



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:42 PM GMT

PDB ID : 3UO9  
Title : Crystal Structure of Human GAC in Complex with Glutamate and BPTES  
Authors : DeLaBarre, B.; Gross, S.; Cheng, F.; Gao, Y.; Jha, A.; Jiang, F.; Song, J.J.; Wei, W.; Hurov, J.B.  
Deposited on : 2011-11-16  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

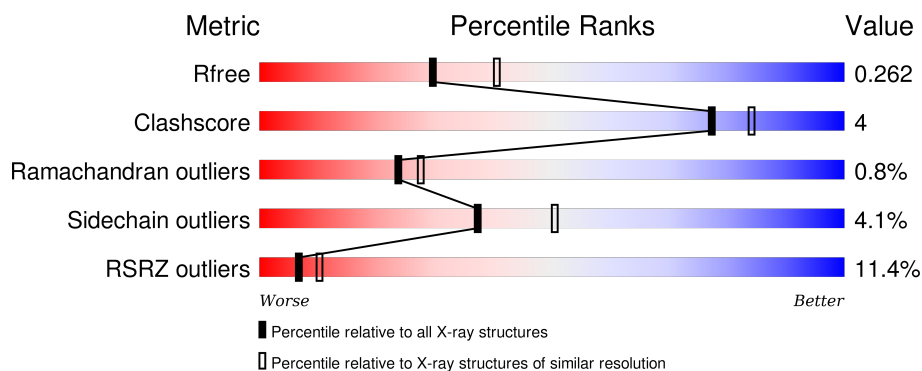
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	534	<div> <div>9%</div> <div>68% 8% • 23%</div> </div>
1	B	534	<div> <div>8%</div> <div>67% 6% • 25%</div> </div>
1	C	534	<div> <div>10%</div> <div>67% 7% •• 24%</div> </div>
1	D	534	<div> <div>7%</div> <div>67% 8% • 24%</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	2	-	-	X	-
2	GOL	C	3	-	-	-	X
2	GOL	D	1	-	-	X	-
3	04A	B	2	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13319 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 Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3208	2044	541	595	28			
1	B	401	Total	C	N	O	S	0	0	0
			3134	2000	527	579	28			
1	C	404	Total	C	N	O	S	0	0	0
			3161	2019	531	583	28			
1	D	408	Total	C	N	O	S	0	0	0
			3191	2034	538	591	28			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	640	HIS	-	EXPRESSION TAG	UNP O94925
A	641	HIS	-	EXPRESSION TAG	UNP O94925
A	642	HIS	-	EXPRESSION TAG	UNP O94925
A	643	HIS	-	EXPRESSION TAG	UNP O94925
A	644	HIS	-	EXPRESSION TAG	UNP O94925
A	645	HIS	-	EXPRESSION TAG	UNP O94925
B	640	HIS	-	EXPRESSION TAG	UNP O94925
B	641	HIS	-	EXPRESSION TAG	UNP O94925
B	642	HIS	-	EXPRESSION TAG	UNP O94925
B	643	HIS	-	EXPRESSION TAG	UNP O94925
B	644	HIS	-	EXPRESSION TAG	UNP O94925
B	645	HIS	-	EXPRESSION TAG	UNP O94925
C	640	HIS	-	EXPRESSION TAG	UNP O94925
C	641	HIS	-	EXPRESSION TAG	UNP O94925
C	642	HIS	-	EXPRESSION TAG	UNP O94925
C	643	HIS	-	EXPRESSION TAG	UNP O94925
C	644	HIS	-	EXPRESSION TAG	UNP O94925
C	645	HIS	-	EXPRESSION TAG	UNP O94925
D	640	HIS	-	EXPRESSION TAG	UNP O94925
D	641	HIS	-	EXPRESSION TAG	UNP O94925
D	642	HIS	-	EXPRESSION TAG	UNP O94925

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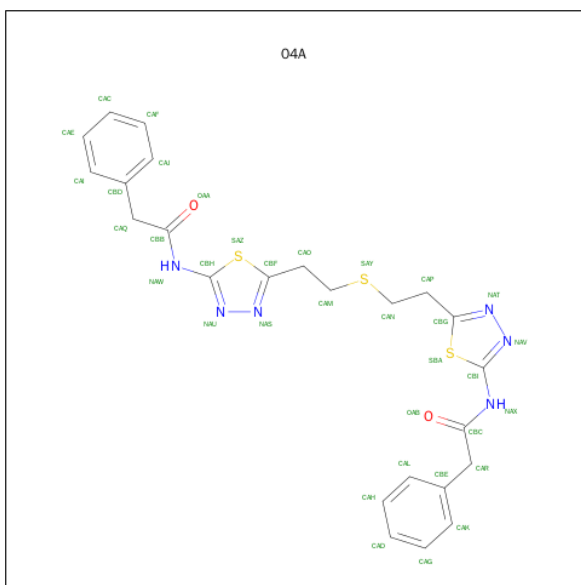
Chain	Residue	Modelled	Actual	Comment	Reference
D	643	HIS	-	EXPRESSION TAG	UNP O94925
D	644	HIS	-	EXPRESSION TAG	UNP O94925
D	645	HIS	-	EXPRESSION TAG	UNP O94925

