



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:09 AM GMT

PDB ID : 1ZXE  
Title : Crystal Structure of eIF2alpha Protein Kinase GCN2: D835N Inactivating Mutant in Apo Form  
Authors : Padyana, A.K.; Qiu, H.; Roll-Mecak, A.; Hinnebusch, A.G.; Burley, S.K.  
Deposited on : 2005-06-07  
Resolution : 2.60 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

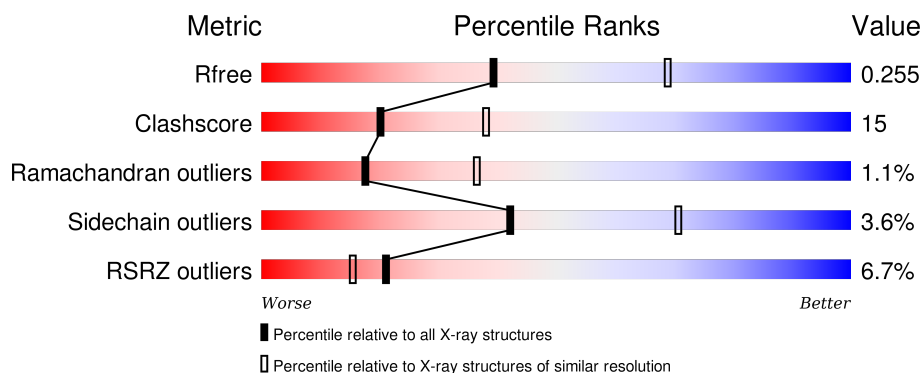
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	303	<div> <div>0%</div> <div>63% 25% 11%</div> </div>
1	B	303	<div> <div>5%</div> <div>64% 18% 17%</div> </div>
1	C	303	<div> <div>5%</div> <div>69% 20% 9%</div> </div>
1	D	303	<div> <div>4%</div> <div>57% 25% 16%</div> </div>
1	E	303	<div> <div>11%</div> <div>54% 31% 13%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	303	

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	398	-	X	-	-
2	GOL	B	498	-	X	-	-
2	GOL	C	998	-	X	-	-
2	GOL	D	698	-	X	-	X
2	GOL	E	998	-	X	-	-
2	GOL	F	998	-	X	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13242 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 Serine/threonine-protein kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	Se	0	0	0
			2222	1427	387	399	1	8			
1	B	252	Total	C	N	O	S	Se	0	0	0
			2081	1336	363	373	1	8			
1	C	275	Total	C	N	O	S	Se	0	0	0
			2259	1448	393	409	1	8			
1	D	256	Total	C	N	O	S	Se	0	0	0
			2117	1358	370	380	1	8			
1	E	264	Total	C	N	O	S	Se	0	0	0
			2181	1399	381	392	1	8			
1	F	249	Total	C	N	O	S	Se	0	0	0
			2067	1328	358	372	1	8			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	592	SER	-	cloning artifact	UNP P15442
A	593	LEU	-	cloning artifact	UNP P15442
A	645	MSE	MET	modified residue	UNP P15442
A	775	MSE	MET	modified residue	UNP P15442
A	788	MSE	MET	modified residue	UNP P15442
A	835	ASN	ASP	engineered	UNP P15442
A	839	MSE	MET	modified residue	UNP P15442
A	889	MSE	MET	modified residue	UNP P15442
A	908	MSE	MET	modified residue	UNP P15442
A	918	MSE	MET	modified residue	UNP P15442
A	926	MSE	MET	modified residue	UNP P15442
A	951	MSE	MET	modified residue	UNP P15442
B	592	SER	-	cloning artifact	UNP P15442
B	593	LEU	-	cloning artifact	UNP P15442
B	645	MSE	MET	modified residue	UNP P15442
B	775	MSE	MET	modified residue	UNP P15442
B	788	MSE	MET	modified residue	UNP P15442

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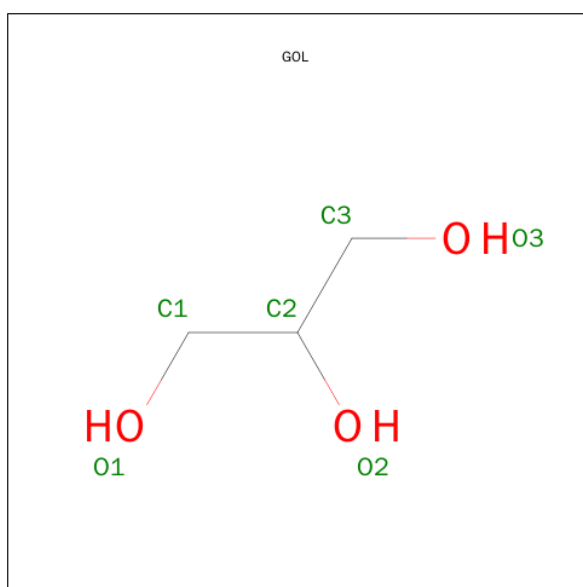
Chain	Residue	Modelled	Actual	Comment	Reference
B	835	ASN	ASP	engineered	UNP P15442
B	839	MSE	MET	modified residue	UNP P15442
B	889	MSE	MET	modified residue	UNP P15442
B	908	MSE	MET	modified residue	UNP P15442
B	918	MSE	MET	modified residue	UNP P15442
B	926	MSE	MET	modified residue	UNP P15442
B	951	MSE	MET	modified residue	UNP P15442
C	592	SER	-	cloning artifact	UNP P15442
C	593	LEU	-	cloning artifact	UNP P15442
C	645	MSE	MET	modified residue	UNP P15442
C	775	MSE	MET	modified residue	UNP P15442
C	788	MSE	MET	modified residue	UNP P15442
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C	908	MSE	MET	modified residue	UNP P15442
C	918	MSE	MET	modified residue	UNP P15442
C	926	MSE	MET	modified residue	UNP P15442
C	951	MSE	MET	modified residue	UNP P15442
D	592	SER	-	cloning artifact	UNP P15442
D	593	LEU	-	cloning artifact	UNP P15442
D	645	MSE	MET	modified residue	UNP P15442
D	775	MSE	MET	modified residue	UNP P15442
D	788	MSE	MET	modified residue	UNP P15442
D	835	ASN	ASP	engineered	UNP P15442
D	839	MSE	MET	modified residue	UNP P15442
D	889	MSE	MET	modified residue	UNP P15442
D	908	MSE	MET	modified residue	UNP P15442
D	918	MSE	MET	modified residue	UNP P15442
D	926	MSE	MET	modified residue	UNP P15442
D	951	MSE	MET	modified residue	UNP P15442
E	592	SER	-	cloning artifact	UNP P15442
E	593	LEU	-	cloning artifact	UNP P15442
E	645	MSE	MET	modified residue	UNP P15442
E	775	MSE	MET	modified residue	UNP P15442
E	788	MSE	MET	modified residue	UNP P15442
E	835	ASN	ASP	engineered	UNP P15442
E	839	MSE	MET	modified residue	UNP P15442
E	889	MSE	MET	modified residue	UNP P15442
E	908	MSE	MET	modified residue	UNP P15442
E	918	MSE	MET	modified residue	UNP P15442
E	926	MSE	MET	modified residue	UNP P15442

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Chain	Residue	Modelled	Actual	Comment	Reference
E	951	MSE	MET	modified residue	UNP P15442
F	592	SER	-	cloning artifact	UNP P15442
F	593	LEU	-	cloning artifact	UNP P15442
F	645	MSE	MET	modified residue	UNP P15442
F	775	MSE	MET	modified residue	UNP P15442
F	788	MSE	MET	modified residue	UNP P15442
F	835	ASN	ASP	engineered	UNP P15442
F	839	MSE	MET	modified residue	UNP P15442
F	889	MSE	MET	modified residue	UNP P15442
F	908	MSE	MET	modified residue	UNP P15442
F	918	MSE	MET	modified residue	UNP P15442
F	926	MSE	MET	modified residue	UNP P15442
F	951	MSE	MET	modified residue	UNP P15442

- 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	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			6	3	3		

