



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2014 – 09:06 AM EDT

PDB ID : 3AXK  
Title : Structure of rice Rubisco in complex with NADP(H)  
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Deposited on : 2011-04-11  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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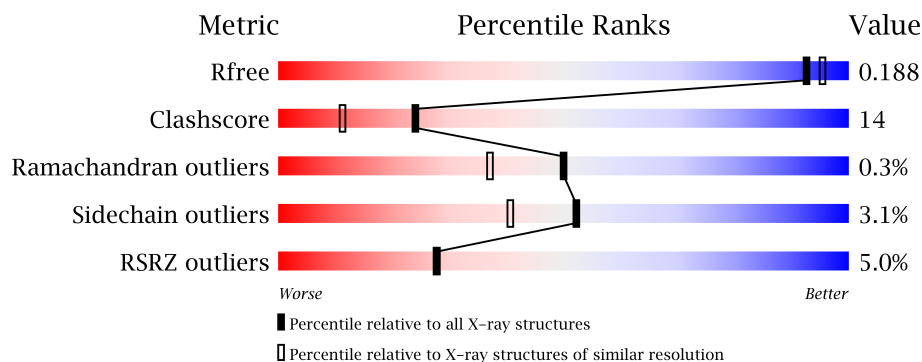
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : **FAILED**  
Xtriage (Phenix) : dev-1439  
EDS : stable23161  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23161

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	477	
1	B	477	
2	S	129	
2	T	129	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	A	501	-	X
3	GOL	A	502	-	X
3	GOL	B	503	-	X
3	GOL	B	504	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	NDP	A	479	-	X
5	NDP	A	480	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9992 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	0
			3384	2141	600	623	20			
1	B	430	Total	C	N	O	S	0	0	0
			3360	2125	597	618	20			

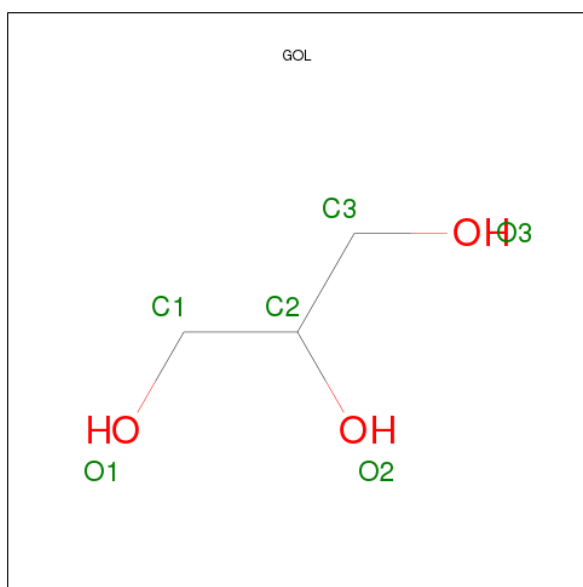
- Molecule 2 is a protein called Ribulose biphosphate carboxylase small chain, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	121	Total	C	N	O	S	0	0	1
			1004	664	161	173	6			
2	T	120	Total	C	N	O	S	0	0	1
			997	659	160	172	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	0	NME	-	AMIDATION	UNP Q0INY7
S	112	CYS	LEU	CONFLICT	UNP Q0INY7
T	0	NME	-	AMIDATION	UNP Q0INY7
T	112	CYS	LEU	CONFLICT	UNP Q0INY7

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

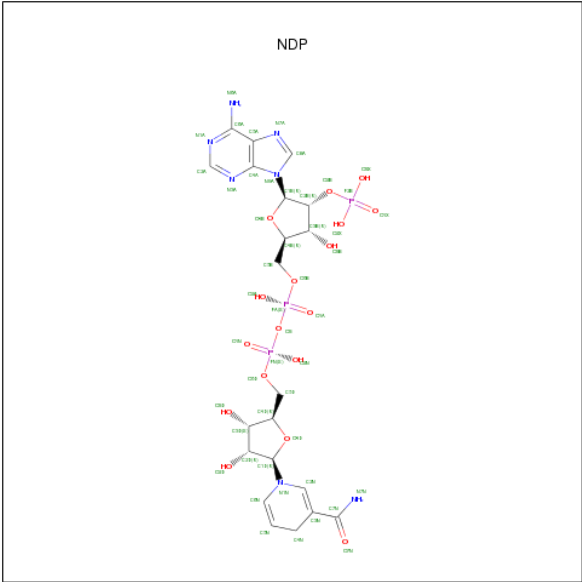


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 6 is water.

