



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:11 AM UTC

PDB ID : 2BEX / pdb\_00002bex  
Title : Crystal structure of Placental Ribonuclease Inhibitor in complex with Human Eosinophil Derived Neurotoxin at 2A resolution  
Authors : Iyer, S.; Holloway, D.E.; Kumar, K.; Shapiro, R.; Acharya, K.R.  
Deposited on : 2004-12-01  
Resolution : 1.99 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

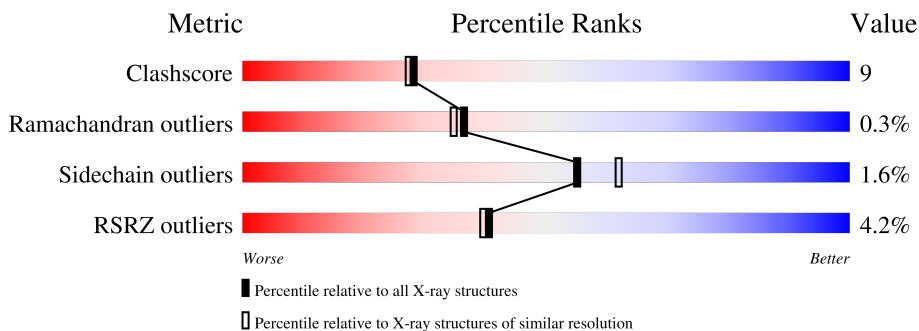
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	460	
1	B	460	
2	C	135	
2	D	135	

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
3	GOL	A	1461	-	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9505 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.

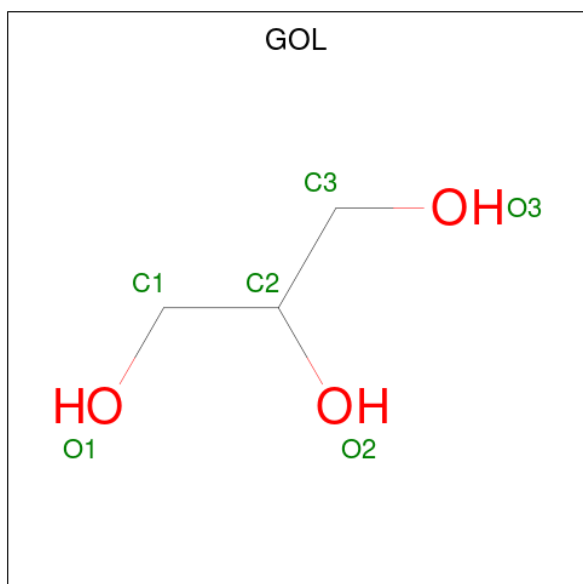
- Molecule 1 is a protein called RIBONUCLEASE INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	456	Total 3381	C 2094	N 589	O 664	S 34	3	0	0
1	B	457	Total 3372	C 2085	N 584	O 669	S 34	3	0	0

- Molecule 2 is a protein called NONSECRETORY RIBONUCLEASE.

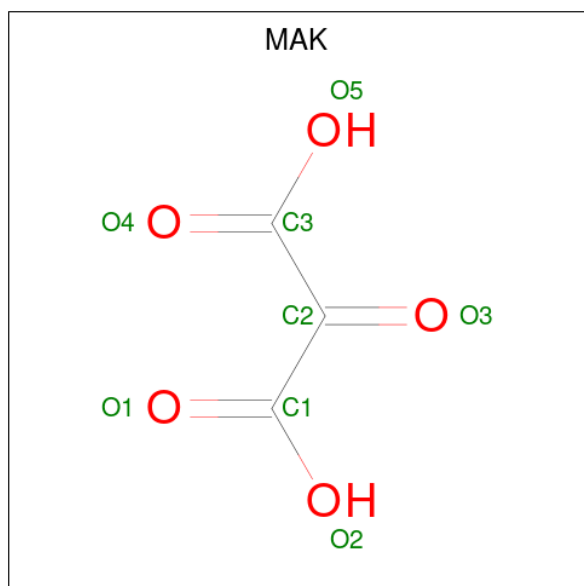
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	135	Total 1071	C 662	N 199	O 197	S 13	0	0	0
2	D	135	Total 1051	C 652	N 193	O 193	S 13	0	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 4 is ALPHA-KETOMALONIC ACID (CCD ID: MAK) (formula:  $C_3H_2O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	3	5		