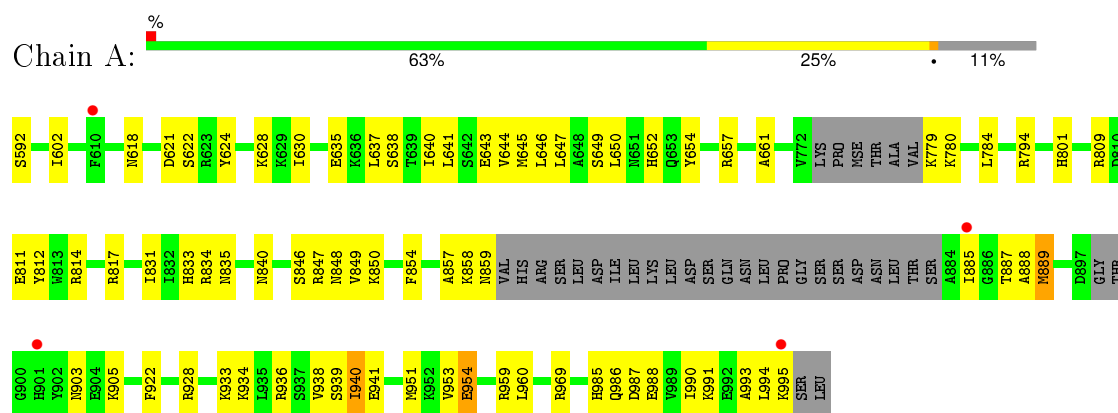
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	67	Total	O	0	0
			67	67		
3	B	51	Total	O	0	0
			51	51		
3	C	57	Total	O	0	0
			57	57		
3	D	72	Total	O	0	0
			72	72		
3	E	11	Total	O	0	0
			11	11		
3	F	21	Total	O	0	0
			21	21		

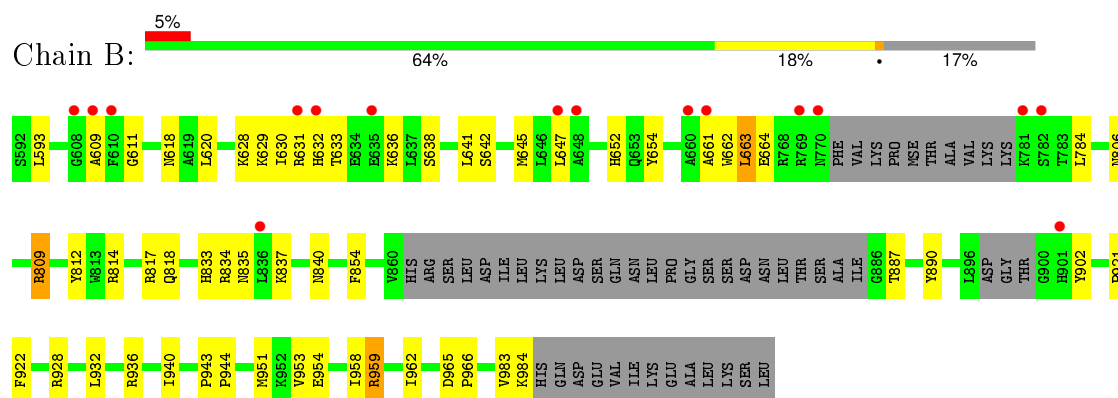
### 3 Residue-property plots

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.

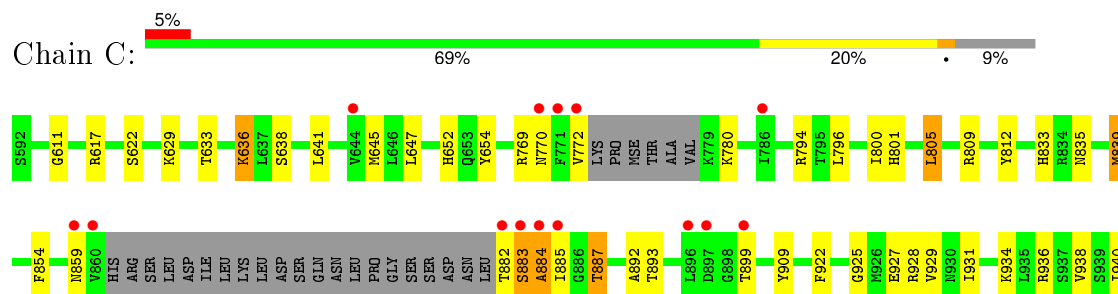
#### • Molecule 1: Serine/threonine-protein kinase



#### • Molecule 1: Serine/threonine-protein kinase



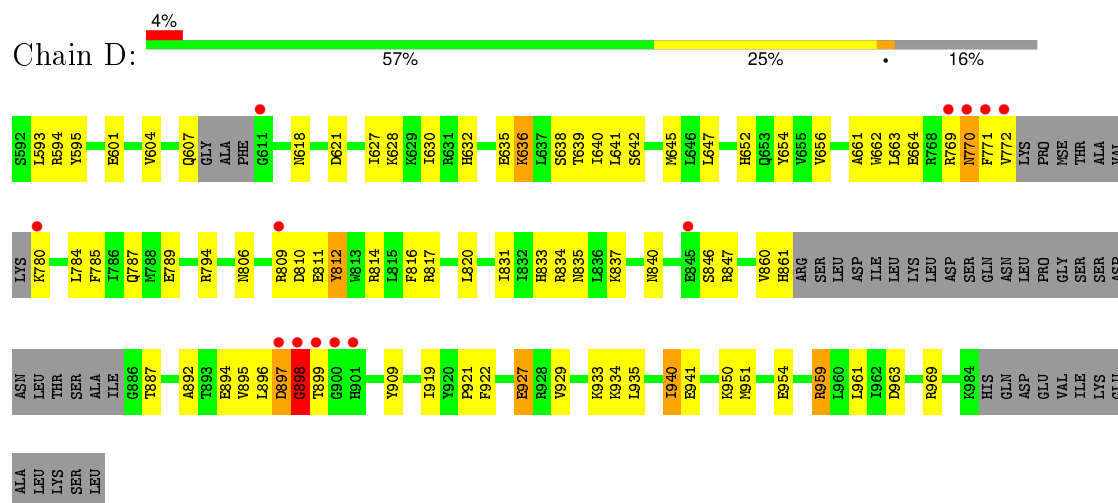
#### • Molecule 1: Serine/threonine-protein kinase