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 3 is N,N'-[SULFANEDIYLBIS(ETHANE-2,1-DIYL-1,3,4-THIADIAZOLE-5,2-DIYL)]BIS(2-PHENYLACETAMIDE) (three-letter code: 04A) (formula:  $C_{24}H_{24}N_6O_2S_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 35	C 24	N 6	O 2	S 3	0	0
3	C	1	Total 35	C 24	N 6	O 2	S 3	0	0

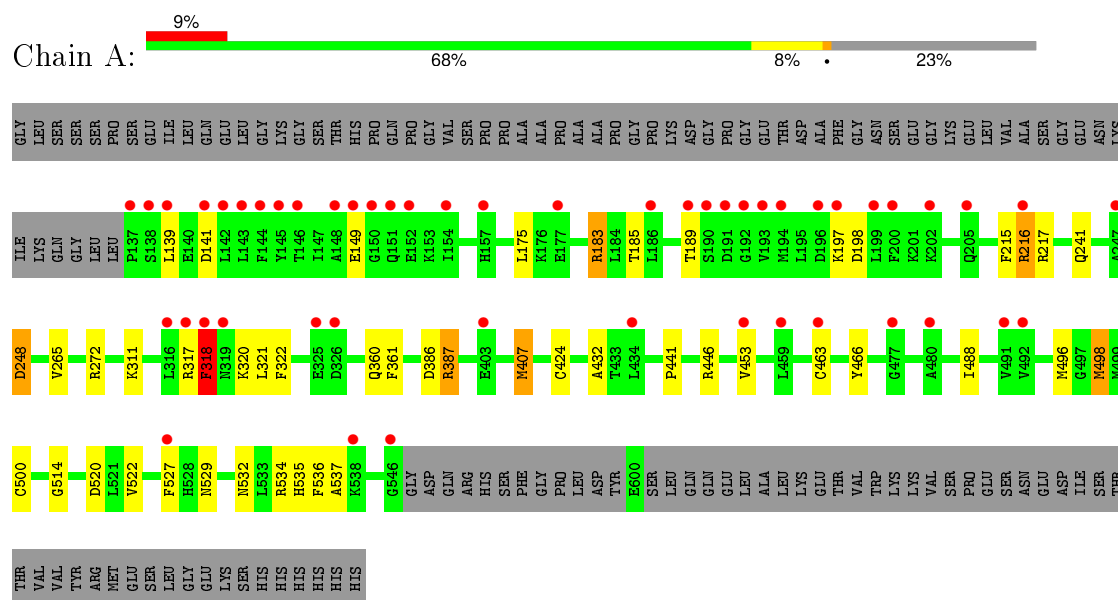
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	115	Total O 115 115	0	0
4	B	132	Total O 132 132	0	0
4	C	145	Total O 145 145	0	0
4	D	139	Total O 139 139	0	0

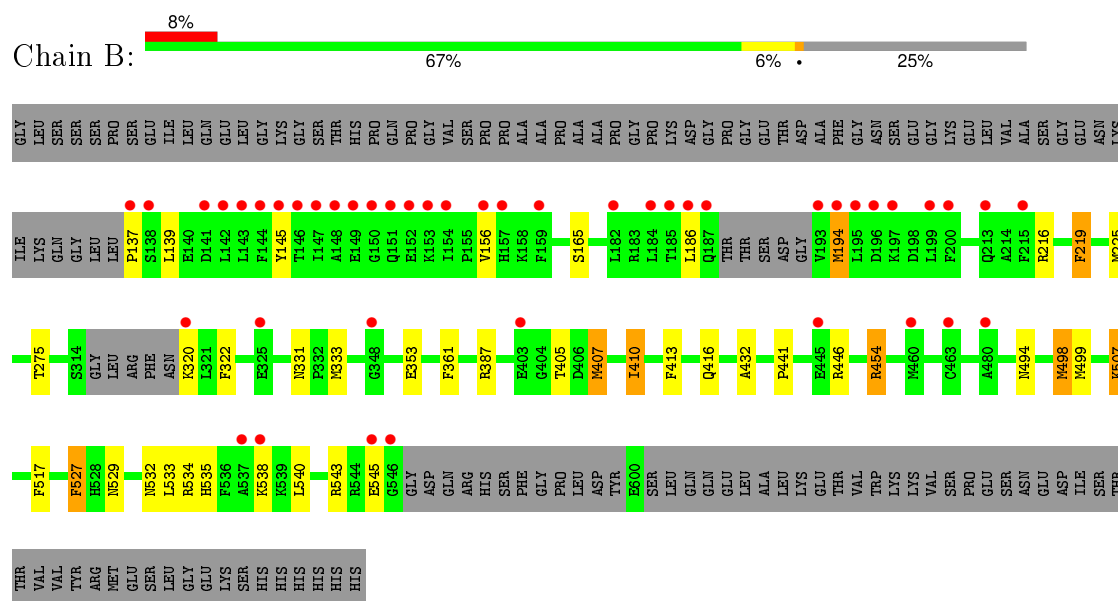
### 3 Residue-property plots [i](#)

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.

