



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:07 PM GMT

PDB ID : 4BHT  
Title : Structural Determinants of Cofactor Specificity and Domain Flexibility in Bacterial Glutamate Dehydrogenases  
Authors : Oliveira, T.; Sharkey, M.; Engel, P.; Khan, A.  
Deposited on : 2013-04-06  
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

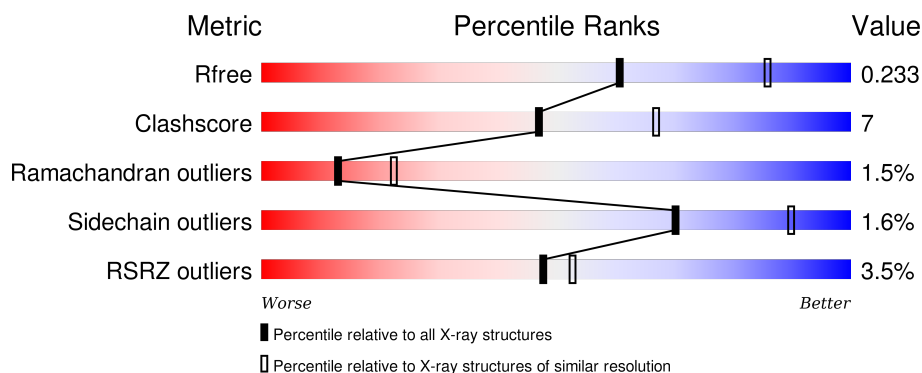
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	447	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	B	447	<div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	C	447	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	D	447	<div> <div>17%</div> <div>72%</div> <div>19%</div> <div>5%</div> <div>.</div> <div>.</div> </div>
1	E	447	<div> <div>2%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	447	 % 93% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	1450	-	-	-	X
2	GOL	A	1451	-	-	-	X
2	GOL	A	1452	-	-	-	X
2	GOL	A	1453	-	-	-	X
2	GOL	A	1454	-	-	X	X
2	GOL	D	1448	-	-	-	X
2	GOL	D	1449	-	-	-	X
2	GOL	E	1448	-	-	-	X
2	GOL	E	1449	-	-	-	X
2	GOL	E	1450	-	-	-	X
2	GOL	F	1448	-	-	-	X
3	EPE	C	1451	-	-	X	X
4	PG4	E	1451	-	-	X	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 41397 atoms, of which 20253 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 NADP-SPECIFIC GLUTAMATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	H	N	O	S	0	4	0
			6752	2136	3362	597	636	21			
1	B	442	Total	C	H	N	O	S	0	1	0
			6719	2125	3346	595	632	21			
1	C	442	Total	C	H	N	O	S	0	1	0
			6717	2124	3345	595	632	21			
1	D	439	Total	C	H	N	O	S	0	1	0
			6684	2113	3330	594	626	21			
1	E	442	Total	C	H	N	O	S	0	0	0
			6706	2121	3339	594	631	21			
1	F	442	Total	C	H	N	O	S	0	2	0
			6732	2129	3353	597	632	21			

- Molecule 2 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
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	E	1	Total	C	H	O	0	0
			14	3	8	3		
2	E	1	Total	C	H	O	0	0
			14	3	8	3		
2	E	1	Total	C	H	O	0	0
			14	3	8	3		
2	F	1	Total	C	H	O	0	0
			14	3	8	3		
2	F	1	Total	C	H	O	0	0
			13	3	7	3		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	H	O	0	0
			31	8	18	5		

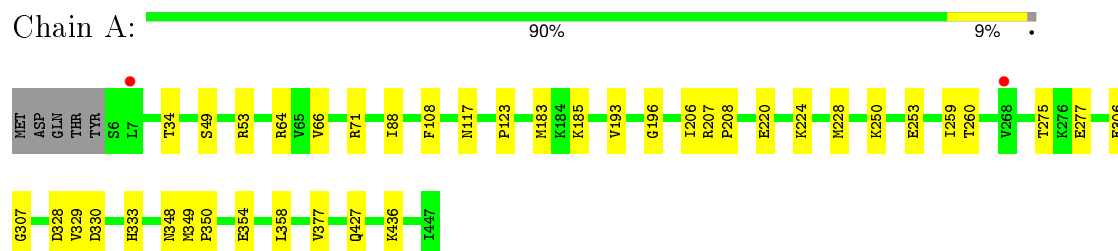
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	160	Total 160	O 160	0	0
5	B	151	Total 151	O 151	0	0
5	C	160	Total 160	O 160	0	0
5	D	103	Total 103	O 103	0	0
5	E	93	Total 93	O 93	0	0
5	F	106	Total 106	O 106	0	0

