



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:18 PM GMT

PDB ID : 4XAJ  
Title : Crystal structure of human NR2E1/TLX  
Authors : Zhi, X.; Zhou, E.; Xu, E.  
Deposited on : 2014-12-14  
Resolution : 3.55 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

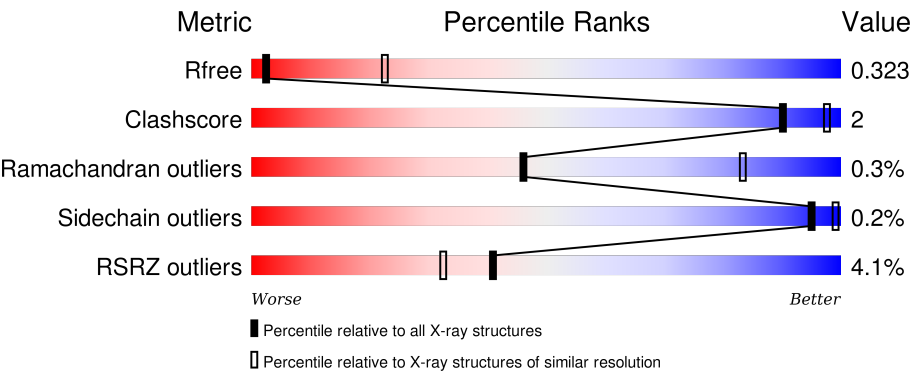
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.55 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 <sub>free</sub>	91344	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)

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. 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	576	<div><div>2%</div><div>91%</div><div>7%</div><div></div></div>
1	B	576	<div><div>%</div><div>96%</div><div></div><div></div></div>
1	C	576	<div><div>3%</div><div>93%</div><div>6%</div><div></div></div>
1	D	576	<div><div>10%</div><div>94%</div><div>5%</div><div></div></div>
2	P	18	<div><div>6%</div><div>100%</div><div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
2	Q	18	 <div>89%11%</div>

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
3	MAL	D	1900	-	-	X	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18097 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 Maltose-binding periplasmic protein,Nuclear receptor subfamily 2 group E member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4424	2847	729	835	13			
1	C	568	Total	C	N	O	S	0	0	0
			4424	2848	729	834	13			
1	B	570	Total	C	N	O	S	0	0	0
			4437	2856	731	836	14			
1	D	568	Total	C	N	O	S	0	0	0
			4424	2848	729	834	13			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0AEY0
A	369	ASN	-	linker	UNP P0AEY0
A	370	ALA	-	linker	UNP P0AEY0
A	371	ALA	-	linker	UNP P0AEY0
A	372	ALA	-	linker	UNP P0AEY0
A	373	GLU	-	linker	UNP P0AEY0
A	374	PHE	-	linker	UNP P0AEY0
A	1257	ARG	LYS	engineered mutation	UNP Q9Y466
A	1259	THR	ASN	engineered mutation	UNP Q9Y466
A	1260	LEU	LYS	engineered mutation	UNP Q9Y466
A	1338	VAL	CYS	engineered mutation	UNP Q9Y466
B	1	MET	-	initiating methionine	UNP P0AEY0
B	369	ASN	-	linker	UNP P0AEY0
B	370	ALA	-	linker	UNP P0AEY0
B	371	ALA	-	linker	UNP P0AEY0
B	372	ALA	-	linker	UNP P0AEY0
B	373	GLU	-	linker	UNP P0AEY0
B	374	PHE	-	linker	UNP P0AEY0
B	1257	ARG	LYS	engineered mutation	UNP Q9Y466
B	1259	THR	ASN	engineered mutation	UNP Q9Y466