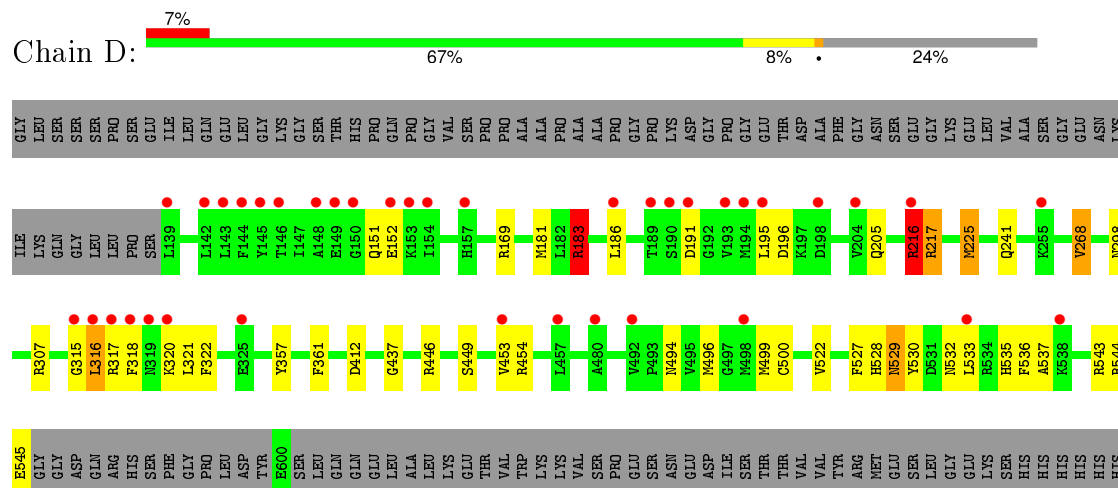
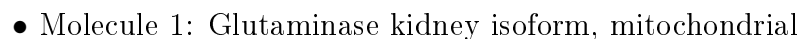
- Molecule 1: Glutaminase kidney isoform, mitochondrial



- Molecule 1: Glutaminase kidney isoform, mitochondrial



- Chain C:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.12Å 139.43Å 177.71Å 90.00° 93.73° 90.00°	Depositor
Resolution (Å)	45.09 – 2.30 46.21 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.09-2.30) 99.0 (46.21-2.28)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.195 , 0.249 0.225 , 0.262	Depositor DCC
$R_{free}$ test set	5390 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 36.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 109070 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13319	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 04A

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	0.96	3/3279 (0.1%)	1.06	18/4424 (0.4%)
1	B	0.93	0/3202	1.03	17/4317 (0.4%)
1	C	0.96	0/3230	1.08	20/4356 (0.5%)
1	D	0.96	1/3261 (0.0%)	1.08	22/4400 (0.5%)
All	All	0.95	4/12972 (0.0%)	1.06	77/17497 (0.4%)

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	6
1	B	0	3
1	C	0	5
1	D	0	6
All	All	0	20

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	463	CYS	CB-SG	-6.58	1.71	1.82
1	A	424	CYS	CB-SG	-6.04	1.72	1.82
1	A	500	CYS	CB-SG	-5.57	1.72	1.81
1	D	500	CYS	CB-SG	-5.51	1.72	1.81

