	1:B:358:PRO:HD3	1.83	0.42
1:C:311:VAL:HA	1:C:372[B]:ILE:HD13	2.00	0.42
1:C:321:LYS:HD3	3:C:501:MYR:O1	2.19	0.42
1:D:318:VAL:HG11	1:D:346:TYR:CE1	2.55	0.42
1:B:196:ILE:HD11	1:B:405:ILE:HG12	2.01	0.42
1:A:327:ALA:HB2	1:A:336:TYR:CE2	2.55	0.42
2:N:87:ARG:HA	2:N:96:PHE:CE1	2.55	0.42
1:C:272:LEU:HB2	1:C:408:LEU:HD21	2.01	0.42
4:C:604:HOH:O	2:N:87:ARG:HG2	2.19	0.41
1:A:380:ASP:HB2	4:A:611:HOH:O	2.20	0.41
1:A:357:LEU:HA	1:A:358:PRO:HD3	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:ALA:HB1	1:D:334:PHE:HB3	2.02	0.41
1:A:302:ASN:O	1:A:303:MET:HG3	2.20	0.41
1:D:362:MET:O	1:D:366:VAL:HG23	2.21	0.41
1:A:251:PHE:CE1	1:A:371:THR:HB	2.56	0.41
1:A:304:THR:HG21	1:A:379:ARG:HH21	1.85	0.41
1:B:354:LEU:HD11	1:B:367:LEU:HD21	2.02	0.41
1:D:381:THR:O	1:D:382:GLN:HB2	2.20	0.40
1:C:341:SER:HA	1:C:342:PRO:HD3	1.90	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	199/218 (91%)	189 (95%)	8 (4%)	2 (1%)	15 17
1	B	200/218 (92%)	193 (96%)	5 (2%)	2 (1%)	15 17
1	C	201/218 (92%)	192 (96%)	8 (4%)	1 (0%)	29 35
1	D	201/218 (92%)	195 (97%)	6 (3%)	0	100 100
2	L	34/41 (83%)	33 (97%)	1 (3%)	0	100 100
2	M	34/41 (83%)	34 (100%)	0	0	100 100
2	N	34/41 (83%)	29 (85%)	4 (12%)	1 (3%)	4 3
2	O	34/41 (83%)	32 (94%)	2 (6%)	0	100 100
All	All	937/1036 (90%)	897 (96%)	34 (4%)	6 (1%)	22 31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	198	THR
1	C	254	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	214	ARG
1	B	254	LYS
1	A	254	LYS
2	N	92	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	186/197 (94%)	183 (98%)	3 (2%)	62 78
1	B	187/197 (95%)	185 (99%)	2 (1%)	73 86
1	C	188/197 (95%)	182 (97%)	6 (3%)	39 54
1	D	188/197 (95%)	183 (97%)	5 (3%)	44 61
2	L	33/38 (87%)	32 (97%)	1 (3%)	41 57
2	M	33/38 (87%)	33 (100%)	0	100 100
2	N	33/38 (87%)	32 (97%)	1 (3%)	41 57
2	O	33/38 (87%)	32 (97%)	1 (3%)	41 57
All	All	881/940 (94%)	862 (98%)	19 (2%)	52 69

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	279	LEU
1	A	305	VAL
1	A	374	LEU
2	L	68	LEU
1	D	240	GLU
1	D	261	LEU
1	D	305	VAL
1	D	339	ASN
1	D	374	LEU
2	O	93	ASP
1	B	305	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	374	LEU
1	C	305	VAL
1	C	313	SER
1	C	360	LYS
1	C	374	LEU
1	C	404	HIS
1	C	410	LYS
2	N	68	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
1	D	220	ASN
1	D	280	ASN
1	B	280	ASN
1	C	280	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 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	MYR	A	501	-	12,15,15	0.20	0	11,15,15	0.73	0
3	MYR	C	501	-	12,15,15	0.20	0	11,15,15	0.70	0
3	MYR	B	501	-	12,15,15	0.17	0	11,15,15	0.74	0
3	MYR	D	501	-	12,15,15	0.20	0	11,15,15	0.70	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	MYR	A	501	-	-	8/11/13/13	-
3	MYR	C	501	-	-	5/11/13/13	-
3	MYR	B	501	-	-	7/11/13/13	-
3	MYR	D	501	-	-	9/11/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	MYR	C1-C2-C3-C4
3	B	501	MYR	C1-C2-C3-C4
3	D	501	MYR	C1-C2-C3-C4
3	D	501	MYR	C10-C11-C12-C13
3	A	501	MYR	C10-C11-C12-C13
3	D	501	MYR	C6-C7-C8-C9
3	C	501	MYR	C11-C10-C9-C8
3	B	501	MYR	C11-C10-C9-C8
3	B	501	MYR	C3-C4-C5-C6
3	D	501	MYR	C7-C8-C9-C10
3	D	501	MYR	C3-C4-C5-C6
3	A	501	MYR	C6-C7-C8-C9
3	A	501	MYR	C3-C4-C5-C6
3	A	501	MYR	C11-C10-C9-C8
3	B	501	MYR	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	501	MYR	C5-C6-C7-C8
3	D	501	MYR	C9-C10-C11-C12
3	C	501	MYR	C11-C12-C13-C14
3	D	501	MYR	C11-C12-C13-C14
3	B	501	MYR	C6-C7-C8-C9
3	B	501	MYR	C11-C12-C13-C14
3	A	501	MYR	C9-C10-C11-C12
3	C	501	MYR	C6-C7-C8-C9
3	C	501	MYR	C4-C5-C6-C7
3	D	501	MYR	C11-C10-C9-C8
3	A	501	MYR	C5-C6-C7-C8
3	B	501	MYR	C5-C6-C7-C8
3	D	501	MYR	C5-C6-C7-C8
3	A	501	MYR	C11-C12-C13-C14

