



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 07:53 am BST

PDB ID : 1GK3  
Title : Histidine Ammonia-Lyase (HAL) Mutant D145A from *Pseudomonas putida*  
Authors : Baedeker, M.; Schulz, G.E.  
Deposited on : 2001-08-07  
Resolution : 2.25 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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

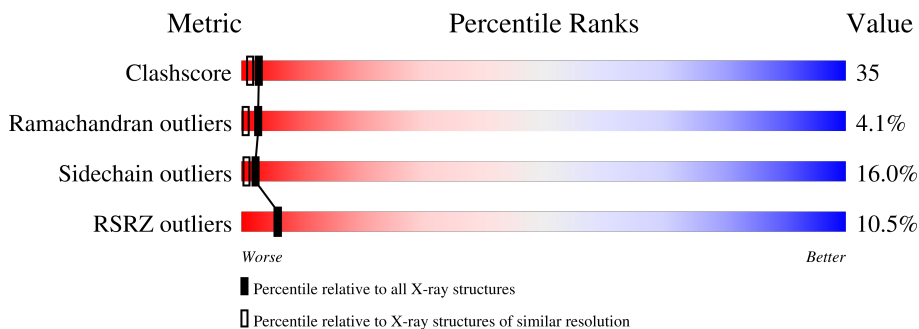
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	509	

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	1511	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3956 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.

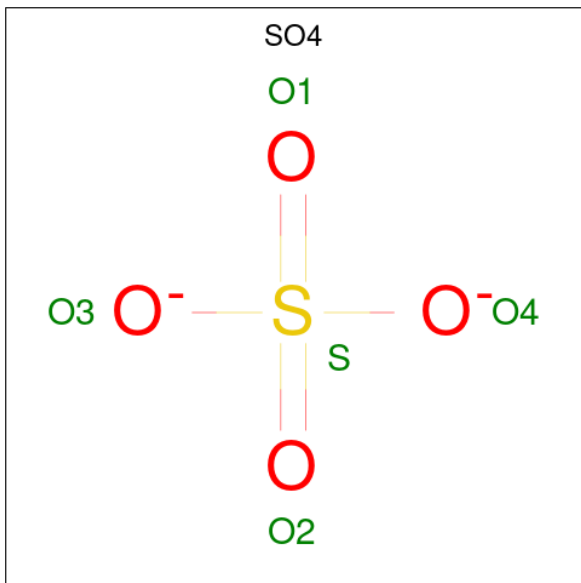
- Molecule 1 is a protein called HISTIDINE AMMONIA-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	509	3761	2359	670	716	16	128	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	ALA	ASP	engineered mutation	UNP P21310
A	273	ALA	CYS	engineered mutation	UNP P21310

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- 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 6 3 3	0	0

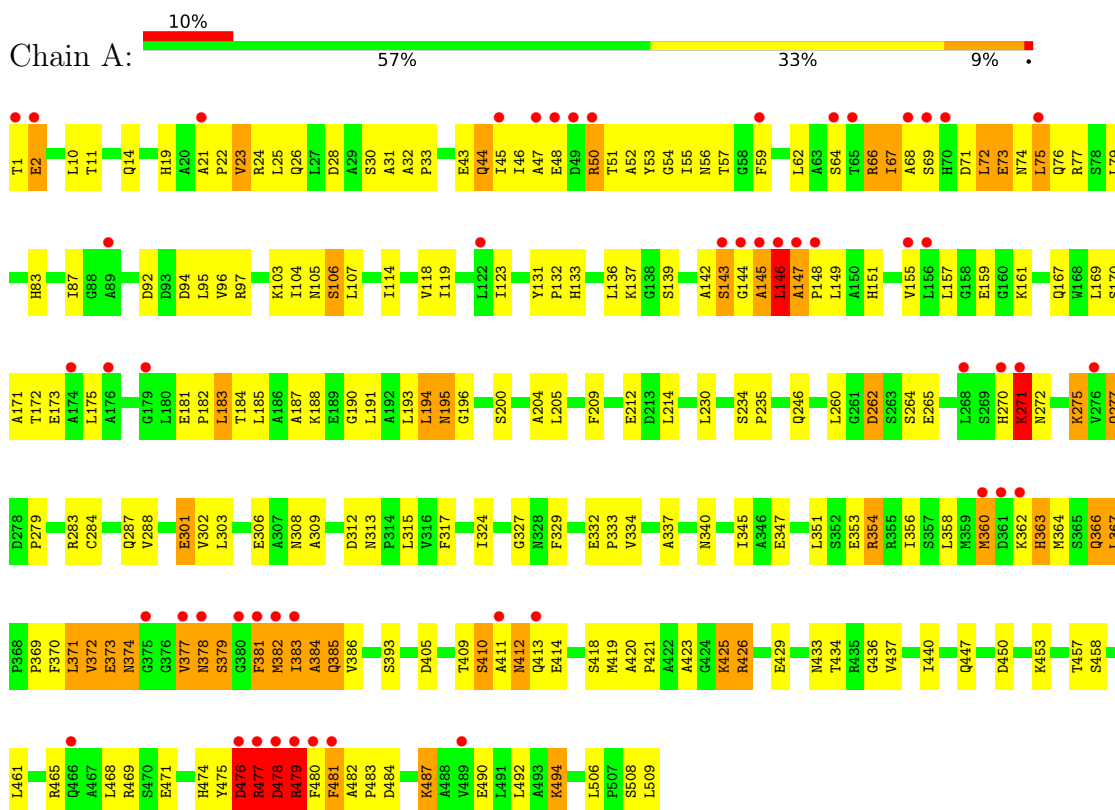
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	184	Total O 184 184	0	0