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	543	ARG	NE-CZ-NH2	-13.25	113.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	454	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	C	534	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	B	407	MET	CG-SD-CE	-8.81	86.10	100.20
1	A	216	ARG	NE-CZ-NH1	8.27	124.43	120.30
1	D	543	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	C	526	ASN	N-CA-CB	7.86	124.75	110.60
1	A	527	PHE	CB-CG-CD2	-7.85	115.31	120.80
1	B	527	PHE	CB-CG-CD2	-7.55	115.52	120.80
1	D	527	PHE	CB-CG-CD2	-7.25	115.73	120.80
1	C	322	PHE	CB-CG-CD1	7.24	125.87	120.80
1	D	527	PHE	CB-CG-CD1	7.19	125.83	120.80
1	B	499	MET	CG-SD-CE	7.12	111.60	100.20
1	D	536	PHE	CB-CG-CD2	7.03	125.72	120.80
1	D	183	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	C	527	PHE	CB-CG-CD1	6.83	125.58	120.80
1	D	322	PHE	CB-CG-CD1	6.83	125.58	120.80
1	C	499	MET	CG-SD-CE	6.81	111.09	100.20
1	C	322	PHE	CB-CG-CD2	-6.80	116.04	120.80
1	D	225	MET	CG-SD-CE	-6.79	89.33	100.20
1	A	322	PHE	CB-CG-CD1	6.74	125.52	120.80
1	D	496	MET	CG-SD-CE	-6.68	89.52	100.20
1	C	216	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	A	407	MET	CG-SD-CE	-6.60	89.64	100.20
1	B	322	PHE	CB-CG-CD1	6.59	125.41	120.80
1	B	387	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	C	216	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	B	194	MET	CG-SD-CE	-6.46	89.87	100.20
1	D	499	MET	CG-SD-CE	6.38	110.41	100.20
1	A	522	VAL	CA-CB-CG2	-6.36	101.37	110.90
1	D	181	MET	CG-SD-CE	-6.32	90.08	100.20
1	D	536	PHE	CB-CG-CD1	-6.26	116.42	120.80
1	A	318	PHE	CB-CG-CD2	6.25	125.17	120.80
1	A	248	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	215	PHE	CB-CG-CD1	-6.23	116.44	120.80
1	A	496	MET	CG-SD-CE	-6.20	90.27	100.20
1	C	454	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	322	PHE	CB-CG-CD2	-6.12	116.51	120.80
1	A	215	PHE	CB-CG-CD2	6.09	125.06	120.80
1	A	183	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	D	322	PHE	CB-CG-CD2	-6.06	116.56	120.80
1	B	527	PHE	CB-CG-CD1	6.02	125.01	120.80
1	C	506	ASP	CB-CG-OD1	6.01	123.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	506	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	D	183	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	C	446	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	D	216	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	C	526	ASN	CA-CB-CG	5.84	126.26	113.40
1	B	543	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	322	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	B	219	PHE	CB-CG-CD1	5.76	124.83	120.80
1	C	508	MET	CG-SD-CE	-5.74	91.01	100.20
1	B	145	TYR	CB-CG-CD1	5.74	124.44	121.00
1	C	527	PHE	CB-CG-CD2	-5.73	116.79	120.80
1	C	446	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	498	MET	CG-SD-CE	-5.72	91.05	100.20
1	C	489	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	272	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	B	219	PHE	CB-CG-CD2	-5.69	116.82	120.80
1	D	357	TYR	CB-CG-CD1	-5.64	117.62	121.00
1	B	454	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	498	MET	CG-SD-CE	-5.60	91.24	100.20
1	D	522	VAL	CA-CB-CG2	-5.56	102.56	110.90
1	C	522	VAL	CA-CB-CG2	-5.56	102.56	110.90
1	B	145	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	A	527	PHE	CB-CG-CD1	5.53	124.67	120.80
1	C	215	PHE	CB-CG-CD1	-5.52	116.94	120.80
1	A	318	PHE	CB-CG-CD1	-5.50	116.95	120.80
1	D	530	TYR	CB-CG-CD1	-5.29	117.82	121.00
1	A	183	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	466	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	B	410	ILE	CA-CB-CG1	-5.13	101.24	111.00
1	D	544	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	545	GLU	N-CA-CB	5.10	119.77	110.60
1	D	545	GLU	N-CA-C	-5.09	97.26	111.00
1	D	268	VAL	CA-CB-CG1	5.04	118.47	110.90
1	C	219	PHE	CB-CG-CD1	5.00	124.30	120.80