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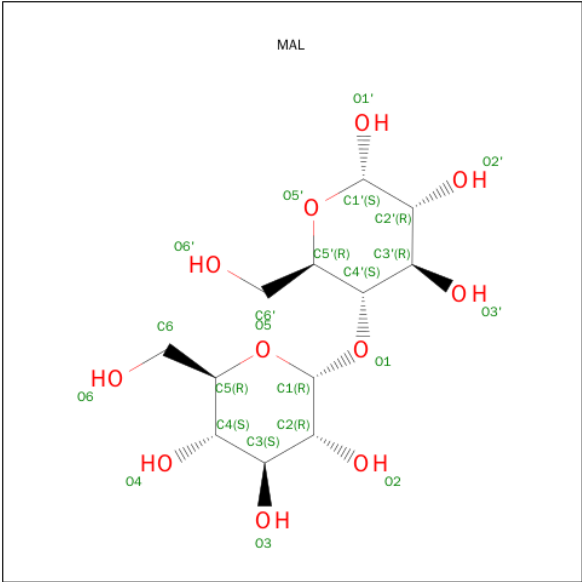
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1260	LEU	LYS	engineered mutation	UNP Q9Y466
B	1338	VAL	CYS	engineered mutation	UNP Q9Y466
C	1	MET	-	initiating methionine	UNP P0AEY0
C	369	ASN	-	linker	UNP P0AEY0
C	370	ALA	-	linker	UNP P0AEY0
C	371	ALA	-	linker	UNP P0AEY0
C	372	ALA	-	linker	UNP P0AEY0
C	373	GLU	-	linker	UNP P0AEY0
C	374	PHE	-	linker	UNP P0AEY0
C	1257	ARG	LYS	engineered mutation	UNP Q9Y466
C	1259	THR	ASN	engineered mutation	UNP Q9Y466
C	1260	LEU	LYS	engineered mutation	UNP Q9Y466
C	1338	VAL	CYS	engineered mutation	UNP Q9Y466
D	1	MET	-	initiating methionine	UNP P0AEY0
D	369	ASN	-	linker	UNP P0AEY0
D	370	ALA	-	linker	UNP P0AEY0
D	371	ALA	-	linker	UNP P0AEY0
D	372	ALA	-	linker	UNP P0AEY0
D	373	GLU	-	linker	UNP P0AEY0
D	374	PHE	-	linker	UNP P0AEY0
D	1257	ARG	LYS	engineered mutation	UNP Q9Y466
D	1259	THR	ASN	engineered mutation	UNP Q9Y466
D	1260	LEU	LYS	engineered mutation	UNP Q9Y466
D	1338	VAL	CYS	engineered mutation	UNP Q9Y466

- Molecule 2 is a protein called Atrophin/grunge.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	18	Total	C	N	O	0	0	0
			148	93	27	28			
2	P	18	Total	C	N	O	0	0	0
			148	93	27	28			

- Molecule 3 is MALTOSE (three-letter code: MAL) (formula: C<sub>12</sub>H<sub>22</sub>O<sub>11</sub>).

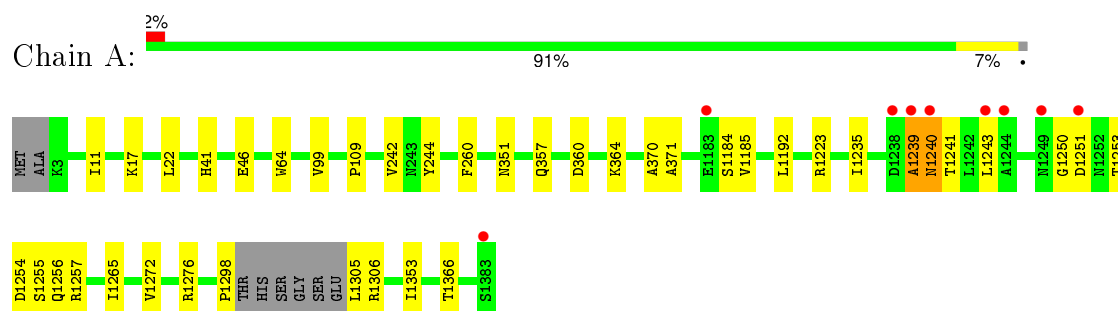


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	12	11		
3	C	1	Total	C	O	0	0
			23	12	11		
3	B	1	Total	C	O	0	0
			23	12	11		
3	D	1	Total	C	O	0	0
			23	12	11		