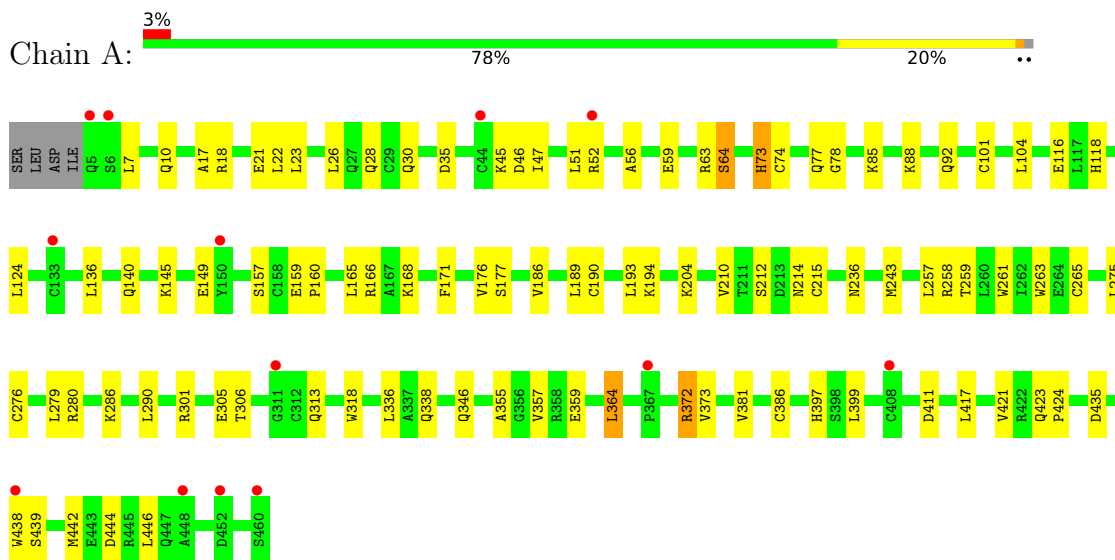
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	257	Total	O	0	0
			257	257		
5	B	246	Total	O	0	0
			246	246		
5	C	65	Total	O	0	0
			65	65		
5	D	48	Total	O	0	0
			48	48		

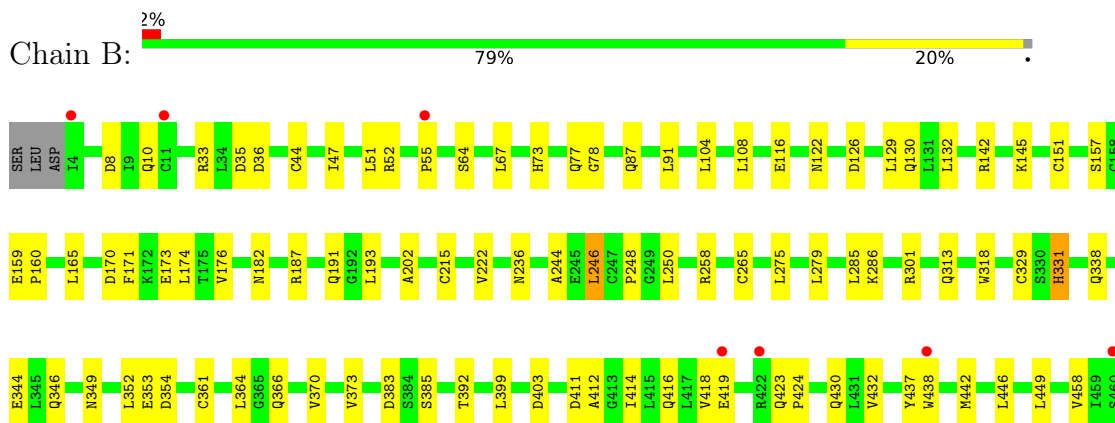
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

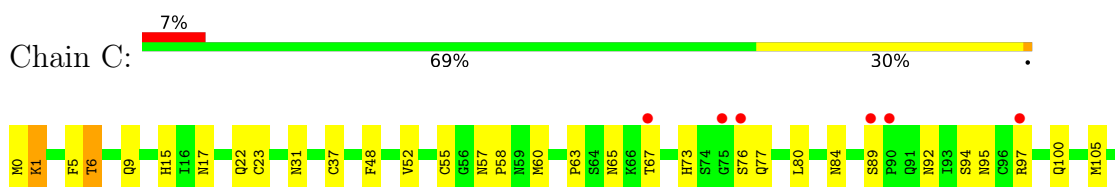
#### • Molecule 1: RIBONUCLEASE INHIBITOR