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	MYR	1	0
3	C	501	MYR	3	0
3	B	501	MYR	1	0
3	D	501	MYR	3	0

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	202/218 (92%)	0.78	25 (12%) 4 5	25, 49, 74, 90	0
1	B	203/218 (93%)	0.54	16 (7%) 12 17	23, 42, 63, 82	0
1	C	203/218 (93%)	0.65	18 (8%) 9 13	27, 45, 74, 91	0
1	D	203/218 (93%)	0.49	14 (6%) 16 22	25, 40, 63, 91	0
2	L	35/41 (85%)	1.09	9 (25%) 0 0	32, 57, 99, 102	0
2	M	35/41 (85%)	1.69	13 (37%) 0 0	29, 74, 106, 115	0
2	N	35/41 (85%)	1.80	11 (31%) 0 0	40, 80, 122, 129	0
2	O	35/41 (85%)	0.39	2 (5%) 23 30	33, 49, 67, 73	0
All	All	951/1036 (91%)	0.71	108 (11%) 5 7	23, 45, 84, 129	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	287	ALA	11.4
2	N	77	THR	8.0
1	C	238	LEU	7.6
2	M	66	GLU	6.8
2	N	76	LYS	6.3
1	C	399	HIS	5.8
2	M	67	ALA	5.8
1	A	399	HIS	4.8
2	L	76	LYS	4.8
1	A	299	SER	4.6
2	M	73[A]	MET	4.6
2	N	73[A]	MET	4.4
1	B	399	HIS	4.3
1	A	398	GLU	4.2
1	B	282	ASN	4.1
2	M	78	ALA	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	69	PHE	4.1
2	L	77	THR	4.1
1	D	332	GLY	4.0
1	A	256	GLY	3.9
2	N	70	ASN	3.9
1	B	202	ARG	3.9
1	C	396	ASN	3.8
2	M	68	LEU	3.8
1	C	361	TYR	3.8
1	C	287	ALA	3.7
1	A	288	GLY	3.7
2	M	79	ASN	3.6
2	L	75	PRO	3.6
1	B	331	ASN	3.6
1	B	398	GLU	3.6
1	C	398	GLU	3.6
2	N	72	VAL	3.5
2	L	78	ALA	3.5
2	M	77	THR	3.4
1	D	399	HIS	3.3
1	D	398	GLU	3.3
1	A	329	PHE	3.3
1	D	331	ASN	3.2
1	B	256	GLY	3.2
1	A	255	LYS	3.2
1	A	199	THR	3.2
2	M	76	LYS	3.1
1	D	288	GLY	3.1
1	C	316	LYS	3.1
1	D	199	THR	3.1
1	C	282	ASN	3.1
1	C	332	GLY	3.1
2	M	75	PRO	3.1
1	B	255	LYS	3.0
2	N	80	VAL	3.0
2	L	79	ASN	3.0
1	A	267	GLN	3.0
1	A	397	SER	2.9
2	N	78	ALA	2.9
1	C	356	HIS	2.9
1	C	360	LYS	2.9
1	B	254	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	361	TYR	2.9
1	A	332	GLY	2.9
2	O	76	LYS	2.8
2	M	97	LYS	2.8
1	A	254	LYS	2.8
1	C	380	ASP	2.8
1	B	287	ALA	2.8
1	A	375	VAL	2.7
2	N	67	ALA	2.7
1	A	264	LYS	2.7
2	M	96	PHE	2.7
1	B	238	LEU	2.7
1	A	376	VAL	2.7
1	C	358	PRO	2.6
2	L	80	VAL	2.6
1	D	333	ARG	2.6
1	D	283	ILE	2.5
1	B	283	ILE	2.5
1	A	307[A]	CYS	2.5
1	D	360	LYS	2.5
1	A	214	ARG	2.5
2	N	68	LEU	2.5
1	A	198	THR	2.4
1	C	283	ILE	2.4
1	C	228	GLY	2.4
2	M	72	VAL	2.4
2	N	97	LYS	2.4
2	L	65	LEU	2.4
2	L	73[A]	MET	2.4
1	A	374	LEU	2.3
1	A	377	THR	2.3
1	A	316	LYS	2.3
2	O	77	THR	2.3
1	A	382	GLN	2.3
1	B	288	GLY	2.3
1	C	214	ARG	2.3
1	D	196	ILE	2.3
1	B	345	GLU	2.2
1	C	379	ARG	2.2
1	B	408	LEU	2.2
1	A	305	VAL	2.2
2	L	96	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	216	PRO	2.2
1	A	322	VAL	2.1
1	A	304	THR	2.1
2	M	94	SER	2.1
1	D	335	VAL	2.1
1	B	327	ALA	2.0
1	D	316	LYS	2.0
1	C	322	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no 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
3	MYR	A	501	16/16	0.85	0.27	38,40,52,55	0
3	MYR	D	501	16/16	0.87	0.24	36,39,45,46	0
3	MYR	B	501	16/16	0.88	0.23	36,39,48,51	0
3	MYR	C	501	16/16	0.88	0.24	39,45,49,50	0

6.5 Other polymers (i)

There are no such residues in this entry.