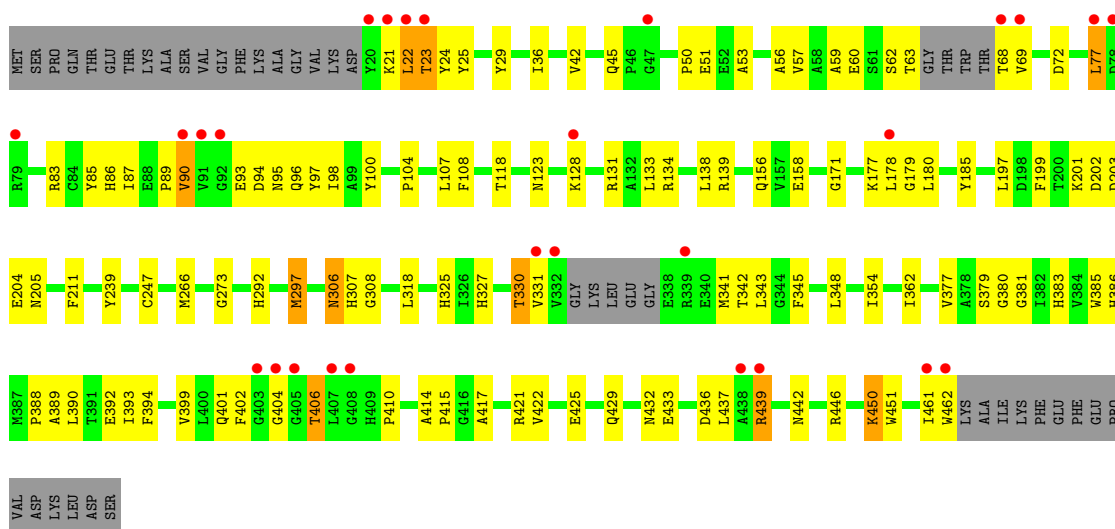
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	427	Total	O	0	0
			427	427		
6	S	162	Total	O	0	0
			162	162		
6	B	389	Total	O	0	0
			389	389		
6	T	147	Total	O	0	0
			147	147		

### 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.

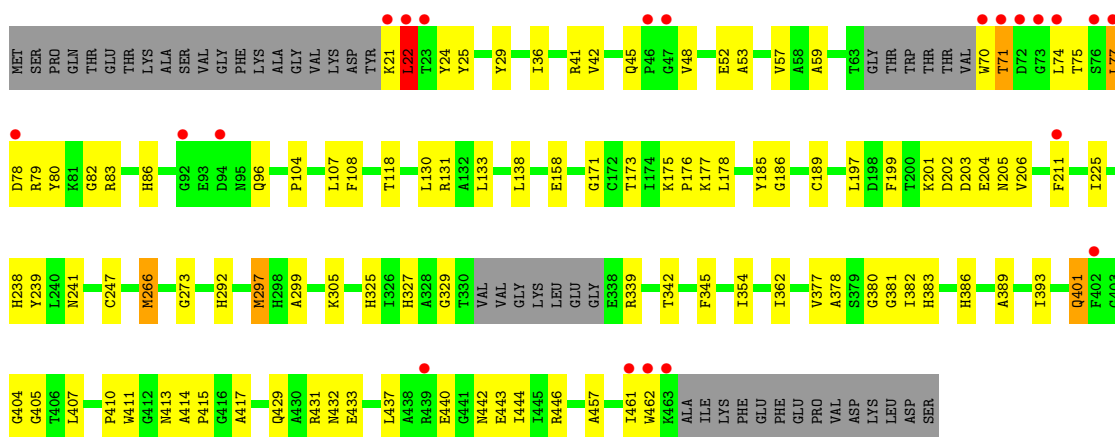
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain A: 



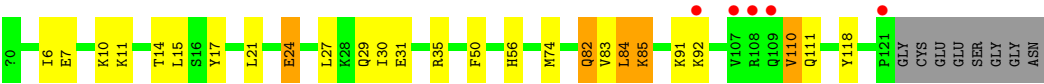
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain B: 



- Molecule 2: Ribulose biphosphate carboxylase small chain, chloroplastic

Chain S: 



● Molecule 2: Ribulose biphosphate carboxylase small chain, chloroplastic

Chain T: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.25Å 110.25Å 199.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.63 – 1.90 39.62 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.8 (39.63-1.90) 94.9 (39.62-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.169 , 0.189 0.169 , 0.188	Depositor DCC
$R_{free}$ test set	3848 reflections (4.54%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 54.1	EDS
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 89311 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9992	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, NME, KCX, NDP