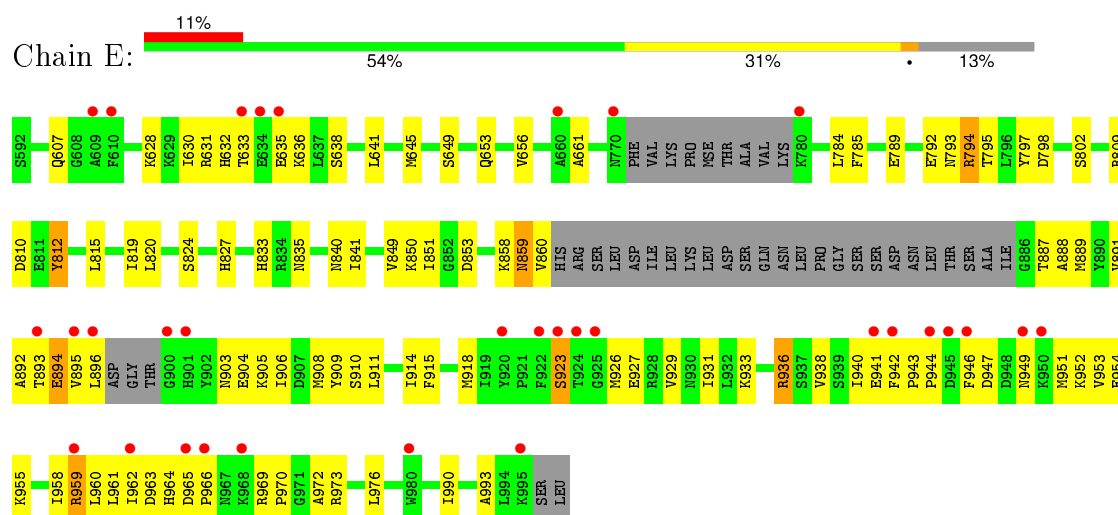




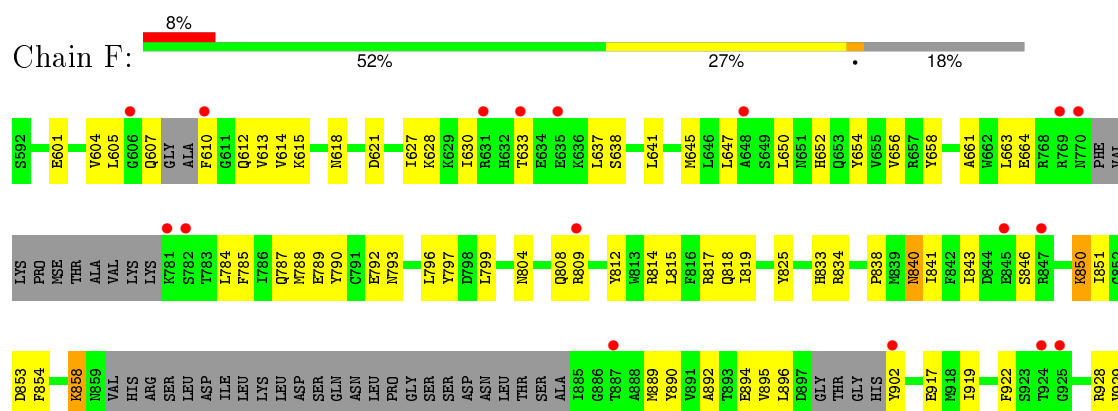
- Molecule 1: Serine/threonine-protein kinase

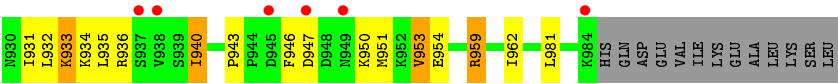


- Molecule 1: Serine/threonine-protein kinase



- Molecule 1: Serine/threonine-protein kinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.56Å 154.14Å 157.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.35 – 2.60 35.35 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.6 (35.35-2.60) 96.8 (35.35-2.35)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.34Å)	Xtriage
Refinement program	CNX 2000.1	Depositor
R, $R_{free}$	0.204 , 0.252 0.210 , 0.255	Depositor DCC
$R_{free}$ test set	1206 reflections (2.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.3	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.9	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 78655 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13242	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.29% 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

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	0.57	0/2257	0.72	1/3021 (0.0%)
1	B	0.63	0/2114	0.75	0/2831
1	C	0.56	0/2295	0.71	1/3075 (0.0%)
1	D	0.55	0/2151	0.73	1/2881 (0.0%)
1	E	0.46	0/2215	0.61	0/2965
1	F	0.45	0/2098	0.58	0/2808
All	All	0.54	0/13130	0.69	3/17581 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	884	ALA	N-CA-C	-8.81	87.21	111.00
1	D	898	GLY	N-CA-C	6.53	129.43	113.10
1	A	657	ARG	NE-CZ-NH2	-5.31	117.64	120.30

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	2222	0	2246	72	0
1	B	2081	0	2098	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2259	0	2283	55	0
1	D	2117	0	2133	65	0
1	E	2181	0	2204	85	0
1	F	2067	0	2085	81	0
2	A	6	0	4	0	0
2	B	6	0	4	0	0
2	C	6	0	4	0	0
2	D	6	0	4	0	0
2	E	6	0	4	0	0
2	F	6	0	4	0	0
3	A	67	0	0	5	0
3	B	51	0	0	5	0
3	C	57	0	0	2	0
3	D	72	0	0	5	0
3	E	11	0	0	0	0
3	F	21	0	0	1	0
All	All	13242	0	13073	383	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 15.