### 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: HISTIDINE AMMONIA-LYASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.81Å 117.11Å 130.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.00 – 2.25 21.22 – 2.25	Depositor EDS
% Data completeness (in resolution range)	91.0 (21.00-2.25) 90.1 (21.22-2.25)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.26Å)	Xtrriage
Refinement program	SHELX	Depositor
R, $R_{free}$	0.221 , 0.280 0.234 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.1	Xtrriage
Anisotropy	0.612	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 98.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	3956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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: SO4, 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	0.39	3/3819 (0.1%)	0.81	8/5180 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	ALA	N-CA	9.57	1.65	1.46
1	A	386	VAL	N-CA	7.80	1.61	1.46
1	A	384	ALA	N-CA	6.76	1.59	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	ALA	N-CA-C	-8.73	87.44	111.00
1	A	146	LEU	C-N-CA	-7.74	102.36	121.70
1	A	465	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	147	ALA	N-CA-CB	-6.76	100.64	110.10
1	A	386	VAL	N-CA-C	5.24	125.16	111.00
1	A	354	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	A	383	ILE	C-N-CA	-5.10	108.96	121.70
1	A	385	GLN	C-N-CA	-5.00	109.19	121.70

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	3761	0	3826	257	1
2	A	5	0	0	1	0
3	A	6	0	8	8	0
4	A	184	0	0	23	0
All	All	3956	0	3834	258	1

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 35.

All (258) 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:383:ILE:HG12	4:A:2138:HOH:O	1.44	1.13
1:A:59:PHE:CZ	3:A:1511:GOL:H11	1.84	1.12
1:A:145:ALA:HB3	1:A:149:LEU:HG	1.20	1.11
1:A:381:PHE:CZ	1:A:447:GLN:HG2	1.84	1.11
1:A:474:HIS:CD2	1:A:476:ASP:HB3	1.87	1.10
1:A:136:LEU:HD12	1:A:136:LEU:O	1.53	1.08
1:A:381:PHE:HZ	1:A:447:GLN:HG2	0.94	1.06
1:A:145:ALA:HB3	1:A:149:LEU:CG	1.85	1.05
1:A:378:ASN:N	1:A:378:ASN:HD22	1.49	1.01
1:A:474:HIS:HD2	1:A:476:ASP:HB3	1.24	0.99
1:A:146:LEU:HD12	4:A:2033:HOH:O	1.63	0.98
1:A:471:GLU:OE1	1:A:487:LYS:HE2	1.61	0.98
1:A:475:TYR:O	1:A:475:TYR:CD1	2.18	0.96
1:A:145:ALA:CB	1:A:149:LEU:HG	1.96	0.96
1:A:44:GLN:O	1:A:48:GLU:HG3	1.64	0.95
1:A:11:THR:OG1	1:A:14:GLN:HG3	1.66	0.95
1:A:144:GLY:C	1:A:146:LEU:H	1.68	0.95
1:A:377:VAL:HB	1:A:378:ASN:ND2	1.84	0.93
1:A:83:HIS:HD2	1:A:146:LEU:HD13	1.27	0.93
1:A:59:PHE:HZ	3:A:1511:GOL:H11	1.30	0.91
1:A:479:ARG:HB2	4:A:2173:HOH:O	1.70	0.90
1:A:381:PHE:HZ	1:A:447:GLN:CG	1.82	0.90
1:A:235:PRO:HG2	4:A:2109:HOH:O	1.73	0.89
1:A:377:VAL:HB	1:A:378:ASN:HD22	1.38	0.88
1:A:55:ILE:O	3:A:1511:GOL:H32	1.75	0.86
1:A:378:ASN:HB3	1:A:478:ASP:OD1	1.77	0.84
1:A:474:HIS:CD2	1:A:476:ASP:CB	2.61