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	0.31	0/3453	0.64	2/4680 (0.0%)
1	B	0.33	0/3429	0.62	2/4644 (0.0%)
2	S	0.33	0/1036	0.57	0/1405
2	T	0.31	0/1028	0.58	0/1393
All	All	0.32	0/8946	0.62	4/12122 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	LEU	CA-CB-CG	-9.99	92.32	115.30
1	A	23	THR	N-CA-C	-5.38	96.47	111.00
1	B	22	LEU	CA-CB-CG	5.30	127.49	115.30
1	B	82	GLY	N-CA-C	-5.16	100.20	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3384	0	3283	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3360	0	3260	96	0
2	S	1004	0	1003	29	0
2	T	997	0	996	17	0
3	A	12	0	16	1	0
3	B	12	0	16	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	96	0	52	12	0
6	A	427	0	0	8	0
6	B	389	0	0	19	0
6	S	162	0	0	7	0
6	T	147	0	0	2	0
All	All	9992	0	8626	247	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (247) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:189:CYS:HB2	6:B:705:HOH:O	1.46	1.12
1:A:331:VAL:HG11	1:A:393:ILE:HD13	1.32	1.10
1:B:382:ILE:HG12	6:B:1125:HOH:O	1.55	1.04
2:S:85:LYS:HE3	2:S:85:LYS:HA	1.40	1.00
1:A:404:GLY:H	5:A:479:NDP:H4D	1.28	0.95
1:A:178:LEU:HD12	1:B:107:LEU:HD22	1.52	0.91
1:A:90:VAL:HG11	1:A:98:ILE:HG12	1.53	0.90
1:A:156:GLN:NE2	2:S:110:VAL:HG11	1.85	0.90
1:A:156:GLN:CD	2:S:110:VAL:HG21	1.92	0.90
1:A:90:VAL:CG1	1:A:98:ILE:HG12	2.02	0.89
1:A:330:THR:HG23	1:A:379:SER:O	1.78	0.82
1:B:389:ALA:O	1:B:393:ILE:HD13	1.80	0.80
6:A:1096:HOH:O	1:B:383:HIS:HB3	1.81	0.79
1:A:201:KCX:HB3	1:A:239:TYR:CD2	2.21	0.76
1:A:331:VAL:CG1	1:A:393:ILE:HD13	2.14	0.76
1:B:104:PRO:HG2	1:B:107:LEU:HG	1.69	0.75
1:A:404:GLY:N	5:A:479:NDP:H4D	2.00	0.74
2:T:109:GLN:O	2:T:110:VAL:HG13	1.87	0.74
1:B:171:GLY:HA3	1:B:401:GLN:OE1	1.86	0.74
1:A:205:ASN:ND2	1:B:118:THR:HG22	2.04	0.73
1:A:156:GLN:CG	2:S:110:VAL:HG21	2.18	0.73
1:A:432:ASN:HD22	2:S:29:GLN:HE22	1.37	0.73
1:B:203:ASP:OD1	6:B:1112:HOH:O	2.05	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:S:85:LYS:HA	2:S:85:LYS:CE	2.18	0.72
1:A:90:VAL:HG22	1:A:97:TYR:HA	1.71	0.72
1:A:442:ASN:HB3	1:A:446:ARG:NH1	2.04	0.72
1:A:104:PRO:HG2	1:A:107:LEU:HG	1.70	0.72
1:A:205:ASN:HD22	1:B:118:THR:HG22	1.55	0.71
1:B:21:LYS:CB	1:B:25:TYR:HB3	2.21	0.70
1:A:156:GLN:HB2	6:A:861:HOH:O	1.92	0.69
1:A:442:ASN:HB3	1:A:446:ARG:HH12	1.57	0.69
1:A:90:VAL:HG22	1:A:97:TYR:CA	2.23	0.69
1:A:21:LYS:O	1:A:25:TYR:HB3	1.92	0.68
1:B:205:ASN:CG	6:B:1112:HOH:O	2.34	0.66