All (383) 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:652:HIS:HD2	1:C:654:TYR:H	1.10	0.95
1:F:601:GLU:HG3	1:F:614:VAL:HG11	1.48	0.93
1:A:784:LEU:HD11	1:B:645:MSE:HE2	1.53	0.89
1:B:837:LYS:HD2	1:B:887:THR:HG21	1.57	0.87
1:E:915:PHE:HA	1:E:918:MSE:HE3	1.56	0.86
1:B:835:ASN:O	1:B:840:ASN:ND2	2.10	0.84
1:A:661:ALA:CB	1:B:645:MSE:HE1	2.08	0.82
1:A:652:HIS:HD2	1:A:654:TYR:H	1.26	0.82
1:D:896:LEU:C	1:D:898:GLY:H	1.81	0.82
1:C:833:HIS:HD2	1:C:835:ASN:H	1.24	0.82
1:B:984:LYS:HD2	1:C:899:THR:HG23	1.60	0.81
1:A:889:MSE:HE3	1:A:936:ARG:HD3	1.63	0.81
1:A:817:ARG:HD2	3:A:19:HOH:O	1.80	0.81
1:D:632:HIS:CE1	1:D:636:LYS:HD3	2.17	0.80
1:A:835:ASN:O	1:A:840:ASN:ND2	2.15	0.79
1:E:661:ALA:HB1	1:F:645:MSE:HE1	1.65	0.79
1:F:889:MSE:HE2	1:F:932:LEU:HB2	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:837:LYS:CD	1:B:887:THR:HG21	2.14	0.77
1:C:652:HIS:CD2	1:C:654:TYR:H	1.99	0.77
1:D:835:ASN:O	1:D:840:ASN:ND2	2.19	0.76
1:A:951:MSE:HB3	1:A:954:GLU:HG2	1.65	0.76
1:B:633:THR:HG23	1:B:636:LYS:H	1.50	0.75
1:F:858:LYS:HD2	1:F:858:LYS:N	2.02	0.75
1:B:806:ASN:ND2	1:B:921:PRO:HB3	2.03	0.74
1:F:652:HIS:HD2	1:F:654:TYR:H	1.35	0.73
1:B:984:LYS:HD2	1:C:899:THR:CG2	2.18	0.73
1:B:959:ARG:HD3	1:B:959:ARG:O	1.90	0.72
1:E:931:ILE:HG23	1:E:943:PRO:HG3	1.71	0.72
1:E:835:ASN:O	1:E:840:ASN:ND2	2.22	0.72
1:F:892:ALA:HB3	1:F:895:VAL:HG23	1.70	0.71
1:A:645:MSE:HE2	1:B:784:LEU:HD11	1.72	0.71
1:E:628:LYS:HE3	1:E:630:ILE:HD11	1.73	0.71
1:B:922:PHE:CE1	1:B:928:ARG:HG3	2.26	0.71
1:F:628:LYS:HD2	1:F:788:MSE:HE1	1.72	0.71
1:B:940:ILE:HD12	1:B:959:ARG:NH1	2.06	0.70
1:F:858:LYS:HD2	1:F:858:LYS:H	1.57	0.70
1:F:934:LYS:HB2	3:F:233:HOH:O	1.90	0.70
1:C:645:MSE:HE3	1:D:641:LEU:HD22	1.72	0.70
1:E:824:SER:HA	1:E:972:ALA:HB1	1.73	0.70
1:F:889:MSE:HE3	1:F:936:ARG:HD2	1.73	0.70
1:A:661:ALA:HB1	1:B:645:MSE:HE1	1.73	0.69
1:D:636:LYS:O	1:D:639:THR:HG22	1.92	0.69
1:D:780:LYS:HA	3:D:131:HOH:O	1.92	0.69
1:C:638:SER:HA	1:C:641:LEU:HG	1.74	0.69
1:D:639:THR:HG23	1:D:640:ILE:HG23	1.75	0.68
1:F:840:ASN:ND2	1:F:853:ASP:HB3	2.08	0.68
1:C:611:GLY:HA3	1:C:629:LYS:O	1.94	0.68
1:F:652:HIS:CD2	1:F:654:TYR:H	2.11	0.68
1:A:809:ARG:HA	1:A:812:TYR:CE1	2.29	0.68
1:E:661:ALA:CB	1:F:645:MSE:HE1	2.23	0.68
1:A:985:HIS:CD2	1:A:987:ASP:H	2.11	0.68
1:C:954:GLU:O	1:C:958:ILE:HG13	1.94	0.68
1:A:643:GLU:CD	1:A:858:LYS:HE2	2.15	0.67
1:A:885:ILE:HG22	1:A:888:ALA:H	1.57	0.67
1:E:784:LEU:HD11	1:F:645:MSE:HE2	1.75	0.67
1:C:833:HIS:CD2	1:C:835:ASN:H	2.12	0.67
1:F:809:ARG:HH21	1:F:950:LYS:HE3	1.60	0.67
1:E:645:MSE:HE2	1:F:641:LEU:HD22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:951:MSE:HB3	1:C:954:GLU:CG	2.25	0.67
1:E:892:ALA:HB1	1:E:894:GLU:OE1	1.95	0.67
1:B:642:SER:HB3	3:B:11:HOH:O	1.94	0.66
1:C:899:THR:HG22	1:C:899:THR:O	1.95	0.66
1:D:897:ASP:O	1:D:897:ASP:OD1	2.13	0.66
1:D:769:ARG:HG2	3:D:188:HOH:O	1.95	0.66
1:A:645:MSE:HE1	1:B:661:ALA:HB1	1.77	0.66
1:A:940:ILE:HD12	1:A:959:ARG:CZ	2.25	0.66
1:D:811:GLU:HG2	1:D:847:ARG:HH12	1.61	0.66
1:B:652:HIS:CD2	1:B:654:TYR:H	2.14	0.65
1:A:645:MSE:HE1	1:B:661:ALA:CB	2.26	0.65
1:D:896:LEU:C	1:D:898:GLY:N	2.50	0.65
1:B:652:HIS:HD2	1:B:654:TYR:H	1.46	0.64
1:F:607:GLN:HG3	1:F:612:GLN:HB3	1.79	0.64
1:D:652:HIS:CD2	1:D:654:TYR:H	2.16	0.64
1:A:833:HIS:O	1:A:834:ARG:HB2	1.97	0.64
1:F:929:VAL:O	1:F:933:LYS:HB2	1.97	0.64
1:A:652:HIS:CD2	1:A:654:TYR:H	2.12	0.64
1:D:642:SER:HB3	3:D:55:HOH:O	1.98	0.64
1:A:784:LEU:HD11	1:B:645:MSE:CE	2.27	0.63
1:D:894:GLU:O	1:D:897:ASP:HB3	1.97	0.63
1:C:769:ARG:HB3	1:C:769:ARG:HH11	1.63	0.63
1:F:889:MSE:HE2	1:F:932:LEU:CB	2.28	0.62
1:A:951:MSE:HB3	1:A:954:GLU:CG	2.29	0.62
1:E:892:ALA:HA	1:E:909:TYR:CD2	2.34	0.62
1:D:860:VAL:HG12	1:D:895:VAL:CG1	2.29	0.62
1:A:953:VAL:HG22	1:A:954:GLU:OE1	1.99	0.62
1:F:962:ILE:HG22	1:F:962:ILE:O	1.99	0.62
1:C:951:MSE:HB3	1:C:954:GLU:HG2	1.82	0.62
1:C:883:SER:HA	1:C:885:ILE:HB	1.82	0.62
1:E:946:PHE:CE2	1:E:955:LYS:HD2	2.35	0.61
1:D:816:PHE:CE2	1:D:820:LEU:HD11	2.35	0.61
1:C:769:ARG:HB3	1:C:769:ARG:NH1	2.16	0.61
1:B:618:ASN:OD1	1:B:620:LEU:HB2	2.01	0.61
1:F:940:ILE:HG21	1:F:959:ARG:HH11	1.67	0.60
1:E:962:ILE:HG22	1:E:962:ILE:O	2.02	0.60
1:E:656:VAL:HG13	1:E:789:GLU:HB3	1.84	0.60
1:C:995:LYS:HE2	1:C:995:LYS:HA	1.82	0.60
1:A:643:GLU:OE2	1:A:858:LYS:HE2	2.01	0.59
1:F:615:LYS:HE2	1:F:790:TYR:CZ	2.37	0.59
1:F:638:SER:HA	1:F:641:LEU:HG	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:860:VAL:HG12	1:D:895:VAL:HG12	1.84	0.59
1:E:840:ASN:OD1	1:E:853:ASP:HB3	2.03	0.59
1:E:954:GLU:O	1:E:958:ILE:HG13	2.03	0.59
1:D:837:LYS:HD3	1:D:887:THR:HG23	1.85	0.59
1:B:638:SER:HA	1:B:641:LEU:HG	1.84	0.58
1:F:953:VAL:HG13	1:F:954:GLU:OE1	2.03	0.58
1:D:595:TYR:OH	1:D:601:GLU:HG3	2.03	0.58
1:C:641:LEU:O	1:C:645:MSE:HG2	2.03	0.58
1:F:833:HIS:O	1:F:834:ARG:HB2	2.04	0.58
1:E:940:ILE:HD12	1:E:940:ILE:N	2.19	0.57
1:D:894:GLU:HA	1:D:897:ASP:HB3	1.85	0.57
1:E:923:SER:OG	1:E:927:GLU:HG2	2.05	0.57
1:D:771:PHE:O	1:D:772:VAL:HG12	2.04	0.57
1:C:925:GLY:O	1:C:929:VAL:HG23	2.03	0.57
1:E:936:ARG:NH1	1:E:936:ARG:HG3	2.20	0.57
1:F:601:GLU:CG	1:F:614:VAL:HG11	2.30	0.57
1:D:628:LYS:HD3	1:D:630:ILE:HD11	1.86	0.57
1:B:951:MSE:HB3	1:B:954:GLU:HG2	1.85	0.57
1:D:806:ASN:ND2	1:D:921:PRO:HB3	2.19	0.57
1:C:645:MSE:HB3	1:D:663:LEU:HB2	1.87	0.56
1:E:990:ILE:O	1:E:993:ALA:HB3	2.05	0.56
1:E:819:ILE:HD13	1:E:841:ILE:HD13	1.87	0.56
1:C:973:ARG:HD2	1:C:977:ASN:HD21	1.69	0.56
1:C:839:MSE:HB2	3:C:28:HOH:O	2.05	0.56
1:F:605:LEU:HB2	1:F:613:VAL:HG13	1.85	0.56
1:A:638:SER:HA	1:A:641:LEU:HG	1.88	0.56
1:E:905:LYS:HG2	1:E:966:PRO:O	2.05	0.56
1:E:820:LEU:HD13	1:E:911:LEU:HD21	1.87	0.56
1:D:593:LEU:HD13	1:D:664:GLU:HG2	1.88	0.56
1:D:769:ARG:O	1:D:770:ASN:C	2.42	0.56
1:D:652:HIS:HD2	1:D:654:TYR:H	1.53	0.56