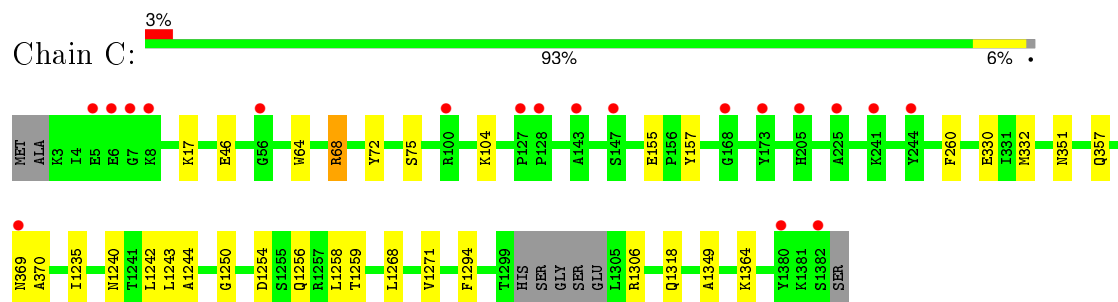
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

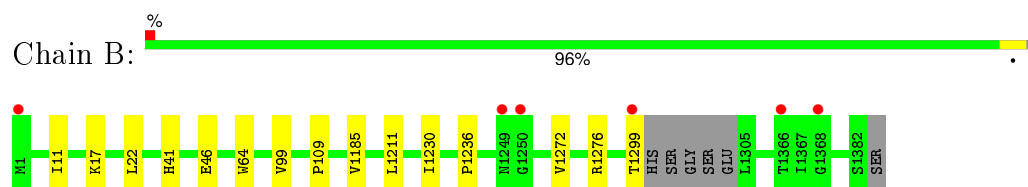
- Molecule 1: Maltose-binding periplasmic protein,Nuclear receptor subfamily 2 group E member 1



- Molecule 1: Maltose-binding periplasmic protein,Nuclear receptor subfamily 2 group E member 1

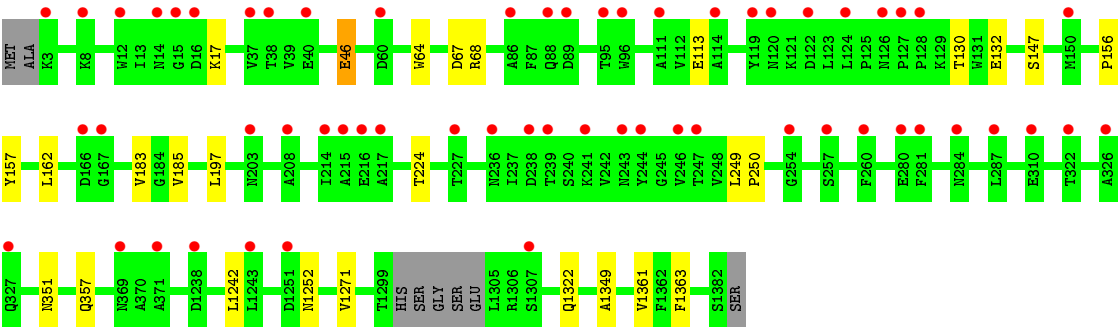


- Molecule 1: Maltose-binding periplasmic protein,Nuclear receptor subfamily 2 group E member 1

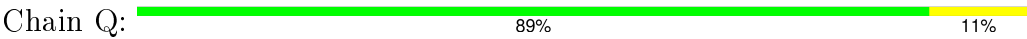


- Molecule 1: Maltose-binding periplasmic protein,Nuclear receptor subfamily 2 group E member 1





