



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:01 PM GMT

PDB ID : 4NGE  
Title : Crystal Structure of Human Presequence Protease in Complex with Amyloid-beta (1-40)  
Authors : King, J.V.; Liang, W.G.; Tang, W.J.  
Deposited on : 2013-11-01  
Resolution : 2.70 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

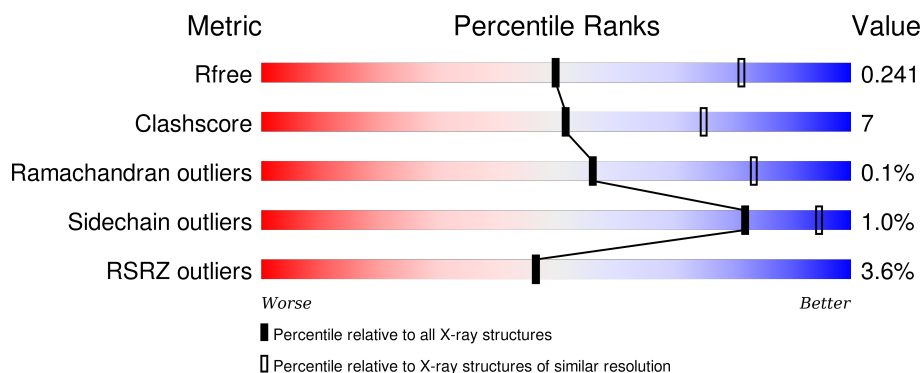
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	1014	<div> <div>4%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
2	B	40	<div> <div>13%</div> <div>13%</div> <div>10%</div> <div>78%</div> </div>
2	E	40	<div> <div>8%</div> <div>8%</div> <div>88%</div> </div>
3	C	7	<div> <div>14%</div> <div>43%</div> <div>43%</div> </div>
3	F	7	<div> <div>14%</div> <div>86%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	1014	

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
6	GOL	A	1102	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16054 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 Presequence protease, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	As	C	N	O	S			
1	A	985	7910	4	5046	1337	1483	40	0	2	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	EXPRESSION TAG	UNP Q5JRX3
A	25	HIS	-	EXPRESSION TAG	UNP Q5JRX3
A	26	HIS	-	EXPRESSION TAG	UNP Q5JRX3
A	27	HIS	-	EXPRESSION TAG	UNP Q5JRX3
A	28	HIS	-	EXPRESSION TAG	UNP Q5JRX3
A	29	HIS	-	EXPRESSION TAG	UNP Q5JRX3
A	30	HIS	-	EXPRESSION TAG	UNP Q5JRX3
A	31	ALA	-	EXPRESSION TAG	UNP Q5JRX3
A	32	ALA	-	EXPRESSION TAG	UNP Q5JRX3
A	107	GLN	GLU	ENGINEERED MUTATION	UNP Q5JRX3
A	328	VAL	ILE	SEE REMARK 999	UNP Q5JRX3
A	397	VAL	ALA	SEE REMARK 999	UNP Q5JRX3
A	1037	ARG	GLN	SEE REMARK 999	UNP Q5JRX3

- Molecule 2 is a protein called Beta-amyloid protein 40.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	9	77	52	11	14	0	0	0
2	E	5	43	31	5	7	0	0	0

- Molecule 3 is a protein called Beta-amyloid protein 40.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			20	12	4	4			
3	F	1	Total	C	N	O	0	0	0
			5	3	1	1			

- Molecule 4 is a protein called Presequence protease, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	987	Total	As	C	N	O	S	0	1	0
			7931	1	5062	1345	1483	40			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	24	MET	-	EXPRESSION TAG	UNP Q5JRX3
D	25	HIS	-	EXPRESSION TAG	UNP Q5JRX3
D	26	HIS	-	EXPRESSION TAG	UNP Q5JRX3
D	27	HIS	-	EXPRESSION TAG	UNP Q5JRX3
D	28	HIS	-	EXPRESSION TAG	UNP Q5JRX3
D	29	HIS	-	EXPRESSION TAG	UNP Q5JRX3
D	30	HIS	-	EXPRESSION TAG	UNP Q5JRX3
D	31	ALA	-	EXPRESSION TAG	UNP Q5JRX3
D	32	ALA	-	EXPRESSION TAG	UNP Q5JRX3
D	107	GLN	GLU	ENGINEERED MUTATION	UNP Q5JRX3
D	328	VAL	ILE	SEE REMARK 999	UNP Q5JRX3
D	397	VAL	ALA	SEE REMARK 999	UNP Q5JRX3
D	1037	ARG	GLN	SEE REMARK 999	UNP Q5JRX3

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

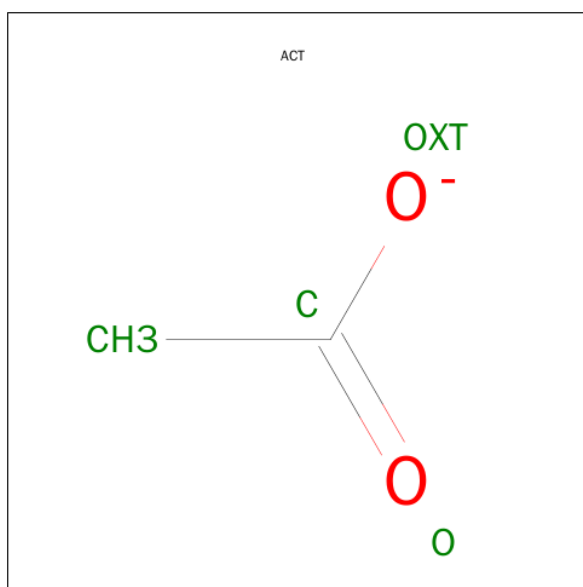
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	E	1	Total	Zn	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

