



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2016 – 03:56 PM EDT

PDB ID : 5LR6  
Title : Crystal Structure of COMT in complex with [3-(2,4-dimethyl-1,3-thiazol-5-yl)-1H-pyrazol-5-yl]-(4-phenylpiperazin-1-yl)methanone  
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Deposited on : 2016-08-18  
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](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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

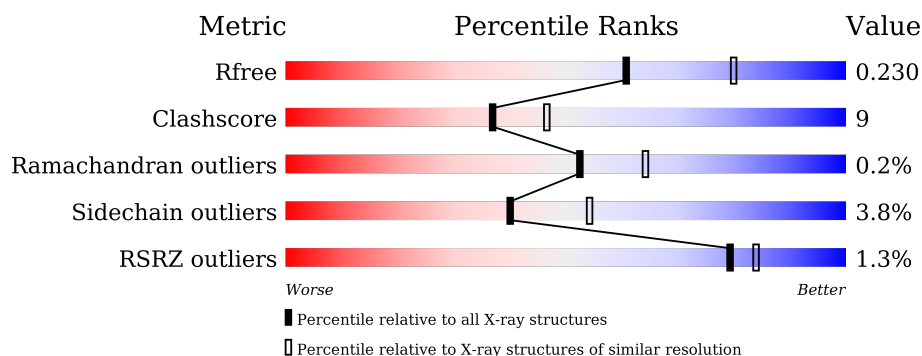
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	221	<div> <div></div> <div>70%25% . .</div> </div>
1	B	221	<div> <div>3%</div> <div>74%21% .</div> </div>
1	C	221	<div> <div>%</div> <div>70%26% . .</div> </div>
1	D	221	<div> <div>%</div> <div>75%21% . .</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7062 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.

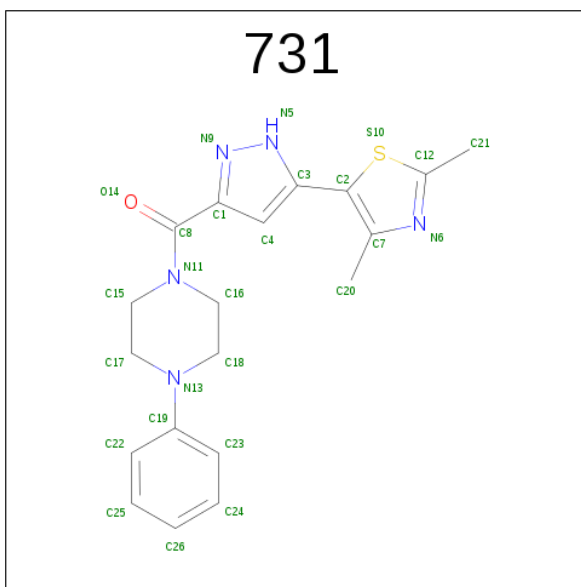
- Molecule 1 is a protein called Catechol O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1654	1051	276	315	12			
1	B	212	Total	C	N	O	S	0	0	0
			1662	1057	276	318	11			
1	C	214	Total	C	N	O	S	0	0	0
			1677	1065	279	322	11			
1	D	214	Total	C	N	O	S	0	0	0
			1666	1058	279	317	12			

There are 8 discrepancies between the modelled and reference sequences:

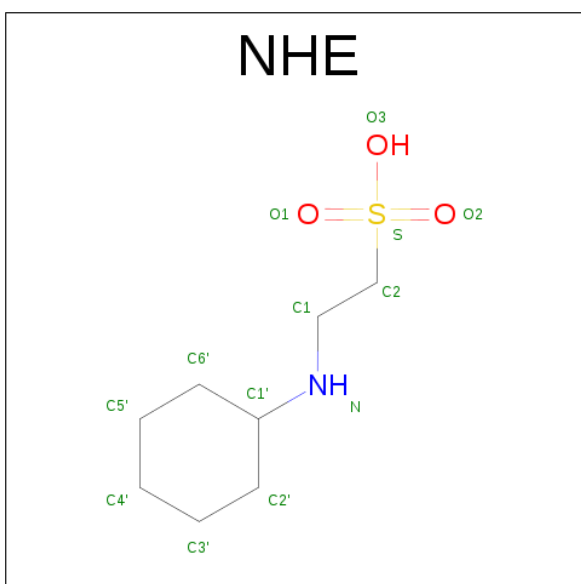
Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ILE	MET	conflict	UNP P22734
A	95	CYS	TYR	conflict	UNP P22734
B	91	ILE	MET	conflict	UNP P22734
B	95	CYS	TYR	conflict	UNP P22734
C	91	ILE	MET	conflict	UNP P22734
C	95	CYS	TYR	conflict	UNP P22734
D	91	ILE	MET	conflict	UNP P22734
D	95	CYS	TYR	conflict	UNP P22734