● Molecule 2: Atrophin/grunge



● Molecule 2: Atrophin/grunge





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.26Å 130.74Å 308.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 3.55 39.90 – 3.55	Depositor EDS
% Data completeness (in resolution range)	97.8 (39.90-3.55) 98.0 (39.90-3.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.273 , 0.314 0.281 , 0.323	Depositor DCC
$R_{free}$ test set	2532 reflections (7.67%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.9	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 32.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	6 of 35524 reflections (0.017%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	18097	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	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 51.47 % 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 5.5865e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MAL

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	0.35	0/4521	0.67	1/6137 (0.0%)
1	B	0.34	0/4534	0.67	0/6156
1	C	0.34	0/4521	0.66	1/6139 (0.0%)
1	D	0.33	0/4521	0.67	2/6139 (0.0%)
2	P	0.30	0/152	0.70	0/206
2	Q	0.30	0/152	0.65	0/206
All	All	0.34	0/18401	0.67	4/24983 (0.0%)

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

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1250	GLY	N-CA-C	5.57	127.03	113.10
1	D	1252	ASN	N-CA-C	5.41	125.60	111.00
1	C	1235	ILE	N-CA-C	-5.39	96.46	111.00
1	D	1322	GLN	CA-CB-CG	5.09	124.61	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	370	ALA	Peptide

## 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	4424	0	4442	22	0
1	B	4437	0	4461	9	0
1	C	4424	0	4444	28	0
1	D	4424	0	4444	23	0
2	P	148	0	140	0	0
2	Q	148	0	140	1	0
3	A	23	0	22	1	0
3	B	23	0	22	1	0
3	C	23	0	22	7	0
3	D	23	0	22	11	0
All	All	18097	0	18159	83	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 2.