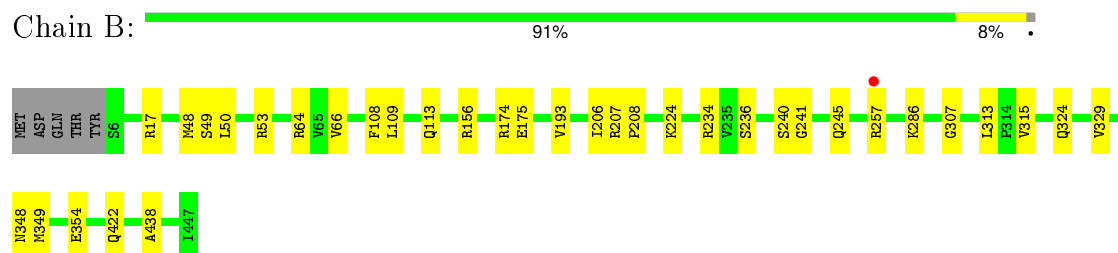
### 3 Residue-property plots [i](#)

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.

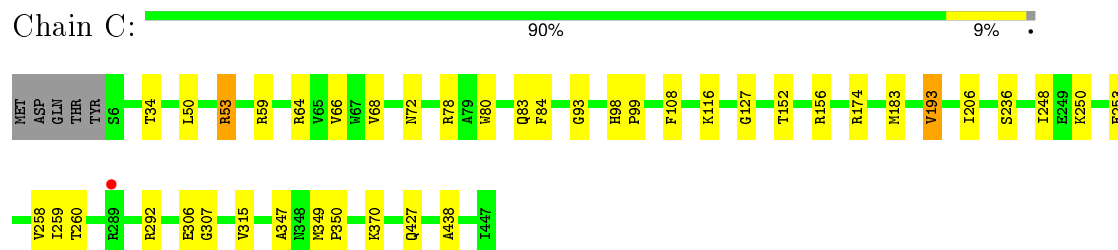
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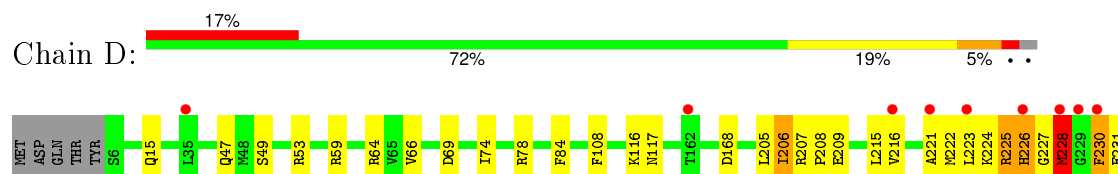
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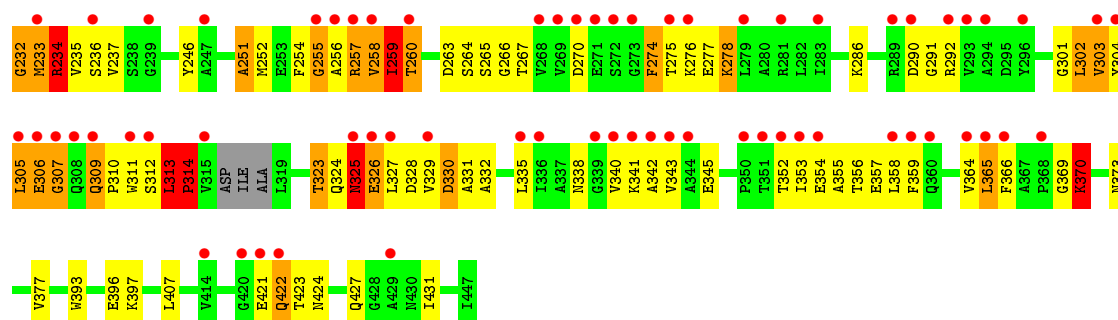
#### • Molecule 1: NADP-SPECIFIC GLUTAMATE DEHYDROGENASE