- Molecule 2 is [5-(2,4-dimethyl-1,3-thiazol-5-yl)-1 {H}-pyrazol-3-yl]-(4-phenylpiperazin-1-yl) methanone (three-letter code: 731) (formula: C<sub>19</sub>H<sub>21</sub>N<sub>5</sub>OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	19	5	1	1		
2	B	1	Total	C	N	O	S	0	0
			26	19	5	1	1		
2	C	1	Total	C	N	O	S	0	0
			26	19	5	1	1		
2	D	1	Total	C	N	O	S	0	0
			26	19	5	1	1		

- Molecule 3 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C<sub>8</sub>H<sub>17</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
3	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
3	C	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
3	D	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- 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		
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

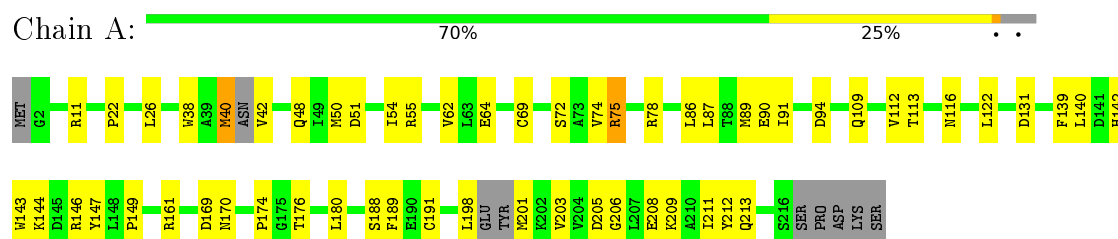
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	59	Total	O	0	0
			59	59		
5	B	57	Total	O	0	0
			57	57		
5	C	68	Total	O	0	0
			68	68		
5	D	59	Total	O	0	0
			59	59		

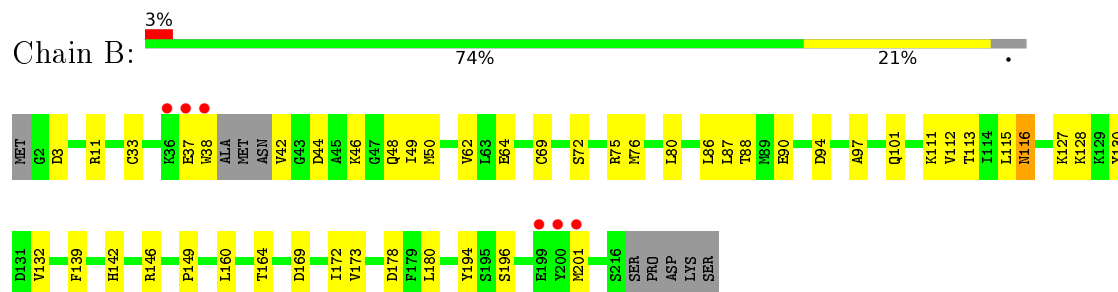
### 3 Residue-property plots

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.