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

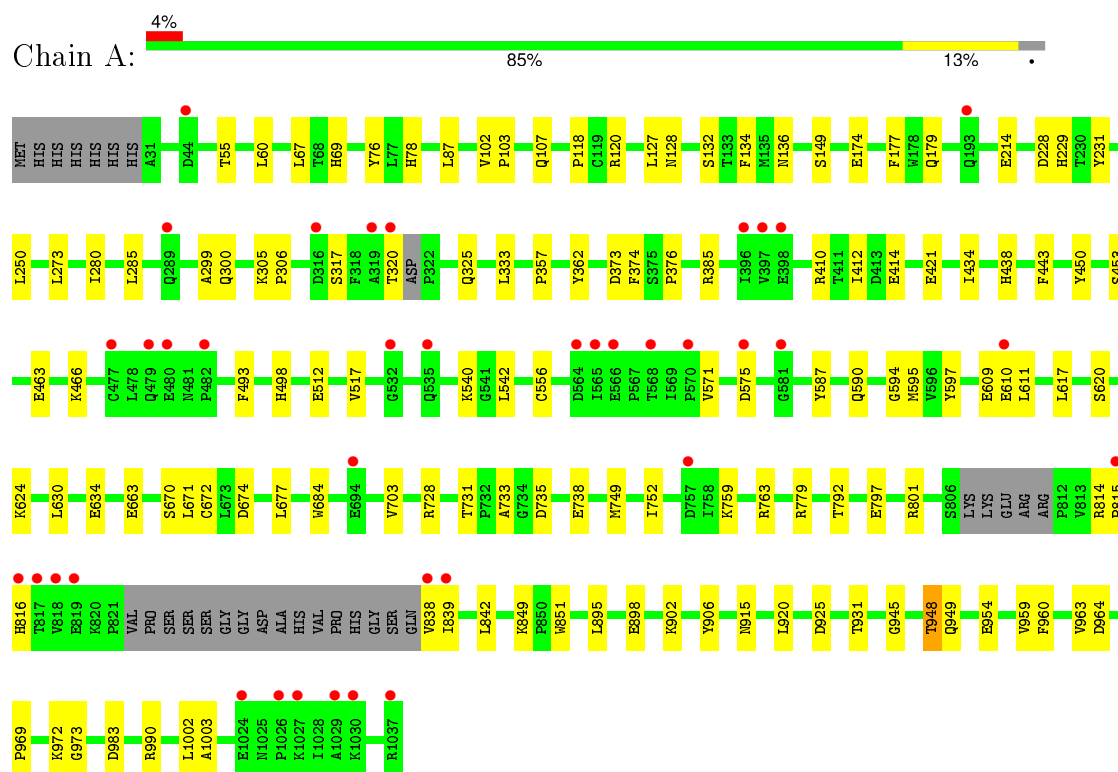
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	11	Total	O	0	0
			11	11		
8	D	28	Total	O	0	0
			28	28		
8	E	1	Total	O	0	0
			1	1		

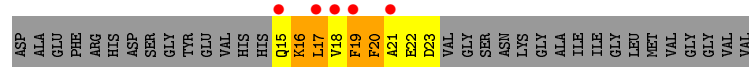
### 3 Residue-property plots [i](#)

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: Presequence protease, mitochondrial



- Molecule 2: Beta-amyloid protein 40



- Molecule 2: Beta-amyloid protein 40



- Molecule 3: Beta-amyloid protein 40



Chain C:  14% 43% 43%




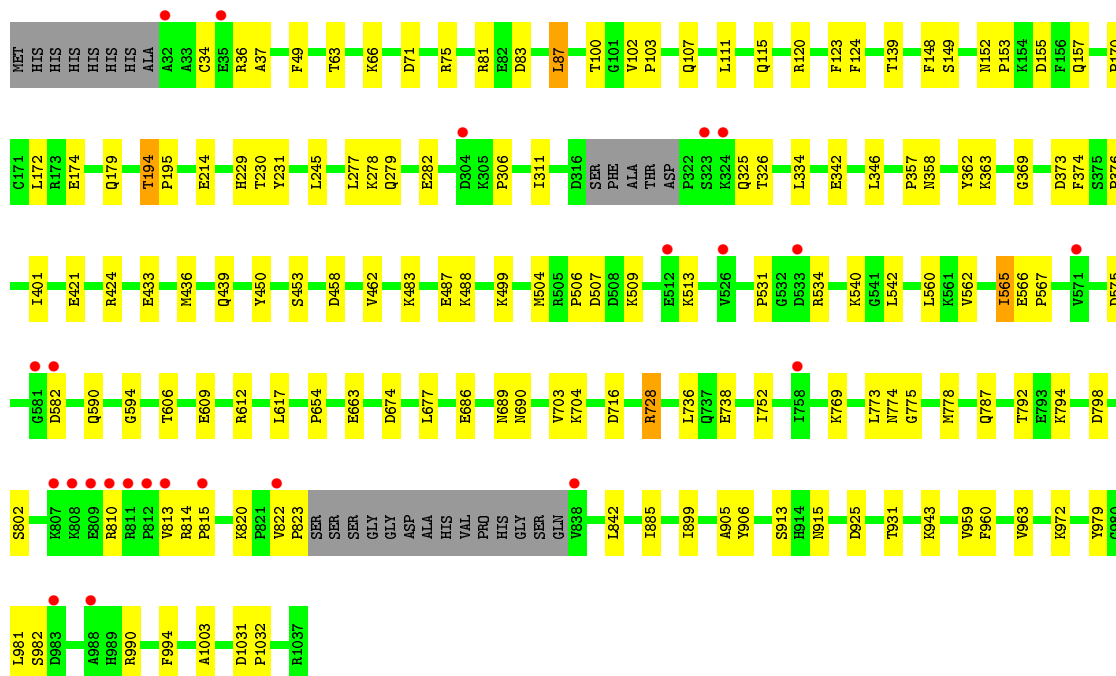
- Molecule 3: Beta-amyloid protein 40

Chain F:  14% 86%



- Molecule 4: Presequence protease, mitochondrial

Chain D:  2% 83% 14%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	247.28 Å   86.18 Å   158.61 Å 90.00°   127.56°   90.00°	Depositor
Resolution (Å)	39.62 – 2.70 39.62 – 2.70	Depositor EDS
% Data completeness (in resolution range)	88.0 (39.62-2.70) 88.4 (39.62-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.29 (at 2.69 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.191 , 0.232 0.207 , 0.241	Depositor DCC
$R_{free}$ test set	3371 reflections (5.52%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.6	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 51.0	EDS
Estimated twinning fraction	0.015 for -h-2*k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 67541 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	16054	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, CAS, ACT, MLZ, MLY

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	0.26	0/7877	0.43	0/10688
2	B	0.46	0/78	1.00	0/103
2	E	0.63	0/44	1.14	0/58
4	D	0.26	0/7885	0.43	1/10709 (0.0%)
All	All	0.26	0/15884	0.44	1/21558 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	87	LEU	CA-CB-CG	5.35	127.59	115.30

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	7910	0	7788	92	0
2	B	77	0	73	31	0
2	E	43	0	37	9	0
3	C	20	0	9	5	0
3	F	5	0	3	3	0
4	D	7931	0	7847	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	E	1	0	0	0	0
6	A	6	0	8	0	0
6	D	12	0	16	0	0
7	A	8	0	6	1	0
8	A	11	0	0	1	0
8	D	28	0	0	5	0
8	E	1	0	0	0	0
All	All	16054	0	15787	217	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 7.