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	ARG	Sidechain
1	A	317	ARG	Sidechain
1	A	387	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	446	ARG	Sidechain
1	A	534	ARG	Sidechain
1	A	536	PHE	Mainchain
1	B	446	ARG	Sidechain
1	B	454	ARG	Sidechain
1	B	534	ARG	Sidechain
1	C	216	ARG	Sidechain
1	C	307	ARG	Sidechain
1	C	318	PHE	Peptide
1	C	446	ARG	Sidechain
1	C	534	ARG	Sidechain
1	D	169	ARG	Sidechain
1	D	183	ARG	Sidechain
1	D	216	ARG	Sidechain
1	D	307	ARG	Sidechain
1	D	446	ARG	Sidechain
1	D	454	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3208	0	3181	14	0
1	B	3134	0	3109	25	0
1	C	3161	0	3136	27	0
1	D	3191	0	3164	29	0
2	A	12	0	16	12	0
2	C	6	0	8	0	0
2	D	6	0	7	16	0
3	B	35	0	22	10	0
3	C	35	0	24	6	0
4	A	115	0	0	2	0
4	B	132	0	0	0	0
4	C	145	0	0	2	0
4	D	139	0	0	3	0
All	All	13319	0	12667	94	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 4.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2:04A:CAE	1:D:317:ARG:HH12	1.19	1.24
3:B:2:04A:HAE	1:D:317:ARG:NH1	1.14	1.10
2:A:2:GOL:H32	1:C:532:ASN:HB2	1.28	1.07
3:B:2:04A:CAE	1:D:317:ARG:NH1	1.80	1.02
1:D:532:ASN:HD22	1:D:535:HIS:H	1.15	0.95
1:D:437:GLY:HA2	2:D:1:GOL:H32	1.49	0.93
1:B:532:ASN:HB2	2:D:1:GOL:H31	1.57	0.86
1:D:437:GLY:HA2	2:D:1:GOL:C3	2.07	0.84
1:C:532:ASN:HD22	1:C:535:HIS:H	1.24	0.82
2:A:2:GOL:H32	1:C:532:ASN:CB	2.12	0.78
3:C:1:04A:OAB	1:D:320:LYS:HD2	1.83	0.77
1:A:532:ASN:HD22	1:A:535:HIS:H	1.30	0.76
3:C:1:04A:HANA	1:D:320:LYS:O	1.90	0.71
1:B:405:THR:HG23	1:B:410:ILE:CD1	2.21	0.71
3:B:2:04A:HAE	1:D:317:ARG:HH12	0.70	0.70
1:D:437:GLY:CA	2:D:1:GOL:H32	2.23	0.68
1:B:532:ASN:HD22	1:B:535:HIS:H	1.43	0.67
2:D:1:GOL:H11	4:D:670:HOH:O	1.92	0.66
1:B:532:ASN:HB2	2:D:1:GOL:C3	2.26	0.66
1:B:507:LYS:HD3	1:B:507:LYS:H	1.62	0.64
2:A:2:GOL:H12	1:C:532:ASN:H	1.63	0.63
1:D:298:ASN:HD22	1:D:449:SER:H	1.48	0.61
1:C:320:LYS:HD2	3:C:1:04A:OAA	2.00	0.60
1:A:529:ASN:HD21	1:C:529:ASN:HD21	1.50	0.60
1:C:250:ILE:HG13	1:C:380:SER:HB3	1.85	0.59
1:B:494:ASN:HD21	1:D:533:LEU:H	1.51	0.58
1:D:437:GLY:CA	2:D:1:GOL:C3	2.78	0.58
2:A:2:GOL:H12	4:A:673:HOH:O	2.04	0.58
1:B:320:LYS:HG2	3:B:2:04A:SBA	2.44	0.57
1:B:405:THR:HG23	1:B:410:ILE:HD12	1.88	0.56
1:B:507:LYS:CD	1:B:507:LYS:H	2.18	0.55
1:C:267:THR:HG23	1:C:269:ASP:H	1.71	0.55
1:B:532:ASN:HB2	2:D:1:GOL:C2	2.36	0.55
1:A:453:VAL:CG1	2:A:2:GOL:H2	2.36	0.55
1:C:525:CYS:O	1:C:526:ASN:CB	2.54	0.54
1:B:494:ASN:ND2	1:D:533:LEU:H	2.05	0.54
1:A:185:THR:O	1:A:189:THR:HG23	2.08	0.54
1:B:413:PHE:HA	1:B:416:GLN:HE21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ASN:HD21	1:C:529:ASN:ND2	2.06	0.54
1:C:267:THR:HG21	1:C:271:GLN:OE1	2.09	0.53
1:B:533:LEU:H	1:D:494:ASN:HD21	1.57	0.53
1:C:320:LYS:NZ	3:C:1:04A:CAJ	2.71	0.53
1:D:453:VAL:HG12	2:D:1:GOL:O2	2.10	0.52
1:A:386:ASP:OD1	2:A:4:GOL:O3	2.28	0.52
1:D:532:ASN:ND2	1:D:535:HIS:H	1.96	0.51
1:D:183:ARG:HD2	4:D:677:HOH:O	2.09	0.51
1:C:320:LYS:HZ2	3:C:1:04A:CAJ	2.24	0.51
2:D:1:GOL:C1	4:D:670:HOH:O	2.55	0.50
1:C:234:LEU:HD22	1:C:520:ASP:HB3	1.92	0.50
1:A:320:LYS:HE3	3:B:2:04A:CAF	2.41	0.50
2:A:2:GOL:C1	4:A:673:HOH:O	2.57	0.50
1:D:453:VAL:HG11	2:D:1:GOL:H32	1.93	0.50
1:B:529:ASN:HD21	1:D:529:ASN:ND2	2.09	0.49
1:C:341:VAL:HA	1:C:344:LEU:HD22	1.94	0.49
1:B:320:LYS:HE2	3:B:2:04A:SBA	2.49	0.49
1:B:320:LYS:CG	3:B:2:04A:SBA	3.01	0.49
2:A:2:GOL:C1	1:C:532:ASN:H	2.26	0.48
1:B:156:VAL:HG21	1:B:186:LEU:HD11	1.94	0.48
1:C:534:ARG:CG	1:C:534:ARG:HH11	2.25	0.48
2:A:2:GOL:H12	1:C:532:ASN:HB2	1.96	0.48
1:B:533:LEU:H	1:D:494:ASN:ND2	2.12	0.47
1:D:315:GLY:C	1:D:317:ARG:H	2.19	0.46
1:D:437:GLY:CA	2:D:1:GOL:H31	2.45	0.46
1:C:525:CYS:O	1:C:540:LEU:O	2.32	0.46
1:A:265:VAL:HG22	1:A:498:MET:HG2	1.97	0.46
1:C:335:ASN:HD22	1:C:388:ASN:HD21	1.62	0.46
1:B:320:LYS:CE	3:B:2:04A:SBA	3.04	0.46
1:D:216:ARG:HH11	1:D:216:ARG:HG3	1.81	0.45
1:A:311:LYS:HZ3	1:C:475:HIS:HE1	1.65	0.45
1:A:320:LYS:HE3	3:B:2:04A:CAJ	2.47	0.45
1:B:532:ASN:CB	2:D:1:GOL:H31	2.36	0.45
1:D:298:ASN:ND2	1:D:449:SER:H	2.13	0.45
1:B:432:ALA:HB1	1:B:441:PRO:HG3	1.99	0.45
1:C:267:THR:CG2	1:C:269:ASP:H	2.29	0.44
3:C:1:04A:SAZ	3:C:1:04A:OAA	2.75	0.44
1:D:437:GLY:N	2:D:1:GOL:C3	2.80	0.44
1:D:437:GLY:HA2	2:D:1:GOL:H31	1.96	0.44
1:A:453:VAL:HG11	2:A:2:GOL:H2	2.00	0.43
1:C:532:ASN:ND2	1:C:535:HIS:H	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:ARG:O	1:D:217:ARG:HB2	2.19	0.43
1:A:318:PHE:HA	1:A:321:LEU:HD23	2.00	0.43
1:B:498:MET:HE1	1:B:517:PHE:CE2	2.53	0.43
1:C:525:CYS:O	1:C:526:ASN:HB3	2.19	0.42
1:D:437:GLY:H	2:D:1:GOL:C3	2.32	0.42
1:B:165:SER:HB2	1:B:225:MET:SD	2.60	0.42
1:C:480:ALA:HB2	1:C:490:LEU:HD12	2.02	0.41
1:A:488:ILE:HD12	1:A:514:GLY:HA3	2.02	0.41
1:B:331:ASN:HD22	1:B:333:MET:H	1.67	0.41
2:A:2:GOL:H31	4:C:720:HOH:O	2.20	0.41
1:A:432:ALA:HB1	1:A:441:PRO:HG3	2.03	0.41
1:C:216:ARG:HD2	1:C:216:ARG:HA	1.87	0.40
2:A:2:GOL:C3	4:C:720:HOH:O	2.68	0.40
1:B:532:ASN:HD22	1:B:535:HIS:N	2.12	0.40
1:C:335:ASN:ND2	1:C:388:ASN:HD21	2.18	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	408/534 (76%)	398 (98%)	7 (2%)	3 (1%)	26	31
1	B	394/534 (74%)	379 (96%)	12 (3%)	3 (1%)	24	27
1	C	397/534 (74%)	385 (97%)	10 (2%)	2 (0%)	34	41
1	D	405/534 (76%)	390 (96%)	10 (2%)	5 (1%)	16	16
All	All	1604/2136 (75%)	1552 (97%)	39 (2%)	13 (1%)	24	27