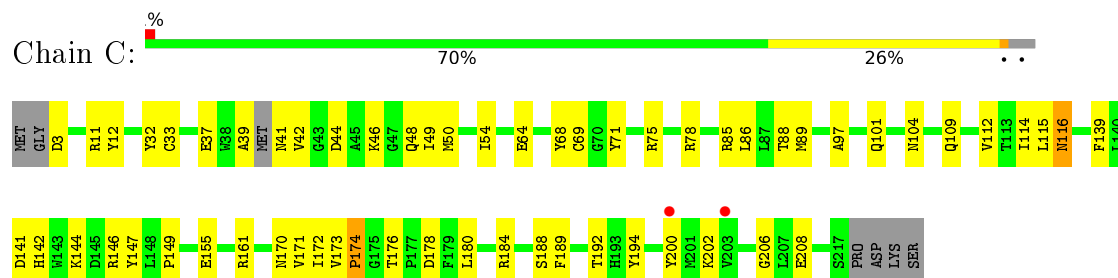
#### • Molecule 1: Catechol O-methyltransferase



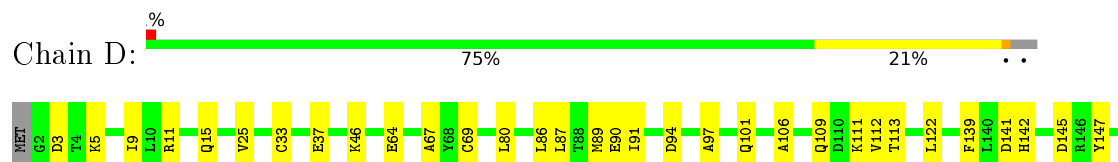
#### • Molecule 1: Catechol O-methyltransferase

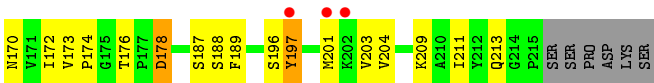


#### • Molecule 1: Catechol O-methyltransferase



#### • Molecule 1: Catechol O-methyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.98Å 103.62Å 78.41Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	46.94 – 2.30 46.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.94-2.30) 94.6 (46.94-2.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.196 , 0.223 0.209 , 0.230	Depositor DCC
$R_{free}$ test set	2455 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 28.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.440 for h,-k,-l	Xtriage
Reported twinning fraction	0.480 for h,-k,-l	Depositor
Outliers	1 of 49981 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7062	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	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 24.78 % 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 3.5885e-03. 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NHE, 731, CL

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	0.54	1/1682 (0.1%)	0.65	0/2276
1	B	0.52	1/1692 (0.1%)	0.61	0/2292
1	C	0.52	1/1707 (0.1%)	0.63	0/2313
1	D	0.53	1/1696 (0.1%)	0.64	0/2299
All	All	0.53	4/6777 (0.1%)	0.63	0/9180

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	69	CYS	CB-SG	-6.66	1.71	1.82
1	A	69	CYS	CB-SG	-6.61	1.71	1.82
1	B	69	CYS	CB-SG	-5.70	1.72	1.81
1	D	69	CYS	CB-SG	-5.68	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1654	0	1665	38	0
1	B	1662	0	1667	24	0
1	C	1677	0	1680	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1666	0	1672	28	0
2	A	26	0	0	2	0
2	B	26	0	0	0	0
2	C	26	0	0	2	0
2	D	26	0	0	0	0
3	A	13	0	16	3	0
3	B	13	0	16	0	0
3	C	13	0	17	0	0
3	D	13	0	17	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	59	0	0	5	0
5	B	57	0	0	3	0
5	C	68	0	0	7	0
5	D	59	0	0	6	0
All	All	7062	0	6750	128	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 9.