All (217) 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)
2:B:16:LYS:HD3	2:B:17:LEU:CD1	1.62	1.27
4:D:575:ASP:OD2	8:D:1218:HOH:O	1.54	1.20
2:B:16:LYS:HG2	2:B:17:LEU:N	1.57	1.13
4:D:562:VAL:O	4:D:565:ILE:HG22	1.54	1.06
2:B:16:LYS:HG2	2:B:17:LEU:H	0.92	1.04
2:B:16:LYS:HD3	2:B:17:LEU:HD12	1.05	1.01
4:D:450:TYR:O	3:F:1:UNK:C	2.09	1.01
4:D:325:GLN:HE21	4:D:506:PRO:HG2	1.25	0.99
2:E:22:GLU:N	2:E:22:GLU:OE1	1.97	0.98
1:A:132:SER:OG	2:B:15:GLN:NE2	1.98	0.96
1:A:134:PHE:CE1	2:B:17:LEU:HD22	2.01	0.95
1:A:320:THR:O	1:A:325:GLN:NE2	2.09	0.86
4:D:686:GLU:OE2	4:D:690:ASN:ND2	2.07	0.86
4:D:565:ILE:HD12	4:D:994:PHE:HZ	1.41	0.86
2:B:16:LYS:CD	2:B:17:LEU:CD1	2.50	0.85
1:A:609:GLU:OE2	1:A:814:ARG:NH2	2.10	0.85
4:D:565:ILE:HD12	4:D:994:PHE:CZ	2.12	0.84
2:B:16:LYS:HD3	2:B:17:LEU:HD13	1.59	0.83
3:C:6:UNK:CB	3:C:7:UNK:HA	2.09	0.82
4:D:453:SER:OG	3:F:1:UNK:CB	2.27	0.82
2:B:16:LYS:CD	2:B:17:LEU:HD12	2.01	0.82
1:A:410:ARG:NH1	1:A:414:GLU:OE2	2.14	0.80
2:B:16:LYS:CG	2:B:17:LEU:N	2.37	0.80
1:A:134:PHE:HE1	2:B:17:LEU:HD22	1.43	0.80
1:A:925:ASP:OD2	1:A:931:THR:OG1	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:609:GLU:OE2	4:D:814:ARG:NH2	2.12	0.79
1:A:728:ARG:HD3	1:A:738:GLU:HG2	1.63	0.79
4:D:925:ASP:OD2	4:D:931:THR:OG1	2.01	0.77
4:D:509:LYS:HB2	4:D:513:LYS:NZ	2.00	0.76
1:A:120:ARG:NH2	1:A:179:GLN:OE1	2.18	0.75
4:D:71:ASP:OD2	8:D:1217:HOH:O	2.05	0.75
4:D:565:ILE:HD13	4:D:566:GLU:O	1.86	0.74
4:D:325:GLN:HE21	4:D:506:PRO:CG	1.98	0.74
1:A:797:GLU:OE2	1:A:801:ARG:NH2	2.21	0.73
4:D:421:GLU:OE1	8:D:1216:HOH:O	2.07	0.73
1:A:1003:ALA:HB2	4:D:542:LEU:HD21	1.71	0.71
1:A:317:SER:OG	8:A:1211:HOH:O	2.08	0.71
2:B:16:LYS:CD	2:B:17:LEU:HD13	2.19	0.70
1:A:214:GLU:HG2	1:A:376:PRO:HG3	1.74	0.69
4:D:565:ILE:CD1	4:D:566:GLU:O	2.42	0.68
4:D:565:ILE:CD1	4:D:994:PHE:HZ	2.07	0.66
2:B:15:GLN:N	2:B:16:LYS:HB2	2.10	0.66
2:E:19:PHE:O	2:E:19:PHE:HD1	1.79	0.66
4:D:325:GLN:NE2	4:D:506:PRO:HG2	2.07	0.65
4:D:565:ILE:HD13	4:D:565:ILE:C	2.16	0.65
1:A:915[B]:ASN:OD1	1:A:915[B]:ASN:N	2.30	0.64
4:D:342:GLU:OE2	4:D:488:MLY:HE2	1.97	0.64
1:A:134:PHE:CZ	2:B:17:LEU:HD22	2.33	0.64
4:D:306:PRO:HB3	4:D:499:LYS:HB3	1.78	0.64
2:B:21:ALA:HB1	2:B:22:GLU:HB3	1.80	0.64
4:D:509:LYS:HB2	4:D:513:LYS:HZ2	1.62	0.63
4:D:107:GLN:NE2	2:E:20:PHE:HB2	2.14	0.63
4:D:913:SER:OG	4:D:915:ASN:OD1	2.11	0.62
1:A:450:TYR:O	3:C:1:UNK:C	2.49	0.61
4:D:325:GLN:NE2	4:D:506:PRO:CG	2.63	0.60
1:A:964:ASP:OD1	1:A:990:ARG:NH1	2.32	0.60
1:A:731:THR:HG22	1:A:733:ALA:H	1.66	0.60
4:D:794:MLY:HH12	4:D:798:ASP:OD2	2.01	0.60
1:A:663:GLU:HB2	1:A:842:LEU:HD22	1.84	0.60
1:A:964:ASP:CG	1:A:990:ARG:HH12	2.06	0.59
4:D:562:VAL:O	4:D:565:ILE:CG2	2.42	0.58
1:A:434:ILE:HG23	1:A:595:MET:HE1	1.86	0.58
1:A:595:MET:HE3	1:A:671:LEU:HD11	1.87	0.57
4:D:703:VAL:HG11	4:D:752:ILE:HG22	1.87	0.57
4:D:194:THR:HG22	4:D:195:PRO:HD2	1.88	0.56
4:D:774:ASN:HB3	8:D:1227:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:66:LYS:HD2	4:D:462:VAL:HG21	1.88	0.56
4:D:509:LYS:HB2	4:D:513:LYS:HZ1	1.70	0.56
2:E:20:PHE:N	2:E:20:PHE:CD1	2.73	0.56
4:D:663:GLU:HB2	4:D:842:LEU:HD22	1.88	0.56
1:A:136:ASN:HD22	2:B:17:LEU:HD23	1.71	0.56
4:D:75:ARG:NH2	4:D:458:ASP:OD1	2.38	0.55
1:A:703:VAL:HG11	1:A:752:ILE:HG22	1.88	0.55
1:A:898:GLU:OE2	1:A:902:MLY:HH12	2.07	0.55