#### • Molecule 1: RIBONUCLEASE INHIBITOR

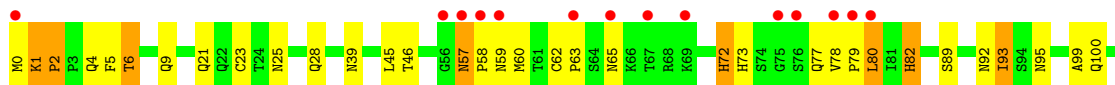


#### • Molecule 2: NONSECRETORY RIBONUCLEASE





● Molecule 2: NONSECRETORY RIBONUCLEASE



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.98Å 91.98Å 257.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 1.99 40.00 – 1.99	Depositor EDS
% Data completeness (in resolution range)	94.9 (40.00-1.99) 95.0 (40.00-1.99)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.18 (at 1.98Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.206 , 0.243 0.211 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtrriage
Anisotropy	0.225	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9505	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, MAK

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	0.54	7/3418 (0.2%)	0.88	12/4633 (0.3%)
1	B	0.54	9/3408 (0.3%)	0.87	8/4625 (0.2%)
2	C	0.75	8/1100 (0.7%)	0.96	4/1505 (0.3%)
2	D	0.84	11/1080 (1.0%)	1.09	14/1479 (0.9%)
All	All	0.61	35/9006 (0.4%)	0.91	38/12242 (0.3%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	82	HIS	ND1-CE1	5.36	1.38	1.32
1	B	331	HIS	ND1-CE1	5.33	1.37	1.32
1	B	73	HIS	ND1-CE1	5.32	1.37	1.32
2	C	73	HIS	ND1-CE1	5.32	1.37	1.32
1	B	313	GLN	CD-OE1	5.31	1.33	1.23
1	A	118	HIS	ND1-CE1	5.30	1.37	1.32
2	D	72	HIS	ND1-CE1	5.29	1.37	1.32
1	A	73	HIS	ND1-CE1	5.28	1.37	1.32
2	C	17	ASN	CG-OD1	5.27	1.33	1.23
1	A	338	GLN	CD-OE1	5.26	1.33	1.23
1	A	397	HIS	ND1-CE1	5.25	1.37	1.32
2	D	25	ASN	CG-OD1	5.22	1.33	1.23
2	D	122	GLN	CD-OE1	5.21	1.33	1.23
2	D	59	ASN	CG-OD1	5.20	1.33	1.23
2	C	22	GLN	CD-OE1	5.19	1.33	1.23
1	B	430	GLN	CD-OE1	5.19	1.33	1.23
1	B	338	GLN	CD-OE1	5.18	1.33	1.23
1	B	77	GLN	CD-OE1	5.18	1.33	1.23
2	D	21	GLN	CD-OE1	5.18	1.33	1.23
2	C	77	GLN	CD-OE1	5.17	1.33	1.23
2	C	116	GLN	CD-OE1	5.14	1.33	1.23
1	A	140	GLN	CD-OE1	5.13	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	GLN	CD-OE1	5.13	1.33	1.23
1	A	28	GLN	CD-OE1	5.11	1.33	1.23
2	C	122	GLN	CD-OE1	5.10	1.33	1.23
2	D	39	ASN	CG-OD1	5.10	1.33	1.23
1	B	366	GLN	CD-OE1	5.08	1.33	1.23
2	D	77	GLN	CD-OE1	5.07	1.33	1.23
1	B	349	ASN	CG-OD1	5.07	1.33	1.23
2	C	65	ASN	CG-OD1	5.07	1.33	1.23
2	D	28	GLN	CD-OE1	5.05	1.33	1.23
1	A	313	GLN	CD-OE1	5.04	1.33	1.23
2	D	57	ASN	CG-OD1	5.04	1.33	1.23
2	C	84	ASN	CG-OD1	5.01	1.33	1.23
2	D	92	ASN	CG-OD1	5.00	1.33	1.23