1:B:241:ASN:HA	1:B:266:MET:HG2	1.77	0.66
1:A:156:GLN:HE22	2:S:110:VAL:HG11	1.59	0.66
1:A:247:CYS:HG	1:B:247:CYS:HG	0.84	0.66
1:B:177:LYS:HG2	1:B:178:LEU:HG	1.78	0.65
1:A:402:PHE:HB2	1:A:406:THR:CG2	2.27	0.65
1:A:330:THR:HG21	1:A:380:GLY:O	1.97	0.65
1:B:414:ALA:HB3	1:B:415:PRO:HD3	1.77	0.65
1:B:178:LEU:HD22	1:B:211:PHE:CZ	2.32	0.65
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.78	0.65
5:A:480:NDP:PN	1:B:381:GLY:H	2.20	0.65
1:B:432:ASN:HD22	2:T:29:GLN:HE22	1.45	0.64
2:T:81:THR:O	2:T:85:LYS:HG2	1.98	0.64
2:S:21:LEU:HA	6:S:1006:HOH:O	1.97	0.64
2:S:10:LYS:HB3	2:S:50:PHE:CZ	2.33	0.64
2:T:105:ASP:OD2	2:T:108:ARG:HG2	1.98	0.64
1:A:93:GLU:O	1:A:96:GLN:HB2	1.98	0.63
1:B:21:LYS:O	1:B:22:LEU:HD23	1.98	0.63
1:A:90:VAL:HG13	1:A:98:ILE:HG12	1.80	0.63
1:B:177:LYS:HD3	1:B:205:ASN:HD22	1.62	0.63
2:T:11:LYS:HG3	2:T:17:TYR:CE1	2.34	0.63
1:A:90:VAL:HG11	1:A:98:ILE:CG1	2.27	0.63
1:B:41:ARG:NH2	1:B:305:LYS:HZ2	1.98	0.62
1:A:45:GLN:OE1	1:A:131:ARG:HG2	1.99	0.62
1:A:45:GLN:CD	1:A:131:ARG:HG2	2.21	0.61
6:A:690:HOH:O	1:B:75:THR:HG21	1.99	0.61
2:S:92:LYS:HD2	6:S:939:HOH:O	2.00	0.61
2:S:35:ARG:HD3	6:S:751:HOH:O	1.99	0.61
1:B:429:GLN:O	1:B:433:GLU:HG3	2.01	0.60
2:S:27:LEU:HD21	2:S:84:LEU:HD12	1.82	0.59
1:B:77:LEU:HD12	6:B:783:HOH:O	2.02	0.59
1:A:36:ILE:HD12	1:A:108:PHE:CE2	2.37	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:T:46:LYS:HE2	6:T:613:HOH:O	2.03	0.59
1:B:41:ARG:NH2	1:B:305:LYS:NZ	2.52	0.58
1:A:45:GLN:HA	1:A:131:ARG:HG3	1.85	0.58
1:B:42:VAL:HG22	1:B:133:LEU:CD1	2.34	0.58
1:B:329:GLY:O	1:B:378:ALA:HA	2.03	0.58
2:S:110:VAL:HG13	2:S:111:GLN:O	2.04	0.58
1:A:21:LYS:O	1:A:25:TYR:N	2.36	0.58
1:A:95:ASN:HB2	6:A:1001:HOH:O	2.04	0.57
1:A:461:ILE:HD11	1:A:462:TRP:CZ3	2.39	0.57
1:A:379:SER:HB3	1:A:401:GLN:HB2	1.86	0.57
1:B:204:GLU:HG2	6:B:1112:HOH:O	2.03	0.57
1:A:178:LEU:HD11	6:B:1121:HOH:O	2.05	0.57
1:B:204:GLU:CD	6:B:1112:HOH:O	2.43	0.57
1:B:79:ARG:NE	6:B:784:HOH:O	2.37	0.56
1:A:343:LEU:HD21	1:A:393:ILE:HG23	1.87	0.56
2:T:27:LEU:O	2:T:31:GLU:HG2	2.06	0.56
1:A:450:LYS:HD2	1:A:450:LYS:N	2.19	0.56
1:A:392:GLU:HG2	1:A:437:LEU:HB2	1.88	0.56
2:S:10:LYS:HB3	2:S:50:PHE:CE1	2.39	0.56
3:B:504:GOL:H11	6:B:654:HOH:O	2.06	0.55
1:A:389:ALA:O	1:A:393:ILE:HD12	2.07	0.55
1:A:197:LEU:HG	1:A:417:ALA:HB1	1.87	0.55
1:A:69:VAL:HG11	1:B:407:LEU:HB2	1.88	0.55
1:B:178:LEU:HD13	1:B:211:PHE:CZ	2.42	0.55