1:A:728:ARG:HG3	1:A:735:ASP:HA	1.88	0.55
1:A:594:GLY:HA2	1:A:674:ASP:OD2	2.07	0.55
4:D:814:ARG:HG3	4:D:815:PRO:HD2	1.90	0.54
4:D:174:GLU:OE2	4:D:540:MLY:HH12	2.07	0.54
4:D:582:ASP:OD1	4:D:582:ASP:N	2.41	0.54
1:A:677:LEU:HD21	1:A:792:THR:HA	1.90	0.54
4:D:606:THR:HG21	4:D:810:ARG:HD3	1.87	0.54
1:A:107:GLN:NE2	2:B:20:PHE:HB2	2.23	0.53
1:A:463:GLU:OE2	1:A:466:MLY:HH12	2.08	0.53
3:C:6:UNK:CB	3:C:7:UNK:CA	2.86	0.53
4:D:373:ASP:OD1	4:D:374:PHE:N	2.39	0.53
4:D:325:GLN:HG3	4:D:506:PRO:HG3	1.90	0.53
1:A:107:GLN:HE22	2:B:20:PHE:HB2	1.73	0.53
4:D:606:THR:HA	4:D:813:VAL:HG23	1.91	0.53
1:A:575:ASP:OD1	1:A:587:TYR:HB2	2.08	0.53
4:D:594:GLY:HA2	4:D:674:ASP:OD2	2.08	0.53
1:A:102:VAL:HG13	1:A:103:PRO:HD3	1.91	0.52
4:D:107:GLN:OE1	4:D:139:THR:OG1	2.19	0.52
4:D:214:GLU:HG2	4:D:376:PRO:HG3	1.92	0.52
4:D:120:ARG:NH2	4:D:179:GLN:OE1	2.41	0.51
1:A:450:TYR:CZ	3:C:6:UNK:CB	2.94	0.51
1:A:948:THR:OG1	1:A:949:GLN:N	2.43	0.51
1:A:906:TYR:CZ	2:B:19:PHE:HB2	2.46	0.51
1:A:895:LEU:HD11	1:A:920:LEU:HD23	1.93	0.51
1:A:542:LEU:HD21	4:D:1003:ALA:HB2	1.92	0.51
1:A:136:ASN:HD22	2:B:17:LEU:HB3	1.76	0.51
1:A:132:SER:OG	2:B:15:GLN:O	2.08	0.50
1:A:797:GLU:HG2	1:A:801:ARG:NH1	2.26	0.50
4:D:107:GLN:HE21	2:E:20:PHE:HB2	1.75	0.50
4:D:775:GLY:HA2	4:D:778:MET:HE2	1.92	0.50
1:A:412:ILE:HD13	1:A:493:PHE:HB3	1.92	0.50
1:A:174:GLU:OE1	1:A:540:LYS:NZ	2.38	0.50
4:D:565:ILE:HD11	4:D:990:ARG:NH2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:507:ASP:CG	4:D:513:LYS:HZ3	2.15	0.50
1:A:610:GLU:HG3	1:A:611:LEU:HG	1.94	0.50
4:D:960:PHE:HA	4:D:963:VAL:HG22	1.94	0.50
4:D:677:LEU:HD21	4:D:792:THR:HA	1.93	0.49
1:A:357:PRO:HA	1:A:362:TYR:CD1	2.47	0.49
1:A:128:ASN:HB3	1:A:954:GLU:HB3	1.95	0.49
4:D:590:GLN:NE2	4:D:972:MLY:HG3	2.28	0.49
2:E:19:PHE:C	2:E:19:PHE:HD1	2.16	0.48
1:A:60:LEU:HD22	1:A:443:PHE:HZ	1.79	0.48
2:E:19:PHE:CD1	2:E:19:PHE:C	2.87	0.48
1:A:849:LYS:HE2	1:A:851:TRP:HZ3	1.78	0.48
4:D:100:THR:HB	4:D:245:LEU:HB2	1.96	0.48
1:A:134:PHE:HE1	2:B:17:LEU:CD2	2.21	0.48
4:D:229:HIS:O	4:D:231:TYR:N	2.46	0.48
4:D:617:LEU:HD11	4:D:703:VAL:HG22	1.95	0.48
1:A:280:ILE:HG22	1:A:285:LEU:HD22	1.95	0.48
4:D:483:LYS:O	4:D:487:GLU:HG3	2.13	0.47
4:D:34:CYS:HG	4:D:63:THR:HG1	1.61	0.47
4:D:36:ARG:HG3	4:D:37:ALA:N	2.30	0.47
1:A:838:VAL:HG23	1:A:839:ILE:HD12	1.96	0.47
1:A:597:TYR:CE2	1:A:671:LEU:HD13	2.49	0.47
1:A:609:GLU:OE2	1:A:814:ARG:CZ	2.62	0.47
4:D:769:MLY:HG2	4:D:773:LEU:HD12	1.96	0.47
1:A:438:HIS:ND1	1:A:597:TYR:OH	2.38	0.47
1:A:617:LEU:HD13	1:A:749:MET:HE1	1.97	0.47
1:A:759:LYS:O	1:A:763:ARG:HG3	2.14	0.47
4:D:433:GLU:HA	4:D:436:MET:HE2	1.95	0.47
4:D:728:ARG:CZ	4:D:738:GLU:HG2	2.45	0.47
4:D:565:ILE:HD12	4:D:994:PHE:CE1	2.49	0.47
1:A:55:THR:HG21	1:A:466:MLY:HE3	1.96	0.47
1:A:373:ASP:OD1	1:A:374:PHE:N	2.45	0.46
4:D:565:ILE:HD13	4:D:566:GLU:C	2.34	0.46
4:D:823:PRO:HB2	4:D:982:SER:HB3	1.98	0.46
4:D:507:ASP:OD2	4:D:513:LYS:NZ	2.45	0.46
1:A:512:GLU:N	1:A:512:GLU:OE1	2.47	0.46
4:D:357:PRO:HA	4:D:362:TYR:CG	2.51	0.46
1:A:229:HIS:O	1:A:231:TYR:N	2.47	0.46
1:A:333:LEU:HD22	1:A:498:HIS:CE1	2.50	0.46
4:D:689:ASN:ND2	4:D:802:SER:O	2.45	0.46
4:D:654:PRO:HG2	4:D:915:ASN:HB3	1.97	0.46
1:A:228:ASP:OD2	1:A:300:GLN:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:102:VAL:HG13	4:D:103:PRO:HD3	1.97	0.46