All (13) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	217	ARG
1	B	527	PHE
1	B	538	LYS
1	C	526	ASN
1	D	217	ARG
1	D	528	HIS
1	D	537	ALA
1	B	219	PHE
1	D	241	GLN
1	A	241	GLN
1	C	197	LYS
1	D	316	LEU
1	A	537	ALA

### 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	356/458 (78%)	342 (96%)	14 (4%)	39	53
1	B	348/458 (76%)	337 (97%)	11 (3%)	46	62
1	C	351/458 (77%)	334 (95%)	17 (5%)	31	42
1	D	354/458 (77%)	338 (96%)	16 (4%)	34	46
All	All	1409/1832 (77%)	1351 (96%)	58 (4%)	37	50

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	LEU
1	A	141	ASP
1	A	149	GLU
1	A	175	LEU
1	A	197	LYS
1	A	198	ASP
1	A	216	ARG
1	A	248	ASP
1	A	318	PHE

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Mol	Chain	Res	Type
1	A	360	GLN
1	A	361	PHE
1	A	387	ARG
1	A	407	MET
1	A	520	ASP
1	B	137	PRO
1	B	139	LEU
1	B	194	MET
1	B	216	ARG
1	B	275	THR
1	B	353	GLU
1	B	361	PHE
1	B	407	MET
1	B	507	LYS
1	B	540	LEU
1	B	545	GLU
1	C	136	LEU
1	C	143	LEU
1	C	153	LYS
1	C	194	MET
1	C	195	LEU
1	C	216	ARG
1	C	218	LYS
1	C	250	ILE
1	C	267	THR
1	C	288	VAL
1	C	344	LEU
1	C	361	PHE
1	C	397	GLU
1	C	505	LEU
1	C	507	LYS
1	C	520	ASP
1	C	540	LEU
1	D	151	GLN
1	D	152	GLU
1	D	186	LEU
1	D	191	ASP
1	D	195	LEU
1	D	196	ASP
1	D	205	GLN
1	D	216	ARG
1	D	225	MET

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Mol	Chain	Res	Type
1	D	268	VAL
1	D	316	LEU
1	D	318	PHE
1	D	321	LEU
1	D	361	PHE
1	D	412	ASP
1	D	529	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	271	GLN
1	A	330	HIS
1	A	335	ASN
1	A	388	ASN
1	A	510	ASN
1	A	529	ASN
1	A	532	ASN
1	B	205	GLN
1	B	207	ASN
1	B	331	ASN
1	B	388	ASN
1	B	416	GLN
1	B	494	ASN
1	B	510	ASN
1	B	532	ASN
1	C	151	GLN
1	C	157	HIS
1	C	205	GLN
1	C	319	ASN
1	C	388	ASN
1	C	461	HIS
1	C	475	HIS
1	C	510	ASN
1	C	519	HIS
1	C	529	ASN
1	C	532	ASN
1	D	187	GLN
1	D	273	HIS
1	D	298	ASN
1	D	330	HIS