2:S:14:THR:HG22	2:S:15:LEU:HG	1.89	0.55
5:A:480:NDP:H3D	1:B:381:GLY:HA2	1.89	0.54
1:B:53:ALA:O	1:B:57:VAL:HG23	2.07	0.54
1:A:29:TYR:CG	1:A:83:ARG:HD2	2.43	0.54
2:T:88:GLU:O	2:T:92:LYS:HD3	2.08	0.54
1:B:178:LEU:CD2	1:B:206:VAL:HG22	2.38	0.54
1:B:382:ILE:HA	1:B:386:HIS:ND1	2.24	0.53
1:A:381:GLY:H	5:A:479:NDP:PN	2.32	0.53
1:B:440:GLU:O	1:B:444:ILE:HG13	2.09	0.53
1:A:21:LYS:O	1:A:25:TYR:CB	2.55	0.53
1:A:123:ASN:HB2	6:A:671:HOH:O	2.09	0.53
2:S:92:LYS:HE2	6:S:1040:HOH:O	2.09	0.53
1:A:177:LYS:HG2	1:A:178:LEU:HG	1.91	0.52
1:A:50:PRO:HG2	1:A:51:GLU:OE2	2.09	0.52
1:A:56:ALA:O	1:A:60:GLU:HG2	2.08	0.52
2:S:85:LYS:HE2	6:S:1039:HOH:O	2.09	0.52
1:A:331:VAL:HG12	1:A:331:VAL:O	2.09	0.52
1:B:48:VAL:HG13	1:B:52:GLU:OE2	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:383:HIS:CE1	1:A:385:TRP:HB2	2.45	0.52
1:A:410:PRO:HD3	1:A:461:ILE:HD13	1.90	0.52
1:B:45:GLN:HA	1:B:131:ARG:HG3	1.91	0.51
1:B:197:LEU:HG	1:B:417:ALA:HB1	1.91	0.51
1:A:297:MET:HG3	1:A:297:MET:O	2.09	0.51
1:B:45:GLN:OE1	1:B:131:ARG:HG2	2.10	0.51
1:B:411:TRP:CD1	2:T:1:MET:HG3	2.46	0.51
1:B:36:ILE:HD12	1:B:108:PHE:CE2	2.45	0.51
1:B:327:HIS:HA	1:B:377:VAL:HB	1.93	0.51
5:A:480:NDP:H1D	6:B:1079:HOH:O	2.10	0.50
1:B:342:THR:HA	1:B:345:PHE:CE2	2.46	0.50
1:A:178:LEU:HB3	1:A:211:PHE:CZ	2.46	0.50
1:A:429:GLN:O	1:A:433:GLU:HG3	2.10	0.50
1:A:439:ARG:HG2	1:A:439:ARG:HH11	1.76	0.50
1:B:173:THR:HA	1:B:201:KCX:HG3	1.93	0.50
1:B:185:TYR:OH	1:B:202:ASP:HA	2.12	0.50
1:A:239:TYR:HB3	1:A:266:MET:HB2	1.94	0.50
1:A:63:THR:HG22	6:B:889:HOH:O	2.11	0.50
5:A:480:NDP:H4D	1:B:404:GLY:H	1.76	0.50
1:A:342:THR:HA	1:A:345:PHE:CE2	2.47	0.50
1:B:292:HIS:HA	1:B:325:HIS:HB2	1.94	0.50
1:A:461:ILE:HD11	1:A:462:TRP:CH2	2.46	0.49
1:B:178:LEU:HD13	1:B:211:PHE:HZ	1.76	0.49
1:B:461:ILE:HD11	1:B:462:TRP:CZ2	2.47	0.49
2:T:35:ARG:HD3	6:T:604:HOH:O	2.12	0.49
1:A:177:LYS:HE2	1:A:203:ASP:OD2	2.13	0.49
1:A:436:ASP:CG	1:A:439:ARG:HD3	2.33	0.49
1:B:178:LEU:HD22	1:B:211:PHE:CE1	2.48	0.49
1:A:421:ARG:O	1:A:425:GLU:HG3	2.12	0.48
1:B:86:HIS:HE1	6:B:652:HOH:O	1.95	0.48
1:B:42:VAL:HG21	1:B:57:VAL:HG21	1.94	0.48
1:A:156:GLN:HG2	2:S:110:VAL:HG21	1.94	0.48
1:B:204:GLU:CG	6:B:1112:HOH:O	2.61	0.48
1:A:377:VAL:CG1	1:A:401:GLN:HG3	2.44	0.48
2:S:27:LEU:CD2	2:S:84:LEU:HD12	2.42	0.48
1:A:133:LEU:H	1:A:307:HIS:CD2	2.31	0.47
1:A:118:THR:HG22	1:B:205:ASN:OD1	2.14	0.47
1:B:442:ASN:O	1:B:446:ARG:HG3	2.14	0.47