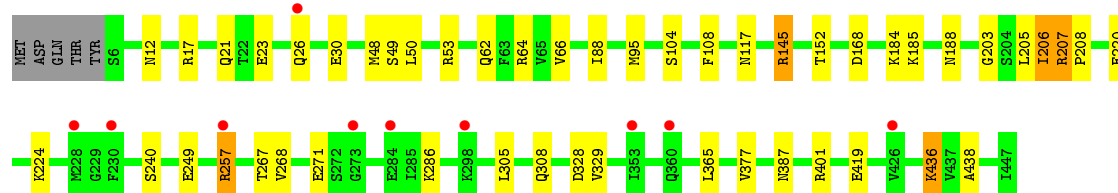
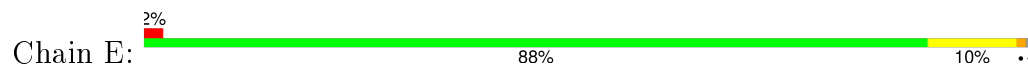
#### • Molecule 1: NADP-SPECIFIC GLUTAMATE DEHYDROGENASE



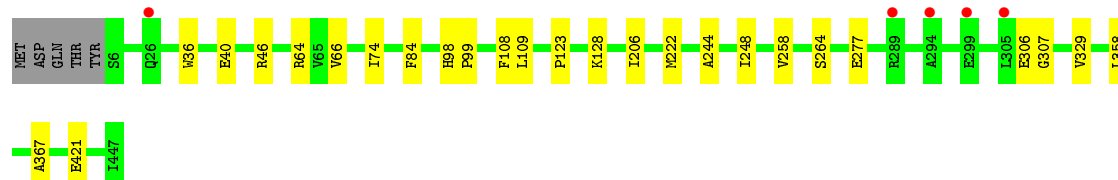




• Molecule 1: NADP-SPECIFIC GLUTAMATE DEHYDROGENASE



• Molecule 1: NADP-SPECIFIC GLUTAMATE DEHYDROGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.97Å 152.86Å 169.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.90 – 2.50 46.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.90-2.50) 99.9 (46.90-2.50)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, $R_{free}$	0.159 , 0.227 0.174 , 0.233	Depositor DCC
$R_{free}$ test set	4557 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.9	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 47.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 91084 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	41397	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	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 24.39 % 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 3.8687e-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, 0.375 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: GOL, PG4, EPE

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	0.73	0/3468	0.79	2/4680 (0.0%)
1	B	0.71	0/3441	0.79	1/4643 (0.0%)
1	C	0.74	1/3440 (0.0%)	0.80	2/4642 (0.0%)
1	D	0.73	0/3421	0.85	8/4613 (0.2%)
1	E	0.70	0/3432	0.75	3/4631 (0.1%)
1	F	0.70	0/3451	0.78	0/4657
All	All	0.72	1/20653 (0.0%)	0.79	16/27866 (0.1%)

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
1	C	0	1
1	D	0	4
1	F	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	193	VAL	CB-CG2	-6.73	1.38	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	326	GLU	C-N-CA	8.10	141.95	121.70
1	A	71	ARG	NE-CZ-NH1	7.36	123.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	69	ASP	CB-CG-OD1	6.74	124.37	118.30
1	B	193	VAL	CG1-CB-CG2	6.64	121.52	110.90
1	D	309	GLN	C-N-CD	6.33	141.68	128.40

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306	GLU	Peptide
1	C	306	GLU	Peptide
1	D	226	HIS	Peptide
1	D	230	PHE	Peptide
1	D	257	ARG	Peptide

## 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	3390	3362	3351	31	0
1	B	3373	3346	3336	32	0
1	C	3372	3345	3334	29	0
1	D	3354	3330	3320	150	0
1	E	3367	3339	3328	42	1
1	F	3379	3353	3341	19	1
2	A	42	56	56	7	0
2	C	18	24	24	5	0
2	D	18	24	24	0	0
2	E	18	24	24	0	0
2	F	12	15	16	1	0
3	C	15	17	18	8	0
4	E	13	18	18	11	0
5	A	160	0	0	4	0
5	B	151	0	0	3	0
5	C	160	0	0	4	1
5	D	103	0	0	7	0
5	E	93	0	0	10	1
5	F	106	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21144	20253	20190	302	2

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.