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	THR	N-CA-C	-7.77	99.32	110.59
2	D	6	THR	N-CA-C	-7.59	99.59	110.59
1	A	73	HIS	CB-CG-CD2	-6.80	122.36	131.20
1	B	73	HIS	CB-CG-CD2	-6.73	122.45	131.20
1	A	397	HIS	CB-CG-CD2	-6.63	122.58	131.20
2	C	73	HIS	CB-CG-CD2	-6.59	122.63	131.20
2	D	72	HIS	CB-CG-CD2	-6.55	122.68	131.20
2	D	82	HIS	CB-CG-CD2	-6.53	122.71	131.20
1	B	331	HIS	CB-CG-CD2	-6.46	122.80	131.20
1	A	118	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	B	370	VAL	N-CA-C	6.18	119.71	113.47
1	B	55	PRO	N-CA-CB	6.05	109.60	103.25
2	D	89	SER	CA-C-N	6.03	126.47	119.47
2	D	89	SER	C-N-CA	6.03	126.47	119.47
1	A	439	SER	N-CA-C	-5.97	101.16	110.42
1	A	386	CYS	N-CA-C	5.95	118.55	111.71
1	B	329	CYS	N-CA-C	5.87	118.47	111.71
1	B	73	HIS	CB-CG-ND1	5.85	131.48	122.70
1	A	73	HIS	CB-CG-ND1	5.82	131.43	122.70
2	D	99	ALA	N-CA-C	-5.76	100.89	110.17
1	A	397	HIS	CB-CG-ND1	5.72	131.28	122.70
2	D	28	GLN	N-CA-C	5.69	117.17	110.97
2	C	73	HIS	CB-CG-ND1	5.67	131.20	122.70
2	D	72	HIS	CB-CG-ND1	5.58	131.08	122.70
1	B	331	HIS	CB-CG-ND1	5.57	131.05	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	HIS	CB-CG-ND1	5.56	131.03	122.70
2	D	82	HIS	CB-CG-ND1	5.55	131.02	122.70
2	D	2	PRO	CA-C-N	5.54	125.64	119.32
2	D	2	PRO	C-N-CA	5.54	125.64	119.32
2	C	15	HIS	N-CA-C	5.50	120.67	113.30
2	D	106	PHE	N-CA-C	-5.37	102.58	110.52
1	A	435	ASP	N-CA-C	5.20	118.57	111.39
1	A	7	LEU	N-CA-C	-5.15	98.17	107.75
2	D	126	VAL	N-CA-C	5.14	114.62	108.45
1	A	64	SER	N-CA-C	5.03	118.53	111.74
1	A	56	ALA	N-CA-C	5.02	116.88	110.61
1	B	91	LEU	N-CA-C	-5.00	104.66	111.56
2	D	93	ILE	N-CA-C	5.00	118.07	111.17

There are no chirality outliers.

There are no planarity outliers.

## 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	3381	0	3394	57	0
1	B	3372	0	3345	49	0
2	C	1071	0	1007	26	0
2	D	1051	0	970	30	0
3	A	6	0	3	0	0
4	B	8	0	1	0	0
5	A	257	0	0	6	0
5	B	246	0	0	2	0
5	C	65	0	0	2	0
5	D	48	0	0	3	0
All	All	9505	0	8720	157	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 9.