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Mol	Chain	Res	Type
1	D	351	ASN
1	D	388	ASN
1	D	494	ASN
1	D	510	ASN
1	D	519	HIS
1	D	529	ASN
1	D	532	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	2	-	5,5,5	0.79	0	5,5,5	1.32	0
2	GOL	A	4	-	5,5,5	0.39	0	5,5,5	0.62	0
3	04A	B	2	-	34,38,38	2.59	7 (20%)	27,49,49	0.80	0
3	04A	C	1	-	34,38,38	2.75	7 (20%)	27,49,49	1.03	2 (7%)
2	GOL	C	3	-	5,5,5	0.36	0	5,5,5	0.72	0
2	GOL	D	1	-	5,5,5	1.29	1 (20%)	5,5,5	1.44	1 (20%)

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	2	-	-	0/4/4/4	0/0/0/0
2	GOL	A	4	-	-	0/4/4/4	0/0/0/0
3	04A	B	2	-	-	0/18/24/24	0/2/4/4
3	04A	C	1	-	-	0/18/24/24	0/2/4/4
2	GOL	C	3	-	-	0/4/4/4	0/0/0/0
2	GOL	D	1	-	-	0/4/4/4	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	04A	CAQ-CBD	-8.57	1.36	1.51
3	B	2	04A	CAQ-CBD	-7.35	1.38	1.51
3	B	2	04A	CAR-CBE	-5.64	1.41	1.51
3	C	1	04A	CAR-CBE	-4.12	1.44	1.51
3	B	2	04A	CBF-SAZ	-4.06	1.60	1.73
3	C	1	04A	CBF-SAZ	-3.20	1.63	1.73
2	D	1	GOL	O2-C2	-2.30	1.36	1.43
3	C	1	04A	CBH-NAW	-2.15	1.33	1.36
3	B	2	04A	CBF-NAS	2.67	1.37	1.33
3	C	1	04A	CBF-NAS	3.18	1.38	1.33
3	B	2	04A	NAT-NAV	3.26	1.44	1.37
3	B	2	04A	CAO-CBF	4.40	1.52	1.49
3	C	1	04A	CAO-CBF	6.79	1.53	1.49
3	B	2	04A	CAP-CBG	7.43	1.53	1.49
3	C	1	04A	CAP-CBG	8.29	1.54	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	04A	CAN-SAY-CAM	-2.51	94.25	101.93
2	D	1	GOL	O1-C1-C2	2.22	120.94	110.18
3	C	1	04A	CAJ-CBD-CAI	2.32	121.84	118.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2	GOL	11	0
2	A	4	GOL	1	0
3	B	2	04A	10	0
3	C	1	04A	6	0
2	D	1	GOL	16	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	411/534 (76%)	0.76	50 (12%) 5 9	17, 28, 70, 82	0
1	B	401/534 (75%)	0.67	45 (11%) 7 10	17, 27, 61, 81	0
1	C	404/534 (75%)	0.74	52 (12%) 5 7	16, 26, 65, 81	0
1	D	408/534 (76%)	0.66	38 (9%) 11 16	15, 26, 66, 78	0
All	All	1624/2136 (76%)	0.71	185 (11%) 7 10	15, 27, 66, 82	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	PHE	8.9
1	C	186	LEU	8.7
1	A	317	ARG	8.6
1	A	546	GLY	7.7
1	B	186	LEU	7.0
1	B	145	TYR	6.9
1	D	317	ARG	6.7
1	B	148	ALA	6.7
1	D	190	SER	6.6
1	B	150	GLY	6.4
1	B	149	GLU	6.2
1	C	195	LEU	6.1
1	A	139	LEU	6.0
1	D	191	ASP	5.9
1	D	144	PHE	5.9
1	A	137	PRO	5.8
1	C	145	TYR	5.7
1	A	191	ASP	5.6
1	C	150	GLY	5.5
1	D	318	PHE	5.5
1	D	316	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	190	SER	5.3
1	C	136	LEU	5.3
1	A	144	PHE	5.2
1	A	142	LEU	5.1
1	C	193	VAL	4.8
1	C	152	GLU	4.8
1	B	195	LEU	4.8
1	C	149	GLU	4.8
1	A	138	SER	4.7
1	A	192	GLY	4.7
1	A	199	LEU	4.6
1	B	154	ILE	4.6
1	D	319	ASN	4.6
1	C	153	LYS	4.5
1	A	149	GLU	4.4
1	A	319	ASN	4.4
1	C	137	PRO	4.4
1	A	194	MET	4.3
1	C	154	ILE	4.3
1	B	546	GLY	4.3
1	B	320	LYS	4.2
1	D	142	LEU	4.2
1	B	144	PHE	4.2
1	D	195	LEU	4.1
1	D	193	VAL	4.0
1	C	142	LEU	4.0
1	C	463	CYS	4.0
1	D	315	GLY	4.0
1	C	196	ASP	4.0
1	C	159	PHE	3.9
1	B	199	LEU	3.9
1	C	156	VAL	3.9