All (128) 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)
3:A:302:NHE:H6'1	2:C:502:731:C24	1.94	0.97
1:C:189:PHE:O	5:C:601:HOH:O	1.94	0.85
1:B:64:GLU:OE2	1:B:72:SER:OG	1.96	0.84
1:A:40:MET:O	1:A:42:VAL:N	2.14	0.81
1:B:90:GLU:OE2	5:B:401:HOH:O	2.05	0.73
1:D:172:ILE:HG22	1:D:173:VAL:HG23	1.72	0.72
1:B:33:CYS:HA	1:B:37:GLU:O	1.93	0.67
1:B:172:ILE:HG22	1:B:173:VAL:HG23	1.75	0.67
1:C:101:GLN:OE1	5:C:602:HOH:O	2.12	0.67
1:C:184:ARG:NH2	1:C:208:GLU:OE1	2.27	0.67
1:A:109:GLN:NE2	5:A:401:HOH:O	2.10	0.66
1:A:94:ASP:OD1	5:A:402:HOH:O	2.14	0.66
1:C:116:ASN:ND2	5:C:604:HOH:O	2.24	0.65
1:D:109:GLN:OE1	1:D:109:GLN:N	2.25	0.65
1:D:141:ASP:OD2	5:D:402:HOH:O	2.15	0.65
1:B:49:ILE:HD13	1:B:194:TYR:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:ASP:OD1	5:D:403:HOH:O	2.15	0.64
1:D:147:TYR:CD2	1:D:176:THR:HG21	2.33	0.63
1:D:33:CYS:HA	1:D:37:GLU:O	1.98	0.63
1:A:147:TYR:CD2	1:A:176:THR:HG21	2.36	0.61
1:C:49:ILE:HD13	1:C:194:TYR:HB3	1.82	0.61
1:B:42:VAL:N	5:B:403:HOH:O	2.33	0.60
1:A:64:GLU:OE2	1:A:72:SER:OG	2.21	0.58
1:A:64:GLU:HG3	1:A:139:PHE:HD2	1.69	0.58
1:D:189:PHE:O	5:D:404:HOH:O	2.17	0.57
1:D:209:LYS:HE3	1:D:211:ILE:HD11	1.85	0.57
1:C:41:ASN:ND2	1:C:141:ASP:OD2	2.34	0.57
1:B:80:LEU:O	1:B:111:LYS:NZ	2.38	0.57
1:C:109:GLN:OE1	1:C:109:GLN:N	2.28	0.57
1:D:145:ASP:N	3:D:302:NHE:O3	2.36	0.56
1:A:38:TRP:CE2	1:C:174:PRO:HB3	2.41	0.56
1:D:64:GLU:HG3	1:D:139:PHE:HD2	1.69	0.56
1:A:198:LEU:HB3	1:A:201:MET:HE3	1.89	0.55
1:B:116:ASN:HB3	5:B:436:HOH:O	2.07	0.55
1:A:90:GLU:OE1	2:A:301:731:N9	2.40	0.54
1:D:3:ASP:OD1	1:D:11:ARG:NH2	2.37	0.54
1:C:75:ARG:O	1:C:78:ARG:NH1	2.39	0.54
1:A:51:ASP:HB3	1:A:55:ARG:NH1	2.22	0.54
1:C:44:ASP:O	1:C:48:GLN:HG2	2.09	0.53
1:D:188:SER:O	1:D:213:GLN:N	2.37	0.53
1:B:64:GLU:HG3	1:B:139:PHE:HD2	1.73	0.53
1:D:15:GLN:O	5:D:405:HOH:O	2.19	0.53
1:C:155:GLU:HB3	5:D:401:HOH:O	2.09	0.52
1:B:146:ARG:HA	1:B:149:PRO:HG2	1.90	0.52
1:C:86:LEU:HD23	1:C:112:VAL:HG13	1.91	0.52