4:D:358:ASN:HB3	4:D:424:ARG:HD2	1.99	0.45
1:A:87:LEU:HD12	1:A:149:SER:HB3	1.97	0.45
1:A:78:HIS:CG	1:A:273:LEU:HD13	2.51	0.45
1:A:779:ARG:NH1	7:A:1104:ACT:H2	2.32	0.45
1:A:320:THR:C	1:A:325:GLN:NE2	2.69	0.45
4:D:612:ARG:HD2	4:D:736:LEU:HD11	1.98	0.45
2:B:22:GLU:HB2	2:B:23:ASP:H	1.54	0.45
4:D:357:PRO:HA	4:D:362:TYR:CD1	2.51	0.45
1:A:731:THR:HG22	1:A:733:ALA:N	2.30	0.45
4:D:531:PRO:HA	4:D:534:ARG:HG2	1.98	0.45
4:D:334:LEU:HD13	4:D:346:LEU:HD23	1.99	0.45
1:A:127:LEU:HD22	2:B:15:GLN:HG3	1.99	0.44
1:A:132:SER:HG	2:B:15:GLN:NE2	2.13	0.44
1:A:972:LYS:HA	1:A:973:GLY:HA2	1.58	0.44
4:D:278:LYS:NZ	4:D:282:GLU:OE2	2.50	0.44
1:A:177:PHE:CD1	1:A:250:LEU:HD22	2.51	0.44
4:D:728:ARG:NH1	4:D:738:GLU:HG2	2.31	0.44
4:D:124:PHE:CE2	2:E:20:PHE:CE1	3.06	0.44
1:A:67:LEU:HB2	1:A:76:TYR:HB3	1.99	0.44
1:A:571:VAL:HG23	1:A:983:ASP:OD2	2.18	0.44
1:A:299:ALA:N	1:A:385:ARG:NH1	2.66	0.44
4:D:325:GLN:HG3	4:D:506:PRO:CG	2.47	0.44
1:A:590:GLN:HB3	1:A:969:PRO:HB3	1.99	0.44
1:A:453:SER:OG	3:C:1:UNK:CB	2.66	0.43
1:A:959:VAL:O	1:A:963:VAL:HG23	2.18	0.43
1:A:815:PRO:HA	1:A:816:HIS:HA	1.49	0.43
4:D:885:ILE:HD13	4:D:959:VAL:HG21	2.00	0.43
1:A:597:TYR:CD2	1:A:671:LEU:HD13	2.54	0.43
4:D:979:TYR:HB2	4:D:981:LEU:HD22	2.01	0.43
1:A:69:HIS:CD2	1:A:285:LEU:HD23	2.53	0.43
4:D:899:ILE:HG22	4:D:905:ALA:HB3	2.00	0.43
4:D:157:GLN:O	4:D:279:GLN:NE2	2.49	0.43
1:A:620:SER:O	1:A:624:MLY:HH12	2.19	0.42
4:D:111:LEU:HB3	4:D:123:PHE:HB2	2.00	0.42
1:A:630:LEU:HD22	1:A:634:GLU:HB3	2.01	0.42
4:D:450:TYR:C	3:F:1:UNK:C	2.84	0.42
1:A:945:GLY:HA3	1:A:1002:LEU:HD21	2.02	0.42
4:D:311:ILE:HG13	4:D:504:MET:HG3	2.01	0.42
4:D:566:GLU:HA	4:D:567:PRO:HD3	1.81	0.42
1:A:960:PHE:O	1:A:964:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:81:ARG:NH2	4:D:439:GLN:OE1	2.53	0.42
4:D:170:PRO:HB2	4:D:172:LEU:HG	2.00	0.42
1:A:814:ARG:HA	1:A:815:PRO:HD2	1.89	0.42
4:D:83:ASP:OD2	8:D:1220:HOH:O	2.21	0.41
1:A:617:LEU:HD11	1:A:703:VAL:HG22	2.01	0.41
1:A:671:LEU:HD12	1:A:672:CYS:N	2.36	0.41
4:D:369:GLY:HA2	4:D:704:MLY:HH21	2.02	0.41
4:D:87:LEU:HD23	4:D:149:SER:HB3	2.01	0.41
4:D:943:MLY:HD3	4:D:943:MLY:HH13	1.81	0.41
1:A:136:ASN:OD1	2:B:20:PHE:HB3	2.20	0.41
4:D:820:LYS:HD3	4:D:842:LEU:HD11	2.02	0.41
2:B:18:VAL:CG2	2:B:19:PHE:N	2.83	0.41
4:D:155:ASP:HB2	4:D:560:LEU:HD11	2.03	0.41
4:D:87:LEU:HD22	4:D:148:PHE:O	2.20	0.41
1:A:134:PHE:CE1	2:B:17:LEU:HD13	2.56	0.41
2:B:16:LYS:O	2:B:17:LEU:C	2.59	0.41
2:B:21:ALA:HB1	2:B:22:GLU:CB	2.49	0.41
1:A:670:SER:CB	1:A:684:TRP:HE1	2.33	0.41
4:D:363:MLY:HH23	4:D:363:MLY:HD2	1.85	0.41
4:D:49:PHE:CD1	4:D:277:LEU:HD22	2.56	0.40
4:D:1031:ASP:HA	4:D:1032:PRO:HD3	1.85	0.40
1:A:305:LYS:HA	1:A:306:PRO:HD3	1.90	0.40
4:D:565:ILE:HD13	4:D:566:GLU:N	2.36	0.40
4:D:906:TYR:OH	2:E:21:ALA:HB2	2.21	0.40
1:A:118:PRO:HG2	1:A:556:CAS:CE2	2.51	0.40
2:B:21:ALA:HB1	2:B:22:GLU:CA	2.52	0.40
4:D:326:THR:HG21	4:D:401:ILE:HD11	2.03	0.40
4:D:152:ASN:HA	4:D:153:PRO:HD2	1.97	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	958/1014 (94%)	933 (97%)	25 (3%)	0	100	100
2	B	7/40 (18%)	3 (43%)	4 (57%)	0	100	100
2	E	3/40 (8%)	3 (100%)	0	0	100	100
4	D	960/1014 (95%)	933 (97%)	26 (3%)	1 (0%)	56	83
All	All	1928/2108 (92%)	1872 (97%)	55 (3%)	1 (0%)	56	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	230	THR