1:B:837:LYS:HG2	1:B:840:ASN:ND2	2.21	0.55
1:A:857:ALA:HB3	1:A:859:ASN:HD22	1.70	0.55
1:B:647:LEU:HD21	1:B:854:PHE:CD2	2.42	0.55
1:D:618:ASN:HB3	1:D:621:ASP:OD1	2.07	0.55
1:E:645:MSE:HE3	1:F:784:LEU:HD11	1.87	0.55
1:B:959:ARG:C	1:B:959:ARG:HD3	2.24	0.55
1:A:650:LEU:HD21	1:A:831:ILE:HD12	1.88	0.55
1:C:883:SER:C	1:C:885:ILE:H	1.95	0.55
1:A:934:LYS:HG3	1:A:941:GLU:HB3	1.89	0.55
1:A:618:ASN:HB3	1:A:621:ASP:OD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:940:ILE:CG2	1:E:959:ARG:HD3	2.37	0.54
1:F:922:PHE:CE2	1:F:931:ILE:HD12	2.42	0.54
1:B:951:MSE:HB3	1:B:954:GLU:CG	2.38	0.54
1:E:649:SER:HB2	1:F:664:GLU:HG2	1.89	0.54
1:B:593:LEU:HD13	1:B:664:GLU:HG2	1.90	0.54
1:E:914:ILE:HG22	1:E:918:MSE:HE2	1.89	0.54
1:E:641:LEU:O	1:E:645:MSE:HG2	2.08	0.54
1:A:985:HIS:HD2	1:A:987:ASP:HB2	1.73	0.54
1:F:951:MSE:HB3	1:F:954:GLU:HB2	1.90	0.54
1:F:641:LEU:O	1:F:645:MSE:HG2	2.07	0.54
1:F:658:TYR:CE2	1:F:788:MSE:HE2	2.43	0.54
1:A:849:VAL:CG1	1:A:850:LYS:N	2.71	0.54
1:F:604:VAL:HA	1:F:614:VAL:HG22	1.89	0.53
1:D:896:LEU:HD12	1:D:896:LEU:N	2.24	0.53
1:D:769:ARG:O	1:D:771:PHE:N	2.41	0.53
1:F:628:LYS:HD2	1:F:788:MSE:CE	2.38	0.53
1:A:661:ALA:HB3	1:B:645:MSE:HE1	1.90	0.53
1:E:951:MSE:HB3	1:E:954:GLU:CG	2.38	0.53
1:A:857:ALA:CB	1:A:859:ASN:HD22	2.21	0.53
1:E:636:LYS:HB3	1:E:636:LYS:HZ2	1.74	0.53
1:A:953:VAL:HG23	1:A:954:GLU:N	2.24	0.53
1:F:959:ARG:C	1:F:959:ARG:HD3	2.30	0.53
1:F:841:ILE:HD12	1:F:851:ILE:CD1	2.39	0.53
1:E:888:ALA:O	1:E:891:VAL:HG12	2.08	0.53
1:A:985:HIS:HD2	1:A:987:ASP:H	1.58	0.52
1:E:910:SER:O	1:E:914:ILE:HG13	2.08	0.52
1:E:638:SER:HA	1:E:641:LEU:HG	1.90	0.52
1:E:909:TYR:OH	1:E:936:ARG:HD3	2.09	0.52
1:E:936:ARG:HH11	1:E:936:ARG:HG3	1.73	0.52
1:B:833:HIS:O	1:B:834:ARG:HB2	2.09	0.52
1:F:661:ALA:HA	1:F:785:PHE:O	2.10	0.52
1:E:942:PHE:HZ	1:E:959:ARG:HG2	1.74	0.52
1:F:840:ASN:HD21	1:F:853:ASP:HB3	1.73	0.52
1:E:896:LEU:HD12	1:E:896:LEU:H	1.75	0.52
1:A:602:ILE:CD1	1:A:624:TYR:HE2	2.21	0.52
1:A:988:GLU:O	1:A:991:LYS:HB2	2.09	0.52
1:C:801:HIS:HE1	3:C:172:HOH:O	1.91	0.52
1:D:951:MSE:HB3	1:D:954:GLU:HG2	1.91	0.52
1:E:966:PRO:HA	1:E:969:ARG:NH1	2.24	0.52
1:C:805:LEU:HD22	1:C:812:TYR:HB3	1.90	0.52
1:F:940:ILE:HG23	1:F:940:ILE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:796:LEU:O	1:C:800:ILE:HG13	2.10	0.51
1:C:645:MSE:HE3	1:D:641:LEU:CD2	2.39	0.51
1:A:986:GLN:O	1:A:990:ILE:HG13	2.10	0.51
1:D:961:LEU:O	1:D:969:ARG:HG2	2.11	0.51
1:D:604:VAL:HG23	3:D:186:HOH:O	2.11	0.51
1:E:942:PHE:CD1	1:E:942:PHE:N	2.79	0.51
1:A:640:ILE:O	1:A:644:VAL:HG23	2.09	0.51
1:B:809:ARG:NE	3:B:157:HOH:O	2.43	0.51
1:E:961:LEU:HD23	1:E:970:PRO:HD2	1.92	0.51
1:D:929:VAL:O	1:D:933:LYS:HB2	2.11	0.51
1:E:889:MSE:HE3	1:E:936:ARG:NH1	2.26	0.51
1:D:647:LEU:HD23	1:D:831:ILE:HD13	1.93	0.51
1:A:645:MSE:HE2	1:B:784:LEU:CD1	2.39	0.50
1:F:647:LEU:HD21	1:F:854:PHE:CD2	2.46	0.50
1:F:796:LEU:HB3	1:F:838:PRO:O	2.12	0.50
1:E:661:ALA:HA	1:E:785:PHE:O	2.11	0.50
1:C:985:HIS:CE1	1:C:987:ASP:OD2	2.65	0.50
1:E:926:MSE:O	1:E:929:VAL:HG22	2.11	0.50
1:C:952:LYS:HB2	1:C:952:LYS:NZ	2.27	0.50
1:E:784:LEU:HD11	1:F:645:MSE:CE	2.39	0.50
1:F:656:VAL:HG13	1:F:789:GLU:HB3	1.94	0.50
1:F:814:ARG:O	1:F:818:GLN:HG3	2.12	0.50
1:F:932:LEU:HA	1:F:935:LEU:HD12	1.94	0.50
1:A:857:ALA:HB2	3:A:204:HOH:O	2.12	0.50
1:A:811:GLU:CD	1:A:814:ARG:HH11	2.15	0.50
1:E:940:ILE:HG21	1:E:959:ARG:HD3	1.94	0.50
1:F:892:ALA:HB1	1:F:894:GLU:OE1	2.11	0.50
1:E:946:PHE:HE2	1:E:955:LYS:HD2	1.76	0.50
1:D:656:VAL:HG13	1:D:789:GLU:HB3	1.94	0.50
1:A:661:ALA:C	1:B:645:MSE:HE1	2.32	0.49
1:A:990:ILE:O	1:A:993:ALA:HB3	2.11	0.49
1:C:833:HIS:HD2	1:C:835:ASN:N	2.02	0.49
1:C:958:ILE:O	1:C:962:ILE:HG12	2.12	0.49
1:E:833:HIS:HD2	1:E:835:ASN:H	1.60	0.49
1:D:894:GLU:C	1:D:897:ASP:HB3	2.33	0.48
1:F:902:TYR:C	1:F:902:TYR:CD1	2.87	0.48
1:A:645:MSE:HE3	1:B:662:TRP:CA	2.43	0.48
1:E:963:ASP:OD1	1:E:964:HIS:N	2.46	0.48
1:D:638:SER:HA	1:D:641:LEU:CD1	2.43	0.48
1:E:915:PHE:CA	1:E:918:MSE:HE3	2.37	0.48
1:A:637:LEU:O	1:A:640:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:799:LEU:CD1	1:F:843:ILE:HG13	2.43	0.48
1:E:827:HIS:CE1	1:E:908:MSE:HE2	2.49	0.48
1:F:601:GLU:HG3	1:F:614:VAL:CG1	2.34	0.48
1:D:663:LEU:HD13	1:D:784:LEU:HD13	1.96	0.48
1:E:645:MSE:CE	1:F:641:LEU:HD22	2.43	0.48
1:F:627:ILE:HD13	1:F:787:GLN:HA	1.95	0.48
1:C:647:LEU:HD21	1:C:854:PHE:CD2	2.49	0.48
1:F:959:ARG:O	1:F:959:ARG:HD3	2.14	0.48
1:D:811:GLU:OE2	1:D:847:ARG:NH1	2.47	0.47
1:C:882:THR:CG2	1:C:883:SER:N	2.77	0.47
1:D:638:SER:HA	1:D:641:LEU:HG	1.96	0.47
1:D:812:TYR:CE2	1:D:919:ILE:HG22	2.49	0.47
1:A:940:ILE:HD12	1:A:959:ARG:NH1	2.30	0.47
1:E:815:LEU:HD22	1:E:849:VAL:HG23	1.96	0.47
1:E:645:MSE:HB3	1:F:663:LEU:HB2	1.97	0.47
1:F:841:ILE:HD12	1:F:851:ILE:HD12	1.96	0.47
1:F:809:ARG:NH2	1:F:950:LYS:HE3	2.28	0.47
1:D:950:LYS:HG3	1:D:951:MSE:HG3	1.97	0.47
1:D:627:ILE:HD13	1:D:787:GLN:HA	1.96	0.47
1:E:903:ASN:O	1:E:906:ILE:HG12	2.14	0.47
1:A:641:LEU:O	1:A:645:MSE:HG2	2.14	0.47
1:B:951:MSE:HE2	3:B:104:HOH:O	2.14	0.47
1:D:940:ILE:HD12	1:D:959:ARG:CZ	2.45	0.47
1:F:889:MSE:HE3	1:F:936:ARG:CD	2.44	0.47
1:C:645:MSE:HE2	1:D:645:MSE:HE2	1.96	0.47
1:A:592:SER:HA	3:A:198:HOH:O	2.14	0.47
1:E:798:ASP:O	1:E:802:SER:HB3	2.14	0.47
1:C:772:VAL:HG22	1:C:780:LYS:NZ	2.30	0.47
1:B:983:VAL:HG13	1:B:983:VAL:O	2.14	0.47
1:C:893:THR:HG21	1:C:964:HIS:CD2	2.50	0.47
1:C:617:ARG:HH12	1:C:622:SER:HB3	1.80	0.47
1:D:922:PHE:HA	1:D:927:GLU:OE2	2.15	0.47
1:E:973:ARG:NH1	1:E:976:LEU:HD13	2.30	0.46
1:E:951:MSE:HB3	1:E:954:GLU:HG2	1.97	0.46
1:E:812:TYR:OH	1:E:951:MSE:HE2	2.15	0.46
1:A:647:LEU:HD21	1:A:854:PHE:CD2	2.50	0.46
1:E:889:MSE:HE1	1:E:933:LYS:HG2	1.98	0.46
1:F:815:LEU:O	1:F:819:ILE:HG13	2.15	0.46
1:F:792:GLU:OE2	1:F:792:GLU:HA	2.15	0.46