All (83) 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:C:64:TRP:HZ2	3:C:1900:MAL:H3	1.27	0.96
1:D:67:ASP:OD2	3:D:1900:MAL:O3	1.96	0.83
1:C:64:TRP:CZ2	3:C:1900:MAL:H3	2.15	0.80
1:A:1255:SER:OG	1:A:1256:GLN:N	2.17	0.76
1:C:17:LYS:NZ	3:C:1900:MAL:O2'	2.15	0.73
1:C:1306:ARG:HA	1:C:1306:ARG:NE	2.05	0.71
1:D:157:TYR:HB2	3:D:1900:MAL:O5	1.95	0.67
1:A:17:LYS:NZ	3:A:1900:MAL:O2'	2.23	0.65
1:D:157:TYR:CD1	3:D:1900:MAL:H1	2.31	0.65
1:D:46:GLU:HG2	1:D:64:TRP:CH2	2.33	0.64
1:C:68:ARG:HB2	1:C:68:ARG:HH11	1.63	0.64
1:A:364:LYS:HA	1:A:364:LYS:HE2	1.82	0.61
1:C:104:LYS:NZ	1:C:1254:ASP:OD2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:GLU:OE2	3:C:1900:MAL:O4	2.19	0.60
1:D:157:TYR:CD2	3:D:1900:MAL:H6'1	2.38	0.59
1:A:41:HIS:O	1:A:41:HIS:ND1	2.41	0.54
1:C:75:SER:HB3	1:C:1244:ALA:HB1	1.90	0.53
1:A:1255:SER:HB3	1:A:1257:ARG:H	1.74	0.53
1:A:1257:ARG:O	1:A:1257:ARG:HG2	2.07	0.53
1:A:1240:ASN:N	1:A:1241:THR:HA	2.24	0.52
1:C:68:ARG:HD3	1:C:72:TYR:CZ	2.45	0.52
1:D:183:VAL:HG22	1:D:185:VAL:H	1.75	0.52
1:D:351:ASN:HB3	1:D:357:GLN:HG2	1.92	0.52
1:D:113:GLU:OE1	3:D:1900:MAL:O2'	2.24	0.52
1:D:130:THR:OG1	1:D:132:GLU:OE1	2.28	0.51
1:C:260:PHE:HB3	1:C:332:MET:CG	2.40	0.51
1:A:1223:ARG:NH1	1:A:1353:ILE:O	2.45	0.50
1:C:68:ARG:HD3	1:C:72:TYR:CE1	2.46	0.50
1:A:1241:THR:HG21	1:A:1265:ILE:HG22	1.93	0.50
1:B:1230:ILE:HG23	1:B:1236:PRO:HD2	1.94	0.49
1:D:1271:VAL:HG22	1:D:1349:ALA:HB1	1.94	0.49
1:A:1272:VAL:O	1:A:1276:ARG:HG2	2.14	0.47
1:C:369:ASN:OD1	1:C:370:ALA:N	2.48	0.47
1:C:1294:PHE:O	1:C:1318:GLN:HB2	2.15	0.46
1:A:1298:PRO:HB2	1:A:1305:LEU:HB2	1.97	0.46
1:D:147:SER:HB3	1:D:224:THR:HG22	1.98	0.46
1:C:260:PHE:HB3	1:C:332:MET:HG3	1.98	0.46
1:C:1256:GLN:O	1:C:1259:THR:N	2.45	0.46
1:C:68:ARG:HD3	1:C:72:TYR:OH	2.16	0.46
1:D:157:TYR:CE1	3:D:1900:MAL:H4'	2.51	0.45
1:C:1271:VAL:HG22	1:C:1349:ALA:HB1	1.98	0.45
1:D:156:PRO:HG2	3:D:1900:MAL:H61	1.99	0.45
1:C:1306:ARG:HA	1:C:1306:ARG:HE	1.81	0.45
1:C:155:GLU:HB3	3:C:1900:MAL:O6	2.17	0.45
1:D:1242:LEU:HD12	1:D:1242:LEU:HA	1.71	0.45
1:A:1253:THR:OG1	1:A:1254:ASP:N	2.49	0.45
1:D:17:LYS:HZ3	3:D:1900:MAL:C1'	2.30	0.45