2:S:11:LYS:HG3	2:S:17:TYR:CE1	2.48	0.47
1:A:442:ASN:O	1:A:446:ARG:HG3	2.14	0.47
1:B:158:GLU:CD	1:B:325:HIS:HE2	2.18	0.47
1:A:327:HIS:HA	1:A:377:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:377:VAL:HG22	1:A:399:VAL:HB	1.97	0.47
1:A:50:PRO:O	1:A:87:ILE:HD13	2.15	0.47
1:A:24:TYR:CG	1:A:59:ALA:HB2	2.49	0.47
1:A:306:ASN:HD22	1:A:306:ASN:N	2.12	0.47
1:B:380:GLY:O	6:B:949:HOH:O	2.21	0.47
1:B:461:ILE:HD11	1:B:462:TRP:CE2	2.50	0.47
1:A:307:HIS:HE1	1:B:299:ALA:O	1.98	0.47
2:T:113:ILE:HG22	2:T:114:SER:N	2.30	0.46
1:A:306:ASN:HD22	1:A:306:ASN:H	1.63	0.46
2:S:85:LYS:HD3	6:S:1038:HOH:O	2.15	0.46
5:A:480:NDP:H4D	1:B:404:GLY:N	2.30	0.46
1:B:178:LEU:HD23	1:B:206:VAL:HG22	1.98	0.46
1:B:70:TRP:N	6:B:1118:HOH:O	2.48	0.46
1:A:211:PHE:HB3	6:B:699:HOH:O	2.14	0.46
1:A:178:LEU:HD22	1:A:211:PHE:HZ	1.81	0.46
6:A:897:HOH:O	2:S:110:VAL:HG22	2.16	0.46
1:A:21:LYS:C	1:A:22:LEU:HG	2.34	0.46
1:A:89:PRO:HA	1:A:97:TYR:CD2	2.51	0.45
1:A:422:VAL:HG13	1:A:451:TRP:CH2	2.52	0.45
1:B:410:PRO:HD3	1:B:461:ILE:HD13	1.97	0.45
1:A:404:GLY:CA	5:A:479:NDP:H4D	2.46	0.45
5:A:480:NDP:O2N	6:B:1125:HOH:O	2.20	0.45
2:S:24:GLU:OE1	2:S:24:GLU:N	2.49	0.45
1:A:86:HIS:NE2	3:A:502:GOL:H11	2.31	0.45
1:A:179:GLY:HA2	1:B:80:TYR:CE2	2.51	0.45
1:B:21:LYS:CB	1:B:25:TYR:CB	2.93	0.45
1:B:393:ILE:HD12	1:B:393:ILE:N	2.32	0.45
1:A:386:HIS:O	1:A:390:LEU:HG	2.17	0.45
1:B:297:MET:O	1:B:297:MET:HG3	2.16	0.45
2:S:14:THR:O	2:S:15:LEU:HB2	2.16	0.45
1:A:331:VAL:CG2	1:A:394:PHE:CE2	3.00	0.44
1:B:339:ARG:NH2	1:B:393:ILE:HG13	2.32	0.44
1:A:45:GLN:HA	1:A:131:ARG:CG	2.47	0.44
1:B:71:THR:HA	1:B:74:LEU:CD2	2.48	0.44
1:A:68:THR:HB	5:A:480:NDP:H72N	1.82	0.44
1:B:239:TYR:HB3	1:B:266:MET:HB3	1.99	0.44
1:B:22:LEU:CD1	1:B:24:TYR:HD2	2.31	0.44
2:T:109:GLN:O	2:T:110:VAL:CG1	2.62	0.44
1:B:225:ILE:HD11	1:B:238:HIS:HB3	1.99	0.43
1:B:431:ARG:HB2	1:B:437:LEU:HD11	1.99	0.43
2:S:91:LYS:HE3	2:S:118:TYR:CD1	2.52	0.43
2:S:30:ILE:HD13	2:S:83:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:T:105:ASP:OD1	2:T:107:VAL:HG22	2.18	0.43
1:A:158:GLU:CD	1:A:325:HIS:HE2	2.18	0.43
1:A:402:PHE:CB	1:A:406:THR:CG2	2.95	0.43
1:B:42:VAL:CG1	1:B:130:LEU:HD22	2.48	0.43
2:T:46:LYS:NZ	2:T:96:ASP:OD2	2.41	0.43
1:B:175:LYS:HB2	1:B:407:LEU:HD13	2.01	0.43
1:A:36:ILE:HD12	1:A:108:PHE:CZ	2.53	0.43
1:A:388:PRO:O	1:A:392:GLU:HB2	2.19	0.43
1:A:345:PHE:HA	1:A:348:LEU:HD12	2.00	0.43