1:A:169:ASP:OD1	1:A:170:ASN:N	2.42	0.52
1:C:97:ALA:O	1:C:101:GLN:HG3	2.10	0.52
1:A:143:TRP:HB3	3:A:302:NHE:HC21	1.90	0.51
1:D:170:ASN:HB3	1:D:174:PRO:HD2	1.92	0.51
1:A:109:GLN:OE1	1:A:109:GLN:N	2.28	0.51
1:C:144:LYS:NZ	1:C:147:TYR:OH	2.38	0.51
1:A:22:PRO:O	1:A:26:LEU:HG	2.10	0.50
1:D:46:LYS:HG2	1:D:196:SER:OG	2.10	0.50
1:B:46:LYS:HG2	1:B:196:SER:OG	2.12	0.50
1:D:5:LYS:O	1:D:9:ILE:HG13	2.13	0.49
1:C:33:CYS:HA	1:C:37:GLU:O	2.10	0.49
1:C:64:GLU:HG3	1:C:139:PHE:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:MET:O	1:A:203:VAL:HG13	2.11	0.49
1:A:50:MET:HE2	1:A:75:ARG:HG2	1.95	0.48
1:C:147:TYR:CD2	1:C:176:THR:HG21	2.48	0.48
1:A:50:MET:O	1:A:54:ILE:HG12	2.14	0.48
1:C:46:LYS:HG3	5:C:653:HOH:O	2.12	0.48
1:D:5:LYS:HG3	1:D:37:GLU:OE1	2.14	0.48
1:A:62:VAL:HB	1:A:86:LEU:HD12	1.96	0.48
1:B:127:LYS:HG2	1:B:132:VAL:O	2.13	0.48
1:D:25:VAL:HG21	1:D:106:ALA:HB2	1.96	0.47
1:B:86:LEU:HD23	1:B:112:VAL:HG13	1.96	0.47
1:C:89:MET:HE2	1:C:115:LEU:HD12	1.96	0.47
1:D:89:MET:HG2	1:D:122:LEU:HD13	1.96	0.47
1:C:50:MET:O	1:C:54:ILE:HG12	2.15	0.47
1:A:191:CYS:HA	1:A:209:LYS:O	2.15	0.47
1:A:38:TRP:NE1	1:C:174:PRO:HB3	2.29	0.46
1:A:170:ASN:HB3	1:A:174:PRO:HD2	1.97	0.46
1:B:160:LEU:HD22	1:B:164:THR:HG21	1.98	0.46
1:B:3:ASP:OD1	1:B:11:ARG:NH2	2.25	0.46
1:B:97:ALA:O	1:B:101:GLN:HG3	2.16	0.46
1:C:3:ASP:OD1	1:C:11:ARG:NH2	2.42	0.46
1:C:42:VAL:HG13	1:C:71:TYR:CE1	2.51	0.46
1:A:74:VAL:O	1:A:78:ARG:HB3	2.16	0.46
1:A:91:ILE:HG22	2:A:301:731:N5	2.31	0.46
1:C:180:LEU:HA	1:C:180:LEU:HD23	1.73	0.46
1:D:87:LEU:HD23	1:D:113:THR:HB	1.97	0.46
1:A:87:LEU:HD23	1:A:113:THR:HB	1.98	0.46
1:C:104:ASN:HB2	5:C:611:HOH:O	2.15	0.45
1:C:172:ILE:HG22	1:C:173:VAL:HG23	1.99	0.45
1:D:201:MET:O	1:D:203:VAL:HG13	2.15	0.45
1:A:146:ARG:HD2	5:A:435:HOH:O	2.14	0.45
1:B:50:MET:HE1	1:B:76:MET:HG3	1.99	0.45
1:C:33:CYS:SG	1:C:39:ALA:HB3	2.55	0.45
1:B:44:ASP:O	1:B:48:GLN:HG2	2.17	0.45
1:C:88:THR:HG22	1:C:114:ILE:HA	1.99	0.45