All (157) 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:A:444:ASP:CB	5:A:2255:HOH:O	2.06	1.02
1:A:63:ARG:HG3	1:A:92:GLN:HB3	1.43	0.96
1:B:414:ILE:HD12	1:B:442:MET:HE3	1.55	0.88
1:A:243:MET:HE1	1:A:275:LEU:HD13	1.57	0.86
1:A:23:LEU:HD21	1:A:46:ASP:HB3	1.58	0.84
2:D:45:LEU:HB2	2:D:79:PRO:HB2	1.62	0.82
1:A:204:LYS:HZ3	2:C:97:ARG:HH22	1.30	0.77
1:A:438:TRP:HZ3	1:A:446:LEU:HD12	1.52	0.74
1:A:372:ARG:HG3	1:A:373:VAL:HG23	1.70	0.74
1:B:414:ILE:CD1	1:B:442:MET:HE3	2.18	0.73
1:A:301:ARG:O	1:A:305:GLU:HG3	1.89	0.73
1:B:438:TRP:CZ3	1:B:446:LEU:HD12	2.24	0.72
1:A:136:LEU:O	1:A:168:LYS:HE3	1.90	0.72
2:C:1:LYS:HE2	2:C:5:PHE:O	1.91	0.70
2:D:80:LEU:HD22	2:D:103:ALA:HB3	1.74	0.70
2:D:23:CYS:SG	2:D:100:GLN:HB3	2.32	0.69
1:B:438:TRP:HZ3	1:B:446:LEU:HD12	1.58	0.69
2:C:105:MET:HB3	2:C:134:ILE:O	1.94	0.68
1:B:279:LEU:HD23	1:B:285:LEU:HD23	1.75	0.68
2:D:1:LYS:HE2	2:D:5:PHE:O	1.95	0.67
1:A:438:TRP:CZ3	1:A:446:LEU:HD12	2.30	0.66
1:A:59:GLU:HG3	1:A:88:LYS:HB2	1.77	0.66
1:A:23:LEU:HD23	1:A:26:LEU:HD12	1.78	0.64
1:B:419:GLU:HG3	5:B:2222:HOH:O	1.97	0.64
1:B:44:CYS:SG	1:B:67:LEU:HD22	2.38	0.64
2:C:89:SER:OG	2:C:95:ASN:HB2	1.98	0.63
1:A:157:SER:C	1:A:160:PRO:HD2	2.24	0.62
1:B:104:LEU:O	1:B:108:LEU:HG	1.98	0.62
2:C:114:ARG:HD2	2:C:123:TYR:O	1.99	0.62
2:D:57:ASN:HB3	2:D:58:PRO:HD2	1.82	0.61
1:A:214:ASN:HA	5:A:2126:HOH:O	2.01	0.61
2:C:23:CYS:SG	2:C:100:GLN:HB3	2.41	0.60
1:A:45:LYS:HD3	1:A:74:CYS:SG	2.41	0.59
1:B:170:ASP:HB2	5:B:2079:HOH:O	2.03	0.58
2:D:60:MET:CE	2:D:73:HIS:HB2	2.34	0.58
1:A:204:LYS:NZ	2:C:97:ARG:HH12	2.02	0.58
1:B:104:LEU:HD23	1:B:132:LEU:HD21	1.85	0.58
1:A:355:ALA:O	1:A:359:GLU:HG3	2.05	0.57
1:A:165:LEU:HD13	1:A:193:LEU:HD23	1.87	0.56
1:B:129:LEU:HD23	1:B:157:SER:HB2	1.87	0.56
2:D:6:THR:OG1	2:D:9:GLN:HG3	2.05	0.56
1:A:204:LYS:HZ3	2:C:97:ARG:NH2	2.01	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:GLU:HG2	1:B:145:LYS:HB2	1.88	0.55
1:B:187:ARG:O	1:B:191:GLN:HG2	2.07	0.55
2:C:80:LEU:C	2:C:80:LEU:HD12	2.33	0.54
2:D:114:ARG:HD2	2:D:123:TYR:O	2.07	0.54
1:B:129:LEU:HD23	1:B:157:SER:CB	2.38	0.54
1:A:45:LYS:HG2	5:A:2018:HOH:O	2.08	0.54
2:D:60:MET:HE3	2:D:73:HIS:HB2	1.90	0.54
1:A:275:LEU:O	1:A:279:LEU:HD13	2.08	0.53
2:C:60:MET:HE2	2:C:63:PRO:HD3	1.91	0.53
2:D:132:ARG:HG3	5:D:2047:HOH:O	2.09	0.53
1:B:171:PHE:HE2	1:B:174:LEU:HB2	1.73	0.53
1:A:318:TRP:CE3	1:A:346:GLN:HG2	2.45	0.52