### 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	857/880 (97%)	854 (100%)	3 (0%)	93	98
2	B	8/31 (26%)	4 (50%)	4 (50%)	0	0
2	E	4/31 (13%)	1 (25%)	3 (75%)	0	0
4	D	859/879 (98%)	852 (99%)	7 (1%)	86	96
All	All	1728/1821 (95%)	1711 (99%)	17 (1%)	82	94

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	421	GLU
1	A	517	VAL
1	A	948	THR
2	B	16	LYS
2	B	17	LEU
2	B	19	PHE
2	B	20	PHE
4	D	115	GLN
4	D	194	THR
4	D	565	ILE

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Mol	Chain	Res	Type
4	D	716	ASP
4	D	728	ARG
4	D	787	GLN
4	D	822	VAL
2	E	19	PHE
2	E	20	PHE
2	E	22	GLU

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	690	ASN
1	A	1025	ASN
2	B	15	GLN
4	D	325	GLN
4	D	852	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

43 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CAS	A	112	1	5,8,9	1.18	0	2,9,11	1.73	1 (50%)
1	CAS	A	171	1	5,8,9	1.28	0	2,9,11	1.67	1 (50%)
1	MLY	A	199	1	9,10,11	0.47	0	9,11,13	0.92	0
1	MLY	A	251	1	9,10,11	0.51	0	9,11,13	0.93	0
1	MLY	A	278	1	9,10,11	0.47	0	9,11,13	0.91	0
1	CAS	A	34	1	5,8,9	1.18	0	2,9,11	1.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	A	363	1	9,10,11	0.51	0	9,11,13	0.93	0
1	MLY	A	41	1	9,10,11	0.51	0	9,11,13	0.88	0
1	MLY	A	431	1	9,10,11	0.50	0	9,11,13	0.91	0
1	MLY	A	466	1	9,10,11	0.47	0	9,11,13	0.99	0
1	MLY	A	513	1	9,10,11	0.47	0	9,11,13	1.03	0
1	MLY	A	525	1	9,10,11	0.46	0	9,11,13	0.94	0
1	CAS	A	556	1	5,8,9	0.91	0	2,9,11	1.45	1 (50%)
1	MLY	A	624	1	9,10,11	0.53	0	9,11,13	0.88	0
1	MLY	A	642	1	9,10,11	0.48	0	9,11,13	0.93	0
1	MLY	A	66	1	9,10,11	0.52	0	9,11,13	0.86	0
1	MLY	A	854	1	9,10,11	0.45	0	9,11,13	1.09	1 (11%)
1	MLY	A	902	1	9,10,11	0.49	0	9,11,13	0.85	0
1	MLY	A	911	1	9,10,11	0.48	0	9,11,13	0.91	0
1	MLY	A	943	1	9,10,11	0.53	0	9,11,13	0.82	0
1	MLZ	A	946	1	8,9,10	1.34	1 (12%)	7,9,11	1.07	0
4	MLY	D	116	4	9,10,11	0.47	0	9,11,13	1.01	0
4	MLY	D	125	4	9,10,11	0.52	0	9,11,13	0.94	1 (11%)
4	MLY	D	207	4	9,10,11	0.52	0	9,11,13	0.90	0
4	MLY	D	287	4	9,10,11	0.51	0	9,11,13	1.00	0
4	MLY	D	290	4	9,10,11	0.48	0	9,11,13	0.92	0
4	MLY	D	363	4	9,10,11	0.51	0	9,11,13	0.91	0
4	MLY	D	488	4	9,10,11	0.49	0	9,11,13	0.95	0
4	MLY	D	525	4	9,10,11	1.12	1 (11%)	9,11,13	1.30	1 (11%)
4	MLY	D	540	4	9,10,11	0.52	0	9,11,13	0.87	0
4	CAS	D	556	4	5,8,9	1.18	0	2,9,11	1.54	0
4	MLY	D	624	4	9,10,11	0.54	0	9,11,13	0.97	1 (11%)
4	MLY	D	642	4	9,10,11	0.44	0	9,11,13	0.98	1 (11%)
4	MLY	D	704	4	9,10,11	0.47	0	9,11,13	0.90	0
4	MLY	D	764	4	9,10,11	0.52	0	9,11,13	0.89	0
4	MLY	D	769	4	9,10,11	0.58	0	9,11,13	0.82	0
4	MLY	D	794	4	9,10,11	0.64	0	9,11,13	0.81	0
4	MLY	D	854	4	9,10,11	0.51	0	9,11,13	1.03	0
4	MLY	D	884	4	9,10,11	0.49	0	9,11,13	0.90	0
4	MLY	D	937	4	9,10,11	0.52	0	9,11,13	0.92	0
4	MLY	D	943	4	9,10,11	0.55	0	9,11,13	0.88	0
4	MLY	D	946	4	9,10,11	0.48	0	9,11,13	0.88	0
4	MLY	D	972	4	9,10,11	0.50	0	9,11,13	0.94	1 (11%)