1	C	537	ALA	3.9
1	D	150	GLY	3.8
1	B	152	GLU	3.8
1	C	197	LYS	3.7
1	C	194	MET	3.7
1	B	159	PHE	3.7
1	C	146	THR	3.7
1	C	546	GLY	3.7
1	A	193	VAL	3.7
1	B	146	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	138	SER	3.6
1	D	139	LEU	3.6
1	B	197	LYS	3.6
1	C	200	PHE	3.6
1	A	148	ALA	3.6
1	D	149	GLU	3.6
1	B	187	GLN	3.6
1	D	157	HIS	3.6
1	B	545	GLU	3.5
1	C	187	GLN	3.5
1	C	144	PHE	3.5
1	D	152	GLU	3.5
1	B	143	LEU	3.4
1	A	152	GLU	3.4
1	A	141	ASP	3.4
1	B	537	ALA	3.4
1	D	538	LYS	3.4
1	A	146	THR	3.3
1	D	320	LYS	3.3
1	B	196	ASP	3.3
1	B	142	LEU	3.3
1	D	145	TYR	3.3
1	B	138	SER	3.3
1	B	325	GLU	3.3
1	C	143	LEU	3.3
1	A	247	ALA	3.2
1	B	137	PRO	3.2
1	D	148	ALA	3.2
1	A	150	GLY	3.2
1	A	316	LEU	3.2
1	D	255	LYS	3.2
1	A	154	ILE	3.2
1	D	154	ILE	3.2
1	B	403	GLU	3.1
1	B	156	VAL	3.1
1	C	199	LEU	3.1
1	B	153	LYS	3.1
1	B	538	LYS	3.1
1	A	325	GLU	3.1
1	C	151	GLN	3.1
1	C	318	PHE	3.0
1	A	151	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	194	MET	3.0
1	C	545	GLU	3.0
1	A	189	THR	3.0
1	A	453	VAL	3.0
1	A	326	ASP	3.0
1	B	194	MET	3.0
1	B	463	CYS	2.9
1	D	216	ARG	2.9
1	A	157	HIS	2.9
1	D	186	LEU	2.9
1	B	200	PHE	2.9
1	C	403	GLU	2.9
1	B	147	ILE	2.9
1	A	216	ARG	2.8
1	A	196	ASP	2.8
1	C	141	ASP	2.8
1	C	225	MET	2.8
1	A	143	LEU	2.7
1	C	148	ALA	2.7
1	C	182	LEU	2.7
1	B	348	GLY	2.7
1	D	453	VAL	2.7
1	B	182	LEU	2.6
1	B	460	MET	2.6
1	C	213	GLN	2.6
1	C	325	GLU	2.6
1	B	151	GLN	2.6
1	A	480	ALA	2.6
1	D	204	VAL	2.6
1	A	527	PHE	2.6
1	A	202	LYS	2.6
1	A	186	LEU	2.6
1	B	193	VAL	2.6
1	C	184	LEU	2.6
1	C	147	ILE	2.6
1	A	492	VAL	2.5
1	B	185	THR	2.5
1	C	205	GLN	2.5
1	C	157	HIS	2.5
1	D	189	THR	2.5
1	A	463	CYS	2.5
1	D	146	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	491	VAL	2.4
1	C	326	ASP	2.4
1	A	459	LEU	2.4
1	A	434	LEU	2.4
1	C	538	LYS	2.4
1	B	184	LEU	2.3
1	C	314	SER	2.3
1	A	200	PHE	2.3
1	D	480	ALA	2.3
1	A	177	GLU	2.3
1	D	325	GLU	2.3
1	A	145	TYR	2.3
1	A	197	LYS	2.3
1	B	157	HIS	2.2
1	C	250	ILE	2.2
1	C	528	HIS	2.2
1	C	319	ASN	2.2
1	A	477	GLY	2.2
1	D	153	LYS	2.2
1	C	530	TYR	2.2
1	C	185	THR	2.2
1	D	533	LEU	2.1
1	B	480	ALA	2.1
1	D	492	VAL	2.1
1	A	538	LYS	2.1
1	A	205	GLN	2.1
1	C	498	MET	2.1
1	C	521	LEU	2.1
1	D	498	MET	2.1
1	B	141	ASP	2.1
1	B	215	PHE	2.0
1	B	213	GLN	2.0
1	A	403	GLU	2.0
1	D	143	LEU	2.0
1	B	445	GLU	2.0
1	D	198	ASP	2.0
1	D	457	LEU	2.0
1	C	525	CYS	2.0

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

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

### 6.3 Carbohydrates [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( $\text{\AA}^2$ )	Q<0.9
2	GOL	C	3	6/6	0.39	0.37	6.04	54,61,61,62	0
2	GOL	A	2	6/6	0.89	0.28	1.56	28,33,37,42	0
2	GOL	D	1	6/6	0.88	0.24	1.32	30,34,35,37	0
3	04A	B	2	35/35	0.78	0.26	0.11	56,69,83,84	0
2	GOL	A	4	6/6	0.81	0.16	-0.07	59,60,61,64	0
3	04A	C	1	35/35	0.89	0.21	-0.30	49,62,90,91	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.