1:C:884:ALA:O	1:C:887:THR:HB	2.15	0.46
1:B:837:LYS:HD3	1:B:887:THR:HG21	1.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:894:GLU:CA	1:D:897:ASP:HB3	2.46	0.46
1:D:846:SER:O	1:D:847:ARG:HB2	2.15	0.46
1:A:953:VAL:CG2	1:A:954:GLU:N	2.78	0.46
1:A:885:ILE:C	1:A:887:THR:H	2.20	0.46
1:B:632:HIS:ND1	1:B:633:THR:HG22	2.32	0.45
1:C:936:ARG:HG2	1:C:936:ARG:HH11	1.81	0.45
1:C:944:PRO:HG2	1:C:945:ASP:H	1.81	0.45
1:A:645:MSE:CE	1:B:784:LEU:HD11	2.42	0.45
1:C:951:MSE:HB3	1:C:954:GLU:HG3	1.97	0.45
1:E:893:THR:C	1:E:895:VAL:H	2.20	0.45
1:D:817:ARG:HG2	3:D:194:HOH:O	2.17	0.45
1:C:899:THR:CG2	1:C:899:THR:O	2.63	0.45
1:B:953:VAL:HG13	3:B:243:HOH:O	2.17	0.45
1:E:927:GLU:O	1:E:931:ILE:HG12	2.17	0.45
1:A:857:ALA:HB3	1:A:859:ASN:ND2	2.31	0.45
1:A:993:ALA:C	1:A:995:LYS:H	2.20	0.45
1:A:846:SER:HB2	1:A:848:ASN:ND2	2.31	0.45
1:C:633:THR:OG1	1:C:636:LYS:HB2	2.17	0.45
1:D:814:ARG:HH12	1:D:847:ARG:HB3	1.82	0.45
1:C:770:ASN:O	1:C:772:VAL:HG13	2.16	0.45
1:A:801:HIS:HE1	3:A:209:HOH:O	1.99	0.45
1:A:645:MSE:HE1	1:B:661:ALA:C	2.38	0.44
1:A:833:HIS:O	1:A:834:ARG:CB	2.65	0.44
1:F:618:ASN:HB3	1:F:621:ASP:OD1	2.17	0.44
1:C:946:PHE:HE2	1:C:955:LYS:HB2	1.82	0.44
1:F:890:TYR:CE2	1:F:917:GLU:OE2	2.70	0.44
1:E:645:MSE:HE3	1:F:784:LEU:CD1	2.47	0.44
1:E:841:ILE:HG12	1:E:851:ILE:HD12	2.00	0.44
1:D:833:HIS:O	1:D:834:ARG:HB2	2.18	0.44
1:E:962:ILE:O	1:E:962:ILE:CG2	2.66	0.44
1:B:983:VAL:O	1:B:984:LYS:HB3	2.17	0.44
1:D:860:VAL:HG22	1:D:861:HIS:CE1	2.53	0.44
1:E:795:THR:HG23	1:E:797:TYR:HB3	2.00	0.44
1:F:922:PHE:CE2	1:F:928:ARG:HA	2.53	0.43
1:B:902:TYR:C	1:B:902:TYR:CD1	2.91	0.43
1:A:960:LEU:O	1:A:969:ARG:HG3	2.18	0.43
1:A:889:MSE:HE1	1:A:933:LYS:HG2	2.01	0.43
1:E:809:ARG:HA	1:E:812:TYR:CE1	2.53	0.43
1:B:628:LYS:HE3	1:B:630:ILE:HD11	1.99	0.43
1:B:887:THR:O	1:B:887:THR:HG22	2.17	0.43
1:A:649:SER:HB3	1:B:663:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:943:PRO:HA	1:E:944:PRO:HD3	1.88	0.43
1:C:809:ARG:HA	1:C:812:TYR:CE2	2.53	0.43
1:C:885:ILE:CG2	1:C:885:ILE:O	2.66	0.43
1:A:628:LYS:HE3	1:A:630:ILE:HD11	2.01	0.43
1:E:942:PHE:HB3	1:E:943:PRO:HD2	2.00	0.43
1:D:963:ASP:O	1:D:969:ARG:HD2	2.19	0.43
1:B:814:ARG:O	1:B:818:GLN:HG3	2.19	0.43
1:E:792:GLU:C	1:E:794:ARG:H	2.22	0.43
1:F:892:ALA:HB3	1:F:895:VAL:CG2	2.44	0.43
1:B:611:GLY:HA3	1:B:629:LYS:O	2.18	0.43
1:A:985:HIS:HD2	1:A:987:ASP:CB	2.31	0.43
1:C:812:TYR:OH	1:C:951:MSE:HE2	2.19	0.43
1:F:814:ARG:NH1	1:F:815:LEU:HD11	2.34	0.43
1:F:799:LEU:HD12	1:F:843:ILE:HG13	2.01	0.43
1:F:943:PRO:O	1:F:946:PHE:HB2	2.18	0.43
1:F:654:TYR:O	1:F:850:LYS:HA	2.18	0.43
1:E:887:THR:C	1:E:889:MSE:H	2.23	0.43
1:A:780:LYS:HA	1:A:780:LYS:HD3	1.76	0.43
1:C:934:LYS:HD2	1:C:941:GLU:OE1	2.18	0.43
1:B:965:ASP:HA	1:B:966:PRO:HD2	1.86	0.43
1:A:885:ILE:HG22	1:A:885:ILE:O	2.19	0.42
1:E:891:VAL:HG13	1:E:936:ARG:NH2	2.34	0.42
1:B:932:LEU:O	1:B:936:ARG:HG3	2.19	0.42
1:A:645:MSE:HE3	1:B:662:TRP:HA	2.01	0.42
1:E:795:THR:CG2	1:E:797:TYR:HB3	2.49	0.42
1:D:935:LEU:HD23	1:D:941:GLU:O	2.19	0.42
1:E:653:GLN:O	1:E:850:LYS:NZ	2.52	0.42
1:B:809:ARG:NH1	3:B:158:HOH:O	2.41	0.42
1:C:922:PHE:CE1	1:C:928:ARG:HG3	2.55	0.42
1:D:639:THR:CG2	1:D:640:ILE:HG23	2.47	0.42
1:E:909:TYR:HE1	1:E:962:ILE:O	2.02	0.42
1:E:936:ARG:HH11	1:E:936:ARG:CG	2.33	0.42
1:F:812:TYR:CE2	1:F:919:ILE:HG22	2.54	0.42
1:D:594:ARG:HD3	1:D:662:TRP:CD2	2.54	0.42
1:E:819:ILE:CD1	1:E:841:ILE:HD13	2.48	0.42
1:C:892:ALA:HA	1:C:909:TYR:CD2	2.54	0.42
1:A:889:MSE:HE3	1:A:936:ARG:CD	2.43	0.42
1:F:658:TYR:HE2	1:F:788:MSE:HE2	1.84	0.42
1:E:960:LEU:HG	1:E:970:PRO:CG	2.49	0.42
1:F:936:ARG:NH2	1:F:936:ARG:HB3	2.34	0.42
1:F:808:GLN:HE21	1:F:808:GLN:HB2	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:887:THR:HG23	1:B:890:TYR:CD1	2.54	0.42
1:F:922:PHE:HE2	1:F:931:ILE:HD12	1.83	0.42
1:C:927:GLU:O	1:C:931:ILE:HG13	2.19	0.42
1:E:953:VAL:HG13	1:E:954:GLU:N	2.35	0.41
1:A:938:VAL:HG23	1:A:939:SER:N	2.35	0.41
1:E:946:PHE:CD2	1:E:955:LYS:HD2	2.55	0.41
1:E:942:PHE:HB3	1:E:943:PRO:CD	2.51	0.41
1:D:894:GLU:HA	1:D:897:ASP:CB	2.48	0.41
1:D:661:ALA:HA	1:D:785:PHE:O	2.20	0.41
1:A:928:ARG:HD3	3:A:52:HOH:O	2.19	0.41
1:B:943:PRO:HA	1:B:944:PRO:HD3	1.87	0.41
1:E:631:ARG:O	1:E:632:HIS:HB2	2.20	0.41
1:E:633:THR:HG22	1:E:635:GLU:H	1.85	0.41
1:F:630:ILE:HG22	1:F:637:LEU:HD21	2.02	0.41
1:F:637:LEU:HD13	1:F:663:LEU:HD11	2.01	0.41
1:D:887:THR:HG22	1:D:887:THR:O	2.19	0.41
1:F:656:VAL:HG23	1:F:851:ILE:O	2.21	0.41
1:E:849:VAL:CG1	1:E:850:LYS:N	2.84	0.41
1:B:958:ILE:O	1:B:962:ILE:HG12	2.20	0.41
1:E:859:ASN:O	1:E:860:VAL:C	2.58	0.41
1:F:650:LEU:HD22	1:F:825:TYR:CE2	2.55	0.41
1:E:963:ASP:OD1	1:E:965:ASP:N	2.53	0.41
1:F:797:TYR:C	1:F:797:TYR:CD1	2.94	0.41
1:B:631:ARG:O	1:B:632:HIS:HB2	2.19	0.41
1:D:934:LYS:HD3	1:D:941:GLU:OE1	2.20	0.41
1:A:922:PHE:CD2	1:A:928:ARG:HA	2.55	0.41
1:D:810:ASP:OD1	1:D:810:ASP:N	2.53	0.41
1:C:965:ASP:OD2	1:C:967:ASN:HB2	2.21	0.41
1:D:809:ARG:NH2	1:D:950:LYS:O	2.54	0.41
1:C:952:LYS:CB	1:C:952:LYS:NZ	2.83	0.41
1:A:811:GLU:OE2	1:A:847:ARG:NH1	2.53	0.41
1:A:635:GLU:OE1	1:A:779:LYS:NZ	2.54	0.41
1:F:628:LYS:HB2	1:F:788:MSE:HE3	2.03	0.40
1:F:962:ILE:CG2	1:F:962:ILE:O	2.68	0.40
1:A:903:ASN:OD1	1:A:905:LYS:HB2	2.21	0.40
1:C:961:LEU:O	1:C:969:ARG:HD2	2.22	0.40
1:F:610:PHE:N	1:F:610:PHE:CD1	2.90	0.40
1:D:892:ALA:HA	1:D:909:TYR:CD2	2.57	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	261/303 (86%)	248 (95%)	11 (4%)	2 (1%)	24	46
1	B	244/303 (80%)	230 (94%)	13 (5%)	1 (0%)	39	65
1	C	269/303 (89%)	251 (93%)	15 (6%)	3 (1%)	17	36
1	D	248/303 (82%)	236 (95%)	8 (3%)	4 (2%)	12	24
1	E	256/303 (84%)	232 (91%)	22 (9%)	2 (1%)	24	46
1	F	239/303 (79%)	214 (90%)	21 (9%)	4 (2%)	11	22
All	All	1517/1818 (83%)	1411 (93%)	90 (6%)	16 (1%)	17	36