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
1	CAS	A	112	1	-	0/0/7/9	0/0/0/0
1	CAS	A	171	1	-	0/0/7/9	0/0/0/0
1	MLY	A	199	1	-	0/7/9/11	0/0/0/0
1	MLY	A	251	1	-	0/7/9/11	0/0/0/0
1	MLY	A	278	1	-	0/7/9/11	0/0/0/0
1	CAS	A	34	1	-	0/0/7/9	0/0/0/0
1	MLY	A	363	1	-	0/7/9/11	0/0/0/0
1	MLY	A	41	1	-	0/7/9/11	0/0/0/0
1	MLY	A	431	1	-	0/7/9/11	0/0/0/0
1	MLY	A	466	1	-	0/7/9/11	0/0/0/0
1	MLY	A	513	1	-	0/7/9/11	0/0/0/0
1	MLY	A	525	1	-	0/7/9/11	0/0/0/0
1	CAS	A	556	1	-	0/0/7/9	0/0/0/0
1	MLY	A	624	1	-	0/7/9/11	0/0/0/0
1	MLY	A	642	1	-	0/7/9/11	0/0/0/0
1	MLY	A	66	1	-	0/7/9/11	0/0/0/0
1	MLY	A	854	1	-	0/7/9/11	0/0/0/0
1	MLY	A	902	1	-	0/7/9/11	0/0/0/0
1	MLY	A	911	1	-	0/7/9/11	0/0/0/0
1	MLY	A	943	1	-	0/7/9/11	0/0/0/0
1	MLZ	A	946	1	-	0/6/8/10	0/0/0/0
4	MLY	D	116	4	-	0/7/9/11	0/0/0/0
4	MLY	D	125	4	-	0/7/9/11	0/0/0/0
4	MLY	D	207	4	-	0/7/9/11	0/0/0/0
4	MLY	D	287	4	-	0/7/9/11	0/0/0/0
4	MLY	D	290	4	-	0/7/9/11	0/0/0/0
4	MLY	D	363	4	-	0/7/9/11	0/0/0/0
4	MLY	D	488	4	-	0/7/9/11	0/0/0/0
4	MLY	D	525	4	-	0/7/9/11	0/0/0/0
4	MLY	D	540	4	-	0/7/9/11	0/0/0/0
4	CAS	D	556	4	-	0/0/7/9	0/0/0/0
4	MLY	D	624	4	-	0/7/9/11	0/0/0/0
4	MLY	D	642	4	-	0/7/9/11	0/0/0/0
4	MLY	D	704	4	-	0/7/9/11	0/0/0/0
4	MLY	D	764	4	-	0/7/9/11	0/0/0/0
4	MLY	D	769	4	-	0/7/9/11	0/0/0/0
4	MLY	D	794	4	-	0/7/9/11	0/0/0/0
4	MLY	D	854	4	-	0/7/9/11	0/0/0/0
4	MLY	D	884	4	-	0/7/9/11	0/0/0/0
4	MLY	D	937	4	-	0/7/9/11	0/0/0/0
4	MLY	D	943	4	-	0/7/9/11	0/0/0/0
4	MLY	D	946	4	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MLY	D	972	4	-	0/7/9/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	525	MLY	CB-CA	-2.90	1.50	1.53
1	A	946	MLZ	CB-CA	-2.05	1.51	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	525	MLY	O-C-CA	-2.46	119.08	125.49
1	A	171	CAS	O-C-CA	-2.28	119.56	125.49
1	A	112	CAS	O-C-CA	-2.23	119.69	125.49
4	D	624	MLY	O-C-CA	-2.09	120.05	125.49
4	D	642	MLY	O-C-CA	-2.08	120.06	125.49
1	A	556	CAS	O-C-CA	-2.04	120.17	125.49
4	D	125	MLY	O-C-CA	-2.04	120.18	125.49
1	A	854	MLY	O-C-CA	-2.02	120.22	125.49
4	D	972	MLY	O-C-CA	-2.01	120.25	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	466	MLY	2	0
1	A	556	CAS	1	0
1	A	624	MLY	1	0
1	A	902	MLY	1	0
4	D	363	MLY	1	0
4	D	488	MLY	1	0
4	D	540	MLY	1	0
4	D	704	MLY	1	0
4	D	769	MLY	1	0
4	D	794	MLY	1	0
4	D	943	MLY	1	0
4	D	972	MLY	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z  > 2$
6	GOL	A	1102	-	5,5,5	0.33	0	5,5,5	0.17	0
7	ACT	A	1103	-	1,3,3	1.34	0	0,3,3	0.00	-
7	ACT	A	1104	-	1,3,3	0.03	0	0,3,3	0.00	-
6	GOL	D	1101	-	5,5,5	0.16	0	5,5,5	0.35	0
6	GOL	D	1102	-	5,5,5	0.33	0	5,5,5	0.16	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
6	GOL	A	1102	-	-	0/4/4/4	0/0/0/0
7	ACT	A	1103	-	-	0/0/0/0	0/0/0/0
7	ACT	A	1104	-	-	0/0/0/0	0/0/0/0
6	GOL	D	1101	-	-	0/4/4/4	0/0/0/0
6	GOL	D	1102	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1104	ACT	1	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	964/1014 (95%)	0.13	38 (3%) 43 43	25, 42, 66, 102	0
2	B	9/40 (22%)	2.97	5 (55%) 0 0	26, 78, 89, 91	0
2	E	5/40 (12%)	2.26	3 (60%) 0 0	71, 73, 93, 99	0
3	C	0/7	-	-	-	-
3	F	0/7	-	-	-	-
4	D	965/1014 (95%)	0.05	24 (2%) 61 61	26, 40, 65, 93	0
All	All	1943/2122 (91%)	0.11	70 (3%) 46 46	25, 41, 67, 102	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	17	LEU	8.1
4	D	512	GLU	5.8
2	B	15	GLN	5.2
4	D	838	VAL	5.0
1	A	479	GLN	4.9
1	A	575	ASP	4.7
4	D	810	ARG	4.7
1	A	398	GLU	4.6
1	A	1027	LYS	4.0
1	A	532	GLY	4.0
4	D	813	VAL	4.0
4	D	807	LYS	3.9
4	D	809	GLU	3.8
1	A	838	VAL	3.8
4	D	811	ARG	3.6
1	A	815	PRO	3.5
2	E	18	VAL	3.5
1	A	397	VAL	3.4