2:D:115:ASP:C	2:D:117:ARG:H	2.17	0.52
1:A:411:ASP:OD1	1:A:442:MET:HG3	2.09	0.52
1:B:129:LEU:HD23	1:B:157:SER:OG	2.10	0.52
1:A:116:GLU:HG2	1:A:145:LYS:HB2	1.92	0.51
1:A:204:LYS:HZ2	2:C:97:ARG:HH12	1.59	0.51
1:B:354:ASP:HA	1:B:385:SER:OG	2.10	0.51
1:B:414:ILE:O	1:B:418:VAL:HG23	2.11	0.51
2:D:2:PRO:HG2	2:D:5:PHE:HD1	1.75	0.51
1:A:275:LEU:HD23	1:A:290:LEU:HD11	1.93	0.50
1:B:383:ASP:OD2	1:B:412:ALA:HB3	2.11	0.50
1:A:10:GLN:HA	1:A:35:ASP:O	2.11	0.50
1:B:126:ASP:O	1:B:130:GLN:HG3	2.11	0.50
1:A:157:SER:O	1:A:160:PRO:HD2	2.11	0.50
1:A:280:ARG:HG2	1:A:306:THR:HG23	1.93	0.49
1:B:215:CYS:HB3	1:B:246:LEU:HD13	1.94	0.49
1:A:166:ARG:NH1	5:A:2099:HOH:O	2.42	0.49
2:D:115:ASP:O	2:D:117:ARG:N	2.46	0.49
2:D:78:VAL:HG13	2:D:79:PRO:HD2	1.95	0.49
1:B:52:ARG:HG3	1:B:78:GLY:HA2	1.94	0.49
1:B:301:ARG:HG3	1:B:331:HIS:CE1	2.48	0.48
2:D:4:GLN:C	2:D:118:ARG:HH22	2.21	0.48
1:B:344:GLU:HG3	1:B:373:VAL:HB	1.95	0.48
2:C:132:ARG:O	2:C:133:ILE:HD12	2.14	0.48
1:A:258:ARG:NH1	1:A:286:LYS:HG3	2.27	0.48
1:A:63:ARG:HG2	1:A:64:SER:N	2.28	0.48
1:B:173:GLU:HG2	1:B:202:ALA:HB3	1.96	0.48
2:C:0:MET:O	2:C:1:LYS:C	2.58	0.47
1:B:159:GLU:HB3	1:B:160:PRO:HD3	1.95	0.47
1:B:403:ASP:HA	1:B:432:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ARG:NH1	1:B:286:LYS:HG3	2.30	0.47
1:A:417:LEU:O	1:A:421:VAL:HG22	2.13	0.47
1:B:142:ARG:HG2	1:B:142:ARG:HH11	1.80	0.47
1:A:63:ARG:HG3	1:A:92:GLN:CB	2.31	0.46
1:A:372:ARG:HA	1:A:399:LEU:HA	1.97	0.46
2:D:63:PRO:HG2	2:D:108:ILE:CD1	2.46	0.46
2:C:48:PHE:O	2:C:52:VAL:HG23	2.16	0.46
2:C:131:ASP:O	2:C:132:ARG:HB2	2.15	0.46
1:A:336:LEU:HD13	1:A:364:LEU:HG	1.97	0.45
1:B:36:ASP:HA	1:B:64:SER:O	2.17	0.45
1:B:361:CYS:HB3	1:B:392:THR:OG1	2.17	0.45
2:C:67:THR:O	2:C:67:THR:HG22	2.17	0.45
1:A:236:ASN:O	1:A:265:CYS:HA	2.16	0.45
1:B:8:ASP:OD2	1:B:33:ARG:HD3	2.16	0.45
2:D:4:GLN:C	2:D:118:ARG:NH2	2.75	0.44
2:C:31:ASN:CG	2:C:37:CYS:HA	2.42	0.44
1:A:186:VAL:HG21	1:A:210:VAL:HG22	1.99	0.44
2:C:92:ASN:CG	2:C:94:SER:HG	2.21	0.44
1:A:17:ALA:O	1:A:21:GLU:HG2	2.16	0.44
1:A:30:GLN:HG3	5:A:2013:HOH:O	2.17	0.44
2:D:2:PRO:HG2	2:D:5:PHE:CD1	2.52	0.44
2:C:114:ARG:CZ	2:C:121:PRO:HA	2.48	0.44
1:A:165:LEU:HD13	1:A:193:LEU:CD2	2.48	0.43
2:D:93:ILE:HD11	5:D:2034:HOH:O	2.17	0.43
1:A:18:ARG:O	1:A:22:LEU:HG	2.18	0.43
2:D:80:LEU:C	2:D:80:LEU:HD23	2.43	0.43
1:A:159:GLU:HB3	1:A:160:PRO:HD3	2.00	0.43