1:B:175:LYS:HA	1:B:176:PRO:C	2.39	0.43
1:B:22:LEU:HD12	1:B:24:TYR:HD2	1.83	0.43
1:B:432:ASN:HD22	2:T:29:GLN:NE2	2.15	0.43
2:T:61:TYR:CD1	2:T:61:TYR:C	2.91	0.43
1:A:439:ARG:HG2	1:A:439:ARG:NH1	2.34	0.43
1:B:186:GLY:O	1:B:189:CYS:HB3	2.19	0.43
1:A:201:KCX:OQ1	1:A:203:ASP:HA	2.19	0.43
1:A:354:ILE:CG2	1:A:362:ILE:HD13	2.49	0.43
1:A:139:ARG:HD2	1:A:139:ARG:C	2.39	0.42
1:B:407:LEU:HD23	1:B:413:ASN:OD1	2.19	0.42
1:A:178:LEU:HD22	1:A:211:PHE:CZ	2.55	0.42
6:A:1096:HOH:O	1:B:405:GLY:CA	2.67	0.42
1:A:354:ILE:HD12	1:A:354:ILE:N	2.34	0.42
1:B:70:TRP:N	6:B:1008:HOH:O	2.53	0.42
1:B:29:TYR:CG	1:B:83:ARG:HD2	2.55	0.42
1:A:204:GLU:HG2	1:A:205:ASN:N	2.34	0.41
1:A:318:LEU:HD13	1:A:318:LEU:C	2.39	0.41
1:A:292:HIS:HA	1:A:325:HIS:HB2	2.02	0.41
1:B:377:VAL:HG11	1:B:401:GLN:HE21	1.85	0.41
1:A:42:VAL:HG22	1:A:133:LEU:CD1	2.50	0.41
1:A:133:LEU:H	1:A:307:HIS:HD2	1.68	0.41
1:A:171:GLY:HA2	1:A:199:PHE:O	2.19	0.41
1:A:134:ARG:HA	1:A:308:GLY:O	2.20	0.41
1:A:273:GLY:HA3	1:B:273:GLY:HA3	2.01	0.41
1:B:339:ARG:HH22	1:B:393:ILE:CD1	2.33	0.41
2:S:74:MET:CE	2:S:82:GLN:NE2	2.84	0.41
1:A:63:THR:HG21	1:A:77:LEU:HD12	2.02	0.41
1:B:171:GLY:HA2	1:B:199:PHE:O	2.19	0.41
2:S:31:GLU:HG3	6:S:771:HOH:O	2.21	0.41
5:A:480:NDP:H4D	1:B:404:GLY:CA	2.51	0.41
1:B:177:LYS:HD3	1:B:205:ASN:ND2	2.30	0.41
1:A:185:TYR:OH	1:A:202:ASP:HA	2.21	0.41
2:T:27:LEU:HG	2:T:84:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:85:TYR:CZ	1:A:100:TYR:HB3	2.56	0.41
1:A:36:ILE:HD12	1:A:108:PHE:CD2	2.55	0.41
1:A:177:LYS:HE2	1:A:203:ASP:CG	2.41	0.41
1:B:354:ILE:CG2	1:B:362:ILE:HD13	2.51	0.41
2:S:6:ILE:HG13	2:S:7:GLU:HG3	2.02	0.41
1:A:436:ASP:OD2	1:A:439:ARG:HD3	2.21	0.40
1:B:457:ALA:O	1:B:461:ILE:HG23	2.22	0.40
1:A:341:MET:HE2	6:A:731:HOH:O	2.21	0.40
1:A:53:ALA:O	1:A:57:VAL:HG23	2.22	0.40
1:A:72:ASP:HB3	1:A:77:LEU:HD23	2.02	0.40
1:A:29:TYR:CD1	1:A:83:ARG:HD2	2.57	0.40
1:B:24:TYR:CD2	1:B:59:ALA:HB2	2.56	0.40
1:B:393:ILE:N	1:B:393:ILE:CD1	2.85	0.40
1:A:385:TRP:CD1	1:A:462:TRP:O	2.75	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	427/477 (90%)	408 (96%)	17 (4%)	2 (0%)	38	23
1	B	423/477 (89%)	408 (96%)	14 (3%)	1 (0%)	56	44
2	S	119/129 (92%)	112 (94%)	7 (6%)	0	100	100
2	T	118/129 (92%)	111 (94%)	7 (6%)	0	100	100
All	All	1087/1212 (90%)	1039 (96%)	45 (4%)	3 (0%)	50	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	B	22	LEU
1	A	62	SER