4	D	808	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	E	19	PHE	3.3
1	A	316	ASP	3.3
1	A	819	GLU	3.2
1	A	1029	ALA	3.1
1	A	757	ASP	3.1
2	B	19	PHE	3.0
1	A	1024	GLU	3.0
1	A	610	GLU	3.0
1	A	477	CYS	2.9
1	A	535	GLN	2.9
4	D	571	VAL	2.8
4	D	581	GLY	2.8
1	A	289	GLN	2.8
1	A	396	ILE	2.8
1	A	44	ASP	2.8
1	A	817	THR	2.7
1	A	320	THR	2.7
1	A	1030	LYS	2.7
4	D	324	LYS	2.7
1	A	1037	ARG	2.6
4	D	35	GLU	2.6
1	A	818	VAL	2.6
4	D	988	ALA	2.6
1	A	566	GLU	2.6
1	A	570	PRO	2.5
1	A	1026	PRO	2.5
4	D	323	SER	2.5
1	A	193	GLN	2.5
1	A	581	GLY	2.5
4	D	983	ASP	2.5
4	D	32	ALA	2.5
4	D	822	VAL	2.4
4	D	582	ASP	2.4
2	B	21	ALA	2.4
1	A	839	ILE	2.4
1	A	816	HIS	2.4
1	A	319	ALA	2.3
2	B	18	VAL	2.3
4	D	533	ASP	2.2
2	E	21	ALA	2.2
1	A	565	ILE	2.2
1	A	482	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	564	ASP	2.2
4	D	526	VAL	2.2
1	A	480	GLU	2.1
4	D	758	ILE	2.1
4	D	815	PRO	2.1
1	A	568	THR	2.1
1	A	694	GLU	2.1
4	D	304	ASP	2.0
4	D	812	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
4	MLY	D	525	11/12	0.88	0.31	-	20,20,20,20	0
1	MLZ	A	946	10/11	0.95	0.15	-	35,40,53,54	0
1	MLY	A	66	11/12	0.96	0.22	-	22,35,61,63	0
1	MLY	A	902	11/12	0.93	0.17	-	27,32,45,51	0
4	MLY	D	937	11/12	0.91	0.20	-	26,31,48,54	0
1	CAS	A	556	9/10	0.89	0.29	-	38,62,116,225	0
4	MLY	D	764	11/12	0.96	0.11	-	38,47,51,56	0
1	MLY	A	624	11/12	0.96	0.13	-	29,33,38,56	0
4	MLY	D	287	11/12	0.96	0.18	-	28,34,44,45	0
1	MLY	A	911	11/12	0.91	0.21	-	34,40,72,73	0
1	MLY	A	363	11/12	0.92	0.15	-	34,39,49,50	0
1	MLY	A	41	11/12	0.93	0.19	-	28,36,48,50	0
1	MLY	A	525	11/12	0.94	0.20	-	38,42,57,61	0
4	MLY	D	624	11/12	0.93	0.18	-	26,34,42,47	0
1	MLY	A	251	11/12	0.96	0.20	-	34,39,49,54	0
1	MLY	A	943	11/12	0.93	0.16	-	30,41,64,66	0
1	MLY	A	513	11/12	0.89	0.33	-	43,53,59,59	0
1	CAS	A	171	9/10	0.82	0.25	-	33,47,64,174	0
4	MLY	D	642	11/12	0.94	0.18	-	32,40,47,51	0
4	MLY	D	972	11/12	0.81	0.29	-	37,54,67,68	0
1	MLY	A	466	11/12	0.94	0.14	-	42,51,59,64	0
1	CAS	A	112	9/10	0.94	0.18	-	44,46,70,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	A	854	11/12	0.94	0.21	-	42,44,51,51	0
4	MLY	D	884	11/12	0.94	0.19	-	24,34,44,55	0
4	MLY	D	794	11/12	0.88	0.21	-	39,47,69,71	0
4	MLY	D	125	11/12	0.95	0.17	-	27,34,52,57	0
4	MLY	D	854	11/12	0.95	0.16	-	27,37,52,53	0
1	MLY	A	431	11/12	0.91	0.19	-	29,37,60,62	0
4	MLY	D	363	11/12	0.89	0.17	-	28,38,55,60	0
4	MLY	D	290	11/12	0.91	0.19	-	33,46,56,59	0
4	MLY	D	946	11/12	0.94	0.17	-	32,39,56,60	0
4	MLY	D	116	11/12	0.94	0.15	-	23,33,45,50	0
4	MLY	D	769	11/12	0.96	0.27	-	36,44,56,60	0
4	MLY	D	207	11/12	0.95	0.17	-	33,40,58,60	0
4	MLY	D	943	11/12	0.94	0.15	-	28,33,52,61	0
1	CAS	A	34	9/10	0.80	0.18	-	44,50,84,149	0
4	CAS	D	556	9/10	0.86	0.32	-	47,57,84,151	0
1	MLY	A	278	11/12	0.94	0.24	-	29,36,54,58	0
4	MLY	D	540	11/12	0.96	0.25	-	31,38,51,54	0
4	MLY	D	488	11/12	0.94	0.17	-	39,43,55,60	0
1	MLY	A	642	11/12	0.95	0.14	-	27,37,40,46	0
1	MLY	A	199	11/12	0.94	0.18	-	31,34,53,67	0
4	MLY	D	704	11/12	0.91	0.18	-	32,38,71,71	0

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

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( $\text{\AA}^2$ )	Q<0.9
6	GOL	A	1102	6/6	0.61	0.26	4.85	48,61,72,75	0
7	ACT	A	1104	4/4	0.71	0.27	0.91	33,59,60,65	0
5	ZN	A	1101	1/1	0.99	0.13	-1.91	44,44,44,44	0
5	ZN	E	101	1/1	0.99	0.11	-1.95	45,45,45,45	0
6	GOL	D	1101	6/6	0.76	0.21	-	56,65,70,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	D	1102	6/6	0.76	0.24	-	44,58,58,65	0
7	ACT	A	1103	4/4	0.47	0.42	-	50,73,77,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.