1:D:162:LEU:HD23	1:D:197:LEU:HG	1.97	0.45
1:B:17:LYS:NZ	3:B:1900:MAL:O2'	2.25	0.45
1:D:157:TYR:CD1	3:D:1900:MAL:H4'	2.51	0.44
1:C:260:PHE:HA	1:C:330:GLU:O	2.18	0.44
1:A:1239:ALA:HB1	1:A:1243:LEU:HB3	2.00	0.44
1:A:1184:SER:OG	1:A:1185:VAL:N	2.50	0.44
1:B:41:HIS:O	1:B:41:HIS:ND1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:GLU:HB3	3:C:1900:MAL:HO6	1.82	0.43
1:C:1256:GLN:C	1:C:1258:LEU:N	2.72	0.43
1:D:17:LYS:NZ	3:D:1900:MAL:C1'	2.82	0.43
1:D:147:SER:O	1:D:224:THR:HA	2.18	0.43
1:A:242:VAL:HG12	1:A:244:TYR:HB3	2.00	0.43
1:A:99:VAL:HG21	1:A:109:PRO:HD3	1.99	0.43
1:C:157:TYR:HB2	3:C:1900:MAL:O5	2.19	0.43
1:D:67:ASP:OD1	1:D:68:ARG:N	2.51	0.43
1:C:260:PHE:HB3	1:C:332:MET:HG2	2.00	0.43
1:B:1211:LEU:HA	1:B:1211:LEU:HD12	1.85	0.42
1:C:1240:ASN:HA	1:C:1243:LEU:HB2	2.01	0.42
1:D:249:LEU:HA	1:D:250:PRO:HD3	1.91	0.42
1:A:351:ASN:HB3	1:A:357:GLN:HG2	2.00	0.42
1:A:1192:LEU:HD11	1:A:1235:ILE:HD12	2.02	0.42
1:B:1299:THR:HG22	1:B:1299:THR:O	2.20	0.42
1:C:1250:GLY:HA2	1:C:1364:LYS:HB3	2.02	0.41
1:D:1242:LEU:HD11	1:D:1361:VAL:HG11	2.01	0.41
1:C:351:ASN:HB3	1:C:357:GLN:HG2	2.02	0.41
1:B:11:ILE:HG21	1:B:22:LEU:HD21	2.03	0.41
1:B:99:VAL:HG21	1:B:109:PRO:HD3	2.03	0.41
1:A:46:GLU:HG2	1:A:64:TRP:CZ2	2.55	0.41
1:B:1272:VAL:O	1:B:1276:ARG:HG2	2.20	0.41
1:A:11:ILE:HG21	1:A:22:LEU:HD21	2.03	0.41
1:D:113:GLU:OE1	3:D:1900:MAL:C2'	2.69	0.40
1:A:360:ASP:O	1:A:364:LYS:HG2	2.22	0.40
2:Q:1828:ARG:HB3	2:Q:1829:PRO:HD3	2.01	0.40
1:B:46:GLU:HG2	1:B:64:TRP:CZ2	2.56	0.40
1:A:1306:ARG:NE	1:A:1306:ARG:HA	2.35	0.40
1:C:1242:LEU:HD21	1:C:1268:LEU:HD23	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	564/576 (98%)	546 (97%)	13 (2%)	5 (1%)	21	67
1	B	566/576 (98%)	548 (97%)	17 (3%)	1 (0%)	52	87
1	C	564/576 (98%)	545 (97%)	19 (3%)	0	100	100
1	D	564/576 (98%)	544 (96%)	20 (4%)	0	100	100
2	P	16/18 (89%)	16 (100%)	0	0	100	100
2	Q	16/18 (89%)	16 (100%)	0	0	100	100
All	All	2290/2340 (98%)	2215 (97%)	69 (3%)	6 (0%)	46	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	371	ALA
1	A	1239	ALA
1	A	1366	THR
1	B	1185	VAL
1	A	1251	ASP
1	A	1240	ASN