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	898	GLY
1	B	609	ALA
1	D	770	ASN
1	E	894	GLU
1	F	896	LEU
1	A	994	LEU
1	C	883	SER
1	D	899	THR
1	E	793	ASN
1	F	804	ASN
1	F	793	ASN
1	F	940	ILE
1	C	859	ASN
1	A	940	ILE
1	C	940	ILE
1	D	940	ILE

### 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	241/263 (92%)	236 (98%)	5 (2%)	61	85
1	B	226/263 (86%)	221 (98%)	5 (2%)	60	83
1	C	246/263 (94%)	240 (98%)	6 (2%)	57	82
1	D	231/263 (88%)	223 (96%)	8 (4%)	43	71
1	E	237/263 (90%)	222 (94%)	15 (6%)	22	44
1	F	226/263 (86%)	215 (95%)	11 (5%)	31	57
All	All	1407/1578 (89%)	1357 (96%)	50 (4%)	42	71

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	622	SER
1	A	646	LEU
1	A	794	ARG
1	A	889	MSE
1	A	954	GLU
1	B	663	LEU
1	B	809	ARG
1	B	812	TYR
1	B	817	ARG
1	B	959	ARG
1	C	636	LYS
1	C	794	ARG
1	C	805	LEU
1	C	839	MSE
1	C	887	THR
1	C	938	VAL
1	D	607	GLN
1	D	635	GLU
1	D	636	LYS
1	D	794	ARG
1	D	812	TYR
1	D	897	ASP

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Mol	Chain	Res	Type
1	D	927	GLU
1	D	959	ARG
1	E	607	GLN
1	E	794	ARG
1	E	810	ASP
1	E	812	TYR
1	E	858	LYS
1	E	859	ASN
1	E	904	GLU
1	E	923	SER
1	E	936	ARG
1	E	938	VAL
1	E	941	GLU
1	E	947	ASP
1	E	949	ASN
1	E	952	LYS
1	E	959	ARG
1	F	633	THR
1	F	817	ARG
1	F	840	ASN
1	F	846	SER
1	F	850	LYS
1	F	858	LYS
1	F	933	LYS
1	F	947	ASP
1	F	953	VAL
1	F	959	ARG
1	F	981	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	607	GLN
1	A	612	GLN
1	A	652	HIS
1	A	793	ASN
1	A	859	ASN
1	A	985	HIS
1	B	607	GLN
1	B	612	GLN
1	B	652	HIS
1	B	967	ASN

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Mol	Chain	Res	Type
1	C	607	GLN
1	C	612	GLN
1	C	652	HIS
1	C	793	ASN
1	C	833	HIS
1	C	967	ASN
1	C	977	ASN
1	D	607	GLN
1	D	612	GLN
1	D	652	HIS
1	D	835	ASN
1	D	967	ASN
1	E	770	ASN
1	E	833	HIS
1	E	949	ASN
1	E	977	ASN
1	F	612	GLN
1	F	652	HIS
1	F	653	GLN
1	F	804	ASN
1	F	808	GLN
1	F	835	ASN
1	F	840	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

6 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	398	-	5,5,5	4.94	5 (100%)	5,5,5	5.57	3 (60%)
2	GOL	B	498	-	5,5,5	4.85	5 (100%)	5,5,5	5.57	3 (60%)
2	GOL	C	998	-	5,5,5	4.89	5 (100%)	5,5,5	5.61	3 (60%)
2	GOL	D	698	-	5,5,5	4.79	5 (100%)	5,5,5	5.62	3 (60%)
2	GOL	E	998	-	5,5,5	4.59	5 (100%)	5,5,5	5.59	3 (60%)
2	GOL	F	998	-	5,5,5	4.77	5 (100%)	5,5,5	5.39	3 (60%)