1:C:146:ARG:HA	1:C:149:PRO:HG2	1.98	0.45
1:D:197:TYR:HE1	1:D:204:VAL:HG22	1.81	0.45
1:A:205:ASP:CG	1:A:206:GLY:H	2.20	0.44
1:C:170:ASN:HB3	1:C:174:PRO:HD2	1.99	0.44
1:C:139:PHE:CE2	1:C:141:ASP:HB2	2.53	0.44
1:C:192:THR:HA	5:C:640:HOH:O	2.17	0.44
1:B:62:VAL:HB	1:B:86:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:VAL:HG22	1:C:206:GLY:O	2.17	0.44
1:C:50:MET:HE2	1:C:75:ARG:HG2	1.98	0.44
1:D:172:ILE:HD11	5:D:432:HOH:O	2.17	0.44
1:D:67:ALA:HB3	1:D:90:GLU:HB2	1.99	0.44
1:A:144:LYS:HB3	1:A:176:THR:HG22	1.99	0.44
1:A:191:CYS:HB3	1:A:208:GLU:OE2	2.18	0.44
1:B:115:LEU:HD22	1:B:130:TYR:CZ	2.53	0.44
1:D:197:TYR:CE1	1:D:204:VAL:HG22	2.54	0.43
1:A:161:ARG:NE	5:A:404:HOH:O	2.25	0.43
3:A:302:NHE:H6'1	2:C:502:731:C23	2.44	0.43
1:B:87:LEU:HD23	1:B:113:THR:HB	2.01	0.43
1:C:12:TYR:CD2	1:C:32:TYR:HB2	2.54	0.43
1:A:89:MET:HE2	1:A:122:LEU:HB3	2.01	0.43
1:C:85:ARG:HG2	5:C:645:HOH:O	2.18	0.43
1:D:97:ALA:O	1:D:101:GLN:HG3	2.19	0.43
1:B:42:VAL:HG22	1:B:169:ASP:OD2	2.19	0.43
1:A:188:SER:HB3	1:A:212:TYR:CE1	2.54	0.42
5:A:434:HOH:O	1:B:128:LYS:HE2	2.20	0.42
1:A:86:LEU:HD23	1:A:112:VAL:HG13	2.01	0.42
1:C:200:TYR:O	1:C:202:LYS:HG3	2.19	0.42
1:A:189:PHE:HA	1:A:211:ILE:O	2.20	0.41
1:D:80:LEU:O	1:D:111:LYS:NZ	2.53	0.41
1:C:50:MET:CE	1:C:75:ARG:HG2	2.50	0.41
1:D:86:LEU:HD23	1:D:112:VAL:HG13	2.02	0.41
1:A:146:ARG:HA	1:A:149:PRO:HG2	2.03	0.41
1:A:144:LYS:HE3	1:A:170:ASN:HB2	2.03	0.40
1:A:180:LEU:HA	1:A:180:LEU:HD23	1.78	0.40
1:A:22:PRO:HB3	1:A:74:VAL:HG13	2.02	0.40
1:A:38:TRP:CZ2	1:C:174:PRO:HB3	2.57	0.40
1:B:180:LEU:HA	1:B:180:LEU:HD23	1.82	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	206/221 (93%)	196 (95%)	10 (5%)	0	100	100
1	B	208/221 (94%)	199 (96%)	9 (4%)	0	100	100
1	C	210/221 (95%)	197 (94%)	11 (5%)	2 (1%)	19	21
1	D	212/221 (96%)	200 (94%)	12 (6%)	0	100	100
All	All	836/884 (95%)	792 (95%)	42 (5%)	2 (0%)	52	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	174	PRO
1	C	68	TYR