The worst 5 of 302 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:230:PHE:CD1	1:D:256:ALA:HB2	1.72	1.25
1:B:234:ARG:HD2	1:B:257:ARG:NH2	1.54	1.21
1:B:234:ARG:CG	1:B:257:ARG:HH21	1.56	1.19
1:B:234:ARG:CD	1:B:257:ARG:HH21	1.55	1.18
1:D:230:PHE:CE1	1:D:256:ALA:HB2	1.80	1.15

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:2125:HOH:O	5:E:2030:HOH:O[4_545]	2.12	0.08
1:E:224:LYS:HZ3	1:F:421:GLU:OE2[1_455]	1.55	0.05

## 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	444/447 (99%)	435 (98%)	7 (2%)	2 (0%)	34	55
1	B	441/447 (99%)	432 (98%)	7 (2%)	2 (0%)	34	55
1	C	441/447 (99%)	432 (98%)	7 (2%)	2 (0%)	34	55
1	D	436/447 (98%)	363 (83%)	43 (10%)	30 (7%)	1	1
1	E	440/447 (98%)	429 (98%)	10 (2%)	1 (0%)	52	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	442/447 (99%)	434 (98%)	6 (1%)	2 (0%)	34	55
All	All	2644/2682 (99%)	2525 (96%)	80 (3%)	39 (2%)	13	22

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ILE
1	B	206	ILE
1	C	206	ILE
1	D	206	ILE
1	D	226	HIS

### 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	350/351 (100%)	349 (100%)	1 (0%)	94	99
1	B	347/351 (99%)	344 (99%)	3 (1%)	84	95
1	C	347/351 (99%)	345 (99%)	2 (1%)	90	97
1	D	345/351 (98%)	324 (94%)	21 (6%)	23	42
1	E	346/351 (99%)	341 (99%)	5 (1%)	74	91
1	F	348/351 (99%)	346 (99%)	2 (1%)	90	97
All	All	2083/2106 (99%)	2049 (98%)	34 (2%)	70	90

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	274	PHE
1	D	313	LEU
1	E	436	LYS
1	D	290	ASP
1	D	47	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	73	GLN
1	D	309	GLN
1	E	242	ASN
1	C	72	ASN
1	E	188	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

20 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	$\# Z  > 2$
2	GOL	A	1448	-	5,5,5	0.69	0	5,5,5	0.96	0
2	GOL	A	1449	-	5,5,5	0.38	0	5,5,5	0.95	0
2	GOL	A	1450	-	5,5,5	0.33	0	5,5,5	0.58	0
2	GOL	A	1451	-	5,5,5	0.53	0	5,5,5	1.43	1 (20%)
2	GOL	A	1452	-	5,5,5	0.41	0	5,5,5	0.42	0
2	GOL	A	1453	-	5,5,5	0.41	0	5,5,5	0.51	0
2	GOL	A	1454	-	5,5,5	0.67	0	5,5,5	1.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	C	1448	-	5,5,5	0.66	0	5,5,5	0.62	0
2	GOL	C	1449	-	5,5,5	0.49	0	5,5,5	0.91	0
2	GOL	C	1450	-	5,5,5	0.22	0	5,5,5	0.72	0
3	EPE	C	1451	-	14,15,15	1.54	4 (28%)	18,20,20	3.11	8 (44%)
2	GOL	D	1448	-	5,5,5	0.34	0	5,5,5	0.38	0
2	GOL	D	1449	-	5,5,5	0.44	0	5,5,5	0.50	0
2	GOL	D	1450	-	5,5,5	0.38	0	5,5,5	0.73	0
2	GOL	E	1448	-	5,5,5	0.45	0	5,5,5	0.92	0
2	GOL	E	1449	-	5,5,5	0.46	0	5,5,5	0.54	0
2	GOL	E	1450	-	5,5,5	0.57	0	5,5,5	0.95	0
4	PG4	E	1451	-	12,12,12	0.97	1 (8%)	11,11,11	0.68	0
2	GOL	F	1448	-	5,5,5	0.37	0	5,5,5	0.42	0
2	GOL	F	1449	-	5,5,5	0.44	0	5,5,5	0.77	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
2	GOL	A	1448	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1449	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1450	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1451	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1452	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1453	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1454	-	-	0/4/4/4	0/0/0/0
2	GOL	C	1448	-	-	0/4/4/4	0/0/0/0
2	GOL	C	1449	-	-	0/4/4/4	0/0/0/0
2	GOL	C	1450	-	-	0/4/4/4	0/0/0/0
3	EPE	C	1451	-	-	0/9/19/19	0/1/1/1
2	GOL	D	1448	-	-	0/4/4/4	0/0/0/0
2	GOL	D	1449	-	-	0/4/4/4	0/0/0/0
2	GOL	D	1450	-	-	0/4/4/4	0/0/0/0
2	GOL	E	1448	-	-	0/4/4/4	0/0/0/0
2	GOL	E	1449	-	-	0/4/4/4	0/0/0/0
2	GOL	E	1450	-	-	0/4/4/4	0/0/0/0
4	PG4	E	1451	-	-	0/10/10/10	0/0/0/0
2	GOL	F	1448	-	-	0/4/4/4	0/0/0/0
2	GOL	F	1449	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1451	EPE	C7-N4	-2.82	1.40	1.47
3	C	1451	EPE	C7-C8	2.10	1.60	1.51
4	E	1451	PG4	O2-C2	2.20	1.51	1.42
3	C	1451	EPE	O1S-S	2.45	1.52	1.45
3	C	1451	EPE	O3S-S	2.63	1.53	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1451	EPE	O3S-S-O1S	-3.73	102.92	111.61
2	A	1451	GOL	O2-C2-C1	2.00	117.83	108.65
3	C	1451	EPE	C9-N1-C2	2.16	116.81	111.27
3	C	1451	EPE	C8-C7-N4	2.96	124.41	113.41
3	C	1451	EPE	C3-C2-N1	2.98	115.96	110.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1451	GOL	1	0
2	A	1452	GOL	1	0
2	A	1454	GOL	5	0
2	C	1448	GOL	2	0
2	C	1449	GOL	1	0
2	C	1450	GOL	2	0
3	C	1451	EPE	8	0
4	E	1451	PG4	11	0
2	F	1449	GOL	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	442/447 (98%)	-0.05	2 (0%) 91 92	21, 34, 57, 117	0
1	B	442/447 (98%)	-0.10	1 (0%) 95 96	20, 32, 57, 129	0
1	C	442/447 (98%)	-0.08	1 (0%) 95 96	22, 31, 48, 78	0
1	D	439/447 (98%)	0.73	74 (16%) 2 2	21, 44, 104, 149	0
1	E	442/447 (98%)	0.15	10 (2%) 64 67	21, 39, 75, 116	0
1	F	442/447 (98%)	0.05	5 (1%) 82 84	20, 36, 68, 120	0
All	All	2649/2682 (98%)	0.12	93 (3%) 48 53	20, 34, 79, 149	0