### 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	347/385 (90%)	335 (96%)	12 (4%)	48	34
1	B	344/385 (89%)	335 (97%)	9 (3%)	59	49
2	S	109/114 (96%)	103 (94%)	6 (6%)	30	16
2	T	108/114 (95%)	107 (99%)	1 (1%)	87	86
All	All	908/998 (91%)	880 (97%)	28 (3%)	52	41

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

Mol	Chain	Res	Type
1	A	23	THR
1	A	77	LEU
1	A	90	VAL
1	A	128	LYS
1	A	138	LEU
1	A	180	LEU
1	A	297	MET
1	A	306	ASN
1	A	330	THR
1	A	406	THR
1	A	439	ARG
1	A	450	LYS
2	S	24	GLU
2	S	56	HIS
2	S	82	GLN
2	S	84	LEU
2	S	85	LYS
2	S	110	VAL
1	B	71	THR
1	B	77	LEU
1	B	78	ASP
1	B	96	GLN
1	B	138	LEU
1	B	266	MET
1	B	297	MET
1	B	401	GLN

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Mol	Chain	Res	Type
1	B	443	GLU
2	T	56	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	205	ASN
1	A	207	ASN
1	A	306	ASN
1	A	307	HIS
2	S	29	GLN
2	S	82	GLN
2	S	109	GLN
1	B	86	HIS
1	B	95	ASN
1	B	156	GLN
1	B	207	ASN
1	B	304	GLN
1	B	442	ASN
2	T	29	GLN
2	T	109	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

Mogul failed to run properly - this section will therefore be empty.

## 5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 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	434/477 (90%)	0.06	27 (6%) 20 20	8, 14, 38, 53	0
1	B	430/477 (90%)	0.00	21 (4%) 28 28	8, 14, 36, 56	0
2	S	121/129 (93%)	0.09	5 (4%) 35 36	9, 20, 32, 49	0
2	T	120/129 (93%)	-0.05	1 (0%) 83 85	11, 19, 30, 43	0
All	All	1105/1212 (91%)	0.03	54 (4%) 28 28	8, 15, 36, 56	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	LEU	9.0
1	A	332	VAL	8.0
1	A	331	VAL	7.3
1	B	77	LEU	6.1
1	A	92	GLY	5.9
1	A	68	THR	5.0
1	A	20	TYR	4.9
1	B	463	LYS	4.7
1	B	22	LEU	4.7
2	S	121	PRO	4.5
1	B	21	LYS	4.3
1	A	462	TRP	4.3
1	B	94	ASP	4.3
1	B	461	ILE	4.0
1	A	79	ARG	3.9
1	A	91	VAL	3.8
1	A	21	LYS	3.6
2	S	107	VAL	3.6
1	B	74	LEU	3.5
2	T	107	VAL	3.3
1	B	439	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	462	TRP	3.2
1	B	72	ASP	3.2
1	B	23	THR	3.1
1	A	461	ILE	3.1
1	B	70	TRP	3.0
1	B	73	GLY	3.0
1	A	23	THR	3.0
1	B	47	GLY	2.9
1	B	211	PHE	2.8
1	A	404	GLY	2.8
1	B	76	SER	2.7
1	A	77	LEU	2.7
2	S	108	ARG	2.6
1	B	71	THR	2.6
1	A	439	ARG	2.6
1	A	339	ARG	2.6
1	B	92	GLY	2.5
1	A	90	VAL	2.5
1	B	46	PRO	2.5
2	S	92	LYS	2.4
1	A	407	LEU	2.4
1	A	403	GLY	2.3
1	B	402	PHE	2.3
1	A	69	VAL	2.3
1	A	128	LYS	2.3
1	A	47	GLY	2.2
1	A	178	LEU	2.2
1	A	438	ALA	2.2
1	A	78	ASP	2.2
2	S	109	GLN	2.2
1	A	405	GLY	2.1
1	A	408	GLY	2.1
1	B	78	ASP	2.1

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

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KCX	B	201	12/13	0.12	0.35	13,19,24,25	0
1	KCX	A	201	12/13	0.11	-0.20	10,17,23,23	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	502	6/6	0.26	29.97	42,47,48,49	0
3	GOL	B	503	6/6	0.31	17.26	32,37,39,42	0
3	GOL	B	504	6/6	0.31	15.45	51,54,55,56	0
3	GOL	A	501	6/6	0.34	10.15	30,32,34,36	0
5	NDP	A	480	48/48	0.42	3.87	46,55,58,59	0
5	NDP	A	479	48/48	0.34	3.32	41,50,55,56	0
4	MG	B	478	1/1	0.07	-1.58	23,23,23,23	0
4	MG	A	478	1/1	0.04	-2.03	29,29,29,29	0

### 6.5 Other polymers

There are no such residues in this entry.