### 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	466/472 (99%)	465 (100%)	1 (0%)	95	99
1	B	467/472 (99%)	467 (100%)	0	100	100
1	C	466/472 (99%)	465 (100%)	1 (0%)	95	99
1	D	466/472 (99%)	464 (100%)	2 (0%)	93	98
2	P	15/15 (100%)	15 (100%)	0	100	100
2	Q	15/15 (100%)	15 (100%)	0	100	100
All	All	1895/1918 (99%)	1891 (100%)	4 (0%)	95	99

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	PHE
1	C	68	ARG
1	D	46	GLU
1	D	1363	PHE

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 ⓘ

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	MAL	A	1900	-	24,24,24	0.54	0	35,35,35	0.71	0
3	MAL	B	1900	-	24,24,24	0.55	0	35,35,35	0.61	0
3	MAL	C	1900	-	24,24,24	0.57	0	35,35,35	0.89	1 (2%)
3	MAL	D	1900	-	24,24,24	0.78	0	35,35,35	1.53	6 (17%)

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	MAL	A	1900	-	-	0/8/48/48	0/2/2/2
3	MAL	B	1900	-	-	0/8/48/48	0/2/2/2
3	MAL	C	1900	-	-	0/8/48/48	0/2/2/2
3	MAL	D	1900	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1900	MAL	C1-O1-C4'	-4.61	105.95	118.01
3	D	1900	MAL	C1'-O5'-C5'	-3.62	106.78	113.47
3	D	1900	MAL	O2'-C2'-C3'	-2.59	104.51	110.34
3	C	1900	MAL	C6-C5-C4	-2.41	107.06	113.02
3	D	1900	MAL	C6-C5-C4	-2.32	107.30	113.02
3	D	1900	MAL	O5'-C5'-C6'	2.06	111.56	106.36
3	D	1900	MAL	O5-C5-C6	2.26	112.07	106.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1900	MAL	1	0
3	B	1900	MAL	1	0
3	C	1900	MAL	7	0
3	D	1900	MAL	11	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	568/576 (98%)	-0.21	9 (1%) 74 66	17, 35, 74, 96	0
1	B	570/576 (98%)	-0.22	6 (1%) 82 74	15, 35, 76, 107	0
1	C	568/576 (98%)	0.26	19 (3%) 50 40	17, 88, 122, 150	0
1	D	568/576 (98%)	0.61	59 (10%) 8 8	18, 116, 185, 210	0
2	P	18/18 (100%)	0.32	1 (5%) 28 22	57, 71, 83, 91	0
2	Q	18/18 (100%)	0.14	0 100 100	50, 63, 90, 91	0
All	All	2310/2340 (98%)	0.11	94 (4%) 41 32	15, 47, 155, 210	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1244	ALA	5.2
1	A	1240	ASN	5.0
1	D	127	PRO	4.8
1	D	111	ALA	4.6
1	D	244	TYR	4.3
1	D	247	THR	4.1
1	D	38	THR	3.9
1	D	287	LEU	3.9
1	D	86	ALA	3.9
1	D	1243	LEU	3.8
1	D	227	THR	3.6
1	D	1307	SER	3.6
1	B	1366	THR	3.5
1	D	216	GLU	3.5
1	B	1249	ASN	3.5
1	C	205	HIS	3.3
1	D	280	GLU	3.3
1	D	310	GLU	3.3
1	D	120	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	241	LYS	3.3
1	A	1238	ASP	3.3
1	D	60	ASP	3.3
1	D	214	ILE	3.2
1	C	5	GLU	3.2
1	B	1368	GLY	3.1
1	D	14	ASN	3.1
1	D	1238	ASP	3.1
1	B	1299	THR	3.1
1	D	16	ASP	3.1
1	C	168	GLY	3.0
1	D	243	ASN	3.0
1	D	326	ALA	3.0
1	D	3	LYS	3.0
1	D	203	ASN	2.9
1	D	88	GLN	2.9
1	A	1243	LEU	2.9
1	A	1239	ALA	2.9
1	D	89	ASP	2.9
1	D	284	ASN	2.9
1	C	7	GLY	2.8
1	A	1383	SER	2.8
1	D	215	ALA	2.8
1	D	238	ASP	2.8
1	D	119	TYR	2.7
1	C	127	PRO	2.7
1	D	239	THR	2.6
1	D	126	ASN	2.6
1	D	114	ALA	2.6
1	D	371	ALA	2.6
1	D	40	GLU	2.6
1	D	246	VAL	2.6
1	D	167	GLY	2.6
1	D	369	ASN	2.5
1	D	254	GLY	2.5
1	D	15	GLY	2.5
1	D	12	TRP	2.5
1	D	236	ASN	2.5
1	C	369	ASN	2.5
1	D	122	ASP	2.5
1	D	327	GLN	2.4
1	D	128	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	173	TYR	2.4
1	D	281	PHE	2.4
1	C	225	ALA	2.4
1	C	241	LYS	2.4
1	C	143	ALA	2.3
1	D	95	THR	2.3
1	C	1380	TYR	2.3
1	D	322	THR	2.3
1	D	8	LYS	2.3
2	P	1814	TYR	2.3
1	D	96	TRP	2.3
1	D	166	ASP	2.2
1	C	128	PRO	2.2
1	C	100	ARG	2.2
1	D	208	ALA	2.2
1	A	1249	ASN	2.2
1	D	260	PHE	2.2
1	D	124	LEU	2.2
1	D	257	SER	2.2
1	A	1251	ASP	2.1
1	A	1183	GLU	2.1
1	D	37	VAL	2.1
1	D	217	ALA	2.1
1	C	1382	SER	2.1
1	C	244	TYR	2.1
1	D	1251	ASP	2.1
1	B	1	MET	2.1
1	D	150	MET	2.1
1	C	6	GLU	2.1
1	C	8	LYS	2.1
1	C	147	SER	2.1
1	B	1250	GLY	2.0
1	C	56	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAL	C	1900	23/23	0.75	0.32	0.58	57,62,68,69	0
3	MAL	D	1900	23/23	0.59	0.44	0.21	84,94,103,104	0
3	MAL	B	1900	23/23	0.94	0.18	-0.76	14,15,16,17	0
3	MAL	A	1900	23/23	0.95	0.16	-1.13	14,15,16,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.