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	226	HIS	10.4
1	D	353	ILE	6.6
1	F	289	ARG	6.3
1	D	279	LEU	6.2
1	D	365	LEU	6.0

### 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
2	GOL	A	1452	6/6	0.93	0.40	10.41	48,64,77,83	0
2	GOL	A	1453	6/6	0.89	0.41	10.34	55,66,75,79	0
2	GOL	A	1450	6/6	0.90	0.34	9.99	47,57,64,65	0
2	GOL	F	1448	6/6	0.93	0.36	9.57	53,64,68,69	0
2	GOL	E	1449	6/6	0.92	0.38	8.80	46,58,69,70	0
2	GOL	A	1451	6/6	0.89	0.33	5.42	40,49,65,66	0
2	GOL	D	1449	6/6	0.91	0.31	3.79	30,43,53,57	0
3	EPE	C	1451	15/15	0.93	0.26	3.27	37,52,73,83	0
4	PG4	E	1451	13/13	0.87	0.24	2.71	43,59,71,77	0
2	GOL	A	1454	6/6	0.87	0.29	2.65	58,69,82,82	0
2	GOL	E	1448	6/6	0.95	0.29	2.36	32,46,59,64	0
2	GOL	D	1448	6/6	0.94	0.22	2.13	30,41,49,52	0
2	GOL	E	1450	6/6	0.93	0.24	2.03	48,59,63,75	0
2	GOL	C	1449	6/6	0.92	0.19	1.37	37,54,65,69	0
2	GOL	C	1448	6/6	0.95	0.18	1.24	42,52,68,82	0
2	GOL	A	1449	6/6	0.90	0.18	1.02	48,58,69,73	0
2	GOL	D	1450	6/6	0.91	0.15	0.46	42,55,70,70	0
2	GOL	A	1448	6/6	0.88	0.21	0.32	47,62,71,79	0
2	GOL	F	1449	6/6	0.87	0.21	0.15	43,63,86,86	0
2	GOL	C	1450	6/6	0.90	0.16	0.11	47,64,77,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.