### 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	181/190 (95%)	172 (95%)	9 (5%)	30	41
1	B	182/190 (96%)	174 (96%)	8 (4%)	35	46
1	C	184/190 (97%)	179 (97%)	5 (3%)	52	70
1	D	181/190 (95%)	175 (97%)	6 (3%)	45	61
All	All	728/760 (96%)	700 (96%)	28 (4%)	40	54

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	40	MET
1	A	48	GLN
1	A	75	ARG
1	A	116	ASN
1	A	131	ASP

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Mol	Chain	Res	Type
1	A	140	LEU
1	A	142	HIS
1	A	213	GLN
1	B	38	TRP
1	B	75	ARG
1	B	88	THR
1	B	94	ASP
1	B	116	ASN
1	B	142	HIS
1	B	178	ASP
1	B	201	MET
1	C	116	ASN
1	C	142	HIS
1	C	161	ARG
1	C	178	ASP
1	C	188	SER
1	D	91	ILE
1	D	94	ASP
1	D	142	HIS
1	D	178	ASP
1	D	187	SER
1	D	197	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	101	GLN

### 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 ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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$
2	731	A	301	-	25,29,29	0.48	0	27,41,41	0.75	0
3	NHE	A	302	-	13,13,13	2.77	2 (15%)	16,17,17	1.49	3 (18%)
2	731	B	301	-	25,29,29	0.46	0	27,41,41	0.91	2 (7%)
3	NHE	B	302	-	13,13,13	2.78	2 (15%)	16,17,17	1.59	3 (18%)
3	NHE	C	501	-	13,13,13	2.47	2 (15%)	16,17,17	1.77	2 (12%)
2	731	C	502	-	25,29,29	0.39	0	27,41,41	0.82	1 (3%)
2	731	D	301	-	25,29,29	0.41	0	27,41,41	0.75	0
3	NHE	D	302	-	13,13,13	2.54	2 (15%)	16,17,17	1.75	2 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	731	A	301	-	-	0/9/26/26	0/4/4/4
3	NHE	A	302	-	-	0/7/15/15	0/1/1/1
2	731	B	301	-	-	0/9/26/26	0/4/4/4
3	NHE	B	302	-	-	0/7/15/15	0/1/1/1
3	NHE	C	501	-	-	0/7/15/15	0/1/1/1
2	731	C	502	-	-	0/9/26/26	0/4/4/4
2	731	D	301	-	-	0/9/26/26	0/4/4/4
3	NHE	D	302	-	-	0/7/15/15	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	NHE	C2-S	-7.62	1.66	1.77
3	D	302	NHE	C2-S	-7.60	1.66	1.77
3	A	302	NHE	C2-S	-7.46	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	NHE	C2-S	-7.35	1.66	1.77
3	C	501	NHE	O3-S	4.61	1.63	1.47
3	D	302	NHE	O3-S	4.64	1.63	1.47
3	B	302	NHE	O2-S	6.05	1.62	1.45
3	A	302	NHE	O2-S	6.21	1.63	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	731	C4-C3-C2	-2.74	125.05	129.24
3	A	302	NHE	O3-S-C2	2.23	109.63	104.99
2	B	301	731	C8-C1-N9	2.26	126.68	120.54
3	B	302	NHE	O3-S-C2	2.33	109.82	104.99
2	C	502	731	C8-C1-N9	2.62	127.64	120.54
3	A	302	NHE	O2-S-C2	2.96	108.96	106.87
3	B	302	NHE	O2-S-C2	3.18	109.12	106.87
3	D	302	NHE	O2-S-C2	3.64	109.44	106.87
3	A	302	NHE	O1-S-C2	3.71	109.49	106.87
3	B	302	NHE	O1-S-C2	4.13	109.79	106.87
3	C	501	NHE	O2-S-C2	4.28	109.89	106.87
3	C	501	NHE	O1-S-C2	4.53	110.07	106.87
3	D	302	NHE	O1-S-C2	5.10	110.47	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	731	2	0
3	A	302	NHE	3	0
2	C	502	731	2	0
3	D	302	NHE	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	212/221 (95%)	-0.45	0 <b>100</b> <b>100</b>	23, 35, 53, 88	0
1	B	212/221 (95%)	-0.28	6 (2%) 56 66	24, 36, 72, 122	0
1	C	214/221 (96%)	-0.37	2 (0%) 85 89	24, 36, 63, 137	0
1	D	214/221 (96%)	-0.35	3 (1%) 78 83	23, 36, 56, 106	0
All	All	852/884 (96%)	-0.36	11 (1%) 79 84	23, 36, 63, 137	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	200	TYR	7.2
1	B	201	MET	6.3
1	B	200	TYR	5.9
1	D	197	TYR	3.2
1	D	202	LYS	2.7
1	B	36	LYS	2.6
1	B	38	TRP	2.5
1	C	203	VAL	2.4
1	B	199	GLU	2.4
1	B	37	GLU	2.3
1	D	201	MET	2.1

### 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. 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	NHE	A	302	13/13	0.95	0.13	1.16	20,25,68,132	0
2	731	B	301	26/26	0.97	0.12	0.15	20,32,50,51	0
3	NHE	D	302	13/13	0.98	0.11	0.07	16,21,32,104	0
2	731	D	301	26/26	0.97	0.11	-0.08	19,35,61,62	0
3	NHE	B	302	13/13	0.98	0.11	-0.10	7,13,36,46	0
3	NHE	C	501	13/13	0.99	0.10	-0.48	17,25,37,65	0
2	731	C	502	26/26	0.97	0.10	-0.70	4,26,42,47	0
2	731	A	301	26/26	0.98	0.09	-1.42	12,26,40,41	0
4	CL	B	303	1/1	0.97	0.07	-	45,45,45,45	0
4	CL	A	303	1/1	0.97	0.08	-	49,49,49,49	0
4	CL	D	303	1/1	0.98	0.06	-	41,41,41,41	0
4	CL	C	503	1/1	0.97	0.11	-	51,51,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.