1:A:257:LEU:HD11	1:A:259:THR:O	2.18	0.43
2:D:62:CYS:HB2	2:D:65:ASN:O	2.18	0.43
1:B:418:VAL:HG13	1:B:449:LEU:HD22	2.01	0.43
1:B:47:ILE:O	1:B:51:LEU:HG	2.18	0.43
1:B:165:LEU:HD13	1:B:193:LEU:CD2	2.49	0.43
2:C:52:VAL:O	2:C:55:CYS:HB2	2.19	0.43
1:B:10:GLN:HA	1:B:35:ASP:O	2.19	0.42
1:B:437:TYR:O	1:B:442:MET:HE1	2.19	0.42
2:C:97:ARG:NH1	5:C:2055:HOH:O	2.52	0.42
2:D:46:THR:HB	2:D:78:VAL:HG11	2.00	0.42
2:D:132:ARG:HG2	2:D:133:ILE:N	2.33	0.42
1:A:423:GLN:HA	1:A:424:PRO:HD3	1.90	0.42
1:B:122:ASN:O	1:B:151:CYS:HA	2.18	0.42
2:D:80:LEU:HD21	2:D:82:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:LEU:O	1:B:353:GLU:HB2	2.19	0.42
2:D:57:ASN:O	2:D:72:HIS:HD2	2.01	0.42
1:B:236:ASN:O	1:B:265:CYS:HA	2.19	0.42
2:C:97:ARG:HD2	5:C:2053:HOH:O	2.18	0.42
1:B:446:LEU:HD13	1:B:458:VAL:HG11	2.01	0.42
2:D:0:MET:O	2:D:1:LYS:C	2.63	0.42
1:A:47:ILE:O	1:A:51:LEU:HG	2.20	0.42
1:B:411:ASP:CG	1:B:442:MET:HG3	2.45	0.42
2:C:23:CYS:SG	2:C:100:GLN:CB	3.08	0.42
1:B:244:ALA:O	1:B:248:PRO:HD3	2.20	0.41
1:B:423:GLN:HA	1:B:424:PRO:HD3	1.94	0.41
1:A:73:HIS:O	1:A:77:GLN:HG2	2.21	0.41
1:B:412:ALA:O	1:B:416:GLN:HG3	2.20	0.41
2:C:6:THR:OG1	2:C:9:GLN:HG3	2.21	0.41
1:A:159:GLU:N	1:A:160:PRO:CD	2.83	0.41
2:C:114:ARG:HB2	2:C:119:ASP:HB2	2.02	0.41
1:B:438:TRP:CH2	1:B:446:LEU:HD12	2.54	0.41
1:A:357:VAL:HG21	1:A:381:VAL:HG22	2.02	0.41
1:A:263:TRP:CD1	1:A:263:TRP:H	2.37	0.41
1:B:318:TRP:CE3	1:B:346:GLN:HG2	2.55	0.41
2:D:63:PRO:HG2	2:D:108:ILE:HD12	2.03	0.41
2:D:57:ASN:O	2:D:72:HIS:CD2	2.73	0.41
2:D:123:TYR:HB2	5:D:2043:HOH:O	2.20	0.41
1:A:52:ARG:CG	1:A:78:GLY:HA2	2.51	0.40
1:A:149:GLU:HG2	1:A:177:SER:HB2	2.03	0.40
1:A:276:CYS:O	1:A:280:ARG:HG3	2.21	0.40
1:A:85:LYS:NZ	5:A:2047:HOH:O	2.53	0.40
1:A:190:CYS:O	1:A:194:LYS:HG3	2.20	0.40
1:B:222:VAL:HG11	1:B:250:LEU:HD23	2.03	0.40
1:A:101:CYS:SG	1:A:124:LEU:HD22	2.62	0.40
1:A:212:SER:O	1:A:215:CYS:HB2	2.22	0.40
2:C:57:ASN:HB3	2:C:58:PRO:HD2	2.03	0.40
1:B:458:VAL:O	2:D:0:MET:HG2	2.21	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	454/460 (99%)	441 (97%)	13 (3%)	0	100	100
1	B	455/460 (99%)	446 (98%)	8 (2%)	1 (0%)	43	42
2	C	133/135 (98%)	125 (94%)	7 (5%)	1 (1%)	16	11
2	D	133/135 (98%)	126 (95%)	6 (4%)	1 (1%)	16	11
All	All	1175/1190 (99%)	1138 (97%)	34 (3%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	116	GLN
2	C	76	SER
1	B	182	ASN