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	398	-	-	0/4/4/4	0/0/0/0
2	GOL	B	498	-	-	0/4/4/4	0/0/0/0
2	GOL	C	998	-	-	0/4/4/4	0/0/0/0
2	GOL	D	698	-	-	0/4/4/4	0/0/0/0
2	GOL	E	998	-	-	0/4/4/4	0/0/0/0
2	GOL	F	998	-	-	0/4/4/4	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	998	GOL	C3-C2	-8.32	1.20	1.52
2	A	398	GOL	C3-C2	-8.21	1.21	1.52
2	D	698	GOL	C3-C2	-8.14	1.21	1.52
2	B	498	GOL	C3-C2	-8.13	1.21	1.52
2	F	998	GOL	C3-C2	-7.91	1.22	1.52
2	E	998	GOL	C3-C2	-7.66	1.23	1.52
2	A	398	GOL	O2-C2	-3.68	1.32	1.43
2	A	398	GOL	C1-C2	-3.50	1.38	1.52
2	C	998	GOL	O2-C2	-3.47	1.33	1.43
2	C	998	GOL	C1-C2	-3.42	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	498	GOL	O2-C2	-3.33	1.33	1.43
2	D	698	GOL	C1-C2	-3.28	1.39	1.52
2	F	998	GOL	C1-C2	-3.27	1.39	1.52
2	E	998	GOL	C1-C2	-3.25	1.39	1.52
2	B	498	GOL	C1-C2	-3.21	1.40	1.52
2	F	998	GOL	O2-C2	-3.01	1.34	1.43
2	D	698	GOL	O2-C2	-2.90	1.34	1.43
2	E	998	GOL	O2-C2	-2.68	1.35	1.43
2	B	498	GOL	O3-C3	3.16	1.56	1.42
2	C	998	GOL	O3-C3	3.19	1.56	1.42
2	A	398	GOL	O3-C3	3.24	1.56	1.42
2	F	998	GOL	O3-C3	3.33	1.56	1.42
2	D	698	GOL	O3-C3	3.39	1.57	1.42
2	E	998	GOL	O3-C3	3.51	1.57	1.42
2	C	998	GOL	O1-C1	4.01	1.59	1.42
2	E	998	GOL	O1-C1	4.07	1.59	1.42
2	D	698	GOL	O1-C1	4.23	1.60	1.42
2	A	398	GOL	O1-C1	4.27	1.60	1.42
2	B	498	GOL	O1-C1	4.49	1.61	1.42
2	F	998	GOL	O1-C1	4.53	1.61	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	998	GOL	O1-C1-C2	2.78	123.65	110.18
2	E	998	GOL	O1-C1-C2	2.90	124.25	110.18
2	D	698	GOL	O1-C1-C2	2.95	124.50	110.18
2	C	998	GOL	O1-C1-C2	3.01	124.79	110.18
2	A	398	GOL	O1-C1-C2	3.23	125.84	110.18
2	B	498	GOL	O1-C1-C2	3.23	125.85	110.18
2	F	998	GOL	O2-C2-C3	6.49	138.40	108.65
2	D	698	GOL	O2-C2-C3	6.75	139.60	108.65
2	B	498	GOL	O2-C2-C3	6.78	139.73	108.65
2	C	998	GOL	O2-C2-C3	6.78	139.74	108.65
2	E	998	GOL	O2-C2-C3	6.84	140.00	108.65
2	A	398	GOL	O2-C2-C3	6.90	140.30	108.65
2	F	998	GOL	O3-C3-C2	9.76	157.52	110.18
2	A	398	GOL	O3-C3-C2	9.84	157.90	110.18
2	B	498	GOL	O3-C3-C2	9.92	158.27	110.18
2	E	998	GOL	O3-C3-C2	10.04	158.87	110.18
2	C	998	GOL	O3-C3-C2	10.11	159.21	110.18
2	D	698	GOL	O3-C3-C2	10.14	159.38	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	261/303 (86%)	-0.06	4 (1%)	76 71	25, 43, 73, 94	0
1	B	244/303 (80%)	0.02	16 (6%)	22 16	21, 38, 72, 94	0
1	C	267/303 (88%)	0.08	14 (5%)	31 24	25, 44, 81, 96	0
1	D	248/303 (81%)	-0.01	13 (5%)	31 24	28, 44, 77, 92	0
1	E	256/303 (84%)	0.62	32 (12%)	5 3	36, 69, 97, 100	0
1	F	241/303 (79%)	0.45	23 (9%)	10 6	40, 69, 91, 102	0
All	All	1517/1818 (83%)	0.18	102 (6%)	21 15	21, 50, 89, 102	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	882	THR	6.0
1	D	899	THR	5.9
1	B	769	ARG	5.8
1	D	772	VAL	5.8
1	E	949	ASN	5.7
1	C	860	VAL	5.4
1	D	897	ASP	5.0
1	C	897	ASP	4.8
1	F	770	ASN	4.7
1	E	980	TRP	4.7
1	C	883	SER	4.6
1	E	900	GLY	4.6
1	B	770	ASN	4.6
1	E	901	HIS	4.5
1	B	609	ALA	4.4
1	D	770	ASN	4.4
1	C	899	THR	4.3
1	E	924	THR	4.2
1	C	770	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	938	VAL	4.0
1	E	995	LYS	4.0
1	B	608	GLY	3.9
1	E	945	ASP	3.9
1	E	922	PHE	3.8
1	E	780	LYS	3.7
1	C	896	LEU	3.7
1	F	949	ASN	3.7
1	E	950	LYS	3.7
1	F	782	SER	3.6
1	C	884	ALA	3.5
1	F	781	LYS	3.5
1	E	896	LEU	3.4
1	F	924	THR	3.3
1	F	769	ARG	3.3
1	D	900	GLY	3.3
1	B	781	LYS	3.3
1	D	901	HIS	3.3
1	C	885	ILE	3.2
1	F	902	TYR	3.2
1	C	772	VAL	3.2
1	B	901	HIS	3.1
1	E	966	PRO	3.1
1	E	660	ALA	3.0
1	E	959	ARG	3.0
1	E	925	GLY	3.0
1	E	633	THR	3.0
1	F	610	PHE	3.0
1	F	606	GLY	2.9
1	F	631	ARG	2.9
1	F	945	ASP	2.9
1	F	847	ARG	2.9
1	F	887	THR	2.8
1	F	845	GLU	2.8
1	E	923	SER	2.8
1	F	809	ARG	2.8
1	B	610	PHE	2.8
1	F	947	ASP	2.8
1	E	770	ASN	2.7
1	E	920	TYR	2.7
1	E	962	ILE	2.7
1	D	769	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	633	THR	2.6
1	D	898	GLY	2.6
1	E	968	LYS	2.6
1	E	610	PHE	2.6
1	B	635	GLU	2.5
1	A	610	PHE	2.5
1	A	995	LYS	2.5
1	B	647	LEU	2.5
1	F	635	GLU	2.5
1	E	895	VAL	2.5
1	F	648	ALA	2.5
1	B	661	ALA	2.4
1	E	944	PRO	2.4
1	E	609	ALA	2.4
1	F	925	GLY	2.4
1	B	782	SER	2.4
1	D	845	GLU	2.4
1	E	965	ASP	2.4
1	C	644	VAL	2.4
1	E	635	GLU	2.4
1	B	632	HIS	2.3
1	E	893	THR	2.3
1	B	648	ALA	2.3
1	A	885	ILE	2.3
1	B	631	ARG	2.3
1	D	611	GLY	2.2
1	D	771	PHE	2.2
1	C	859	ASN	2.2
1	E	946	PHE	2.2
1	A	901	HIS	2.2
1	F	937	SER	2.2
1	B	836	LEU	2.1
1	B	660	ALA	2.1
1	D	780	LYS	2.1
1	E	941	GLU	2.1
1	E	942	PHE	2.1
1	E	634	GLU	2.1
1	C	771	PHE	2.1
1	F	984	LYS	2.1
1	D	809	ARG	2.0
1	C	786	ILE	2.0



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

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

## 6.3 Carbohydrates [i](#)

There are no 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	F	998	6/6	0.70	0.33	3.64	77,81,82,82	0
2	GOL	D	698	6/6	0.88	0.26	2.94	46,56,58,65	0
2	GOL	C	998	6/6	0.94	0.20	1.51	37,47,49,52	0
2	GOL	A	398	6/6	0.95	0.18	0.85	33,46,50,61	0
2	GOL	E	998	6/6	0.88	0.19	0.79	48,57,60,62	0
2	GOL	B	498	6/6	0.96	0.21	0.71	40,47,50,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.