### 5.3.2 Protein sidechains [i](#)

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	379/396 (96%)	372 (98%)	7 (2%)	51	58
1	B	375/396 (95%)	370 (99%)	5 (1%)	61	68
2	C	123/127 (97%)	122 (99%)	1 (1%)	73	80
2	D	117/127 (92%)	114 (97%)	3 (3%)	40	44
All	All	994/1046 (95%)	978 (98%)	16 (2%)	55	62

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LEU
1	A	171	PHE
1	A	176	VAL
1	A	189	LEU
1	A	261	TRP
1	A	364	LEU
1	A	372	ARG
1	B	176	VAL
1	B	246	LEU
1	B	275	LEU
1	B	364	LEU
1	B	399	LEU
2	C	1	LYS
2	D	1	LYS
2	D	80	LEU
2	D	95	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	GLN
1	B	178	ASN
1	B	331	HIS
2	C	104	ASN
2	D	25	ASN
2	D	59	ASN
2	D	72	HIS
2	D	92	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

2 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
4	MAK	B	1461	-	7,7,7	1.66	2 (28%)	9,9,9	0.65	0
3	GOL	A	1461	-	5,5,5	4.85	5 (100%)	5,5,5	6.17	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
4	MAK	B	1461	-	-	0/8/8/8	-
3	GOL	A	1461	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1461	GOL	C3-C2	-8.44	1.19	1.51
3	A	1461	GOL	O1-C1	-4.36	1.24	1.42
3	A	1461	GOL	O2-C2	-3.14	1.34	1.43
3	A	1461	GOL	C1-C2	-3.00	1.40	1.51
4	B	1461	MAK	O2-C1	2.94	1.38	1.30
3	A	1461	GOL	O3-C3	2.89	1.54	1.42
4	B	1461	MAK	O5-C3	2.07	1.36	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1461	GOL	O3-C3-C2	11.33	161.40	110.38
3	A	1461	GOL	O2-C2-C3	6.96	137.99	109.18
3	A	1461	GOL	O1-C1-C2	3.57	126.44	110.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1461	GOL	C1-C2-C3-O3
3	A	1461	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	456/460 (99%)	0.03	13 (2%) 53 52	10, 19, 35, 46	1 (0%)
1	B	457/460 (99%)	0.03	7 (1%) 72 71	11, 21, 37, 45	1 (0%)
2	C	135/135 (100%)	0.51	9 (6%) 24 22	15, 27, 39, 44	0
2	D	135/135 (100%)	0.92	21 (15%) 5 4	14, 33, 47, 50	0
All	All	1183/1190 (99%)	0.19	50 (4%) 40 39	10, 22, 39, 50	2 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	ILE	6.6
1	A	133	CYS	5.5
1	A	6	SER	3.9
2	D	67	THR	3.9
2	D	116	GLN	3.5
2	C	117	ARG	3.3
1	B	11	CYS	3.1
2	D	75	GLY	3.1
1	A	367	PRO	3.0
1	A	452	ASP	3.0
1	B	55	PRO	2.9
1	B	422	ARG	2.9
2	C	76	SER	2.9
2	D	56	GLY	2.8
2	D	80	LEU	2.7
2	D	63	PRO	2.7
1	A	311	GLY	2.7
1	B	460	SER	2.7
2	D	59	ASN	2.7
2	D	76	SER	2.6
2	D	103	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	106	PHE	2.4
2	D	78	VAL	2.4
2	D	79	PRO	2.4
2	D	65	ASN	2.4
1	A	408	CYS	2.4
2	D	123	TYR	2.4
2	C	67	THR	2.3
2	C	90	PRO	2.3
1	A	438	TRP	2.3
2	D	57	ASN	2.3
2	D	58	PRO	2.3
1	A	52	ARG	2.3
2	C	97	ARG	2.3
2	C	89	SER	2.3
1	B	419	GLU	2.3
2	C	75	GLY	2.2
1	A	460	SER	2.2
1	A	5	GLN	2.2
1	A	448	ALA	2.2
2	D	134	ILE	2.2
2	C	133	ILE	2.2
2	D	69	LYS	2.2
1	B	438	TRP	2.1
2	D	104	ASN	2.1
2	D	120	PRO	2.1
1	A	44	CYS	2.0
2	C	132	ARG	2.0
2	D	0	MET	2.0
1	A	150	TYR	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 oligosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAK	B	1461	8/8	0.69	0.17	26,31,33,34	0
3	GOL	A	1461	6/6	0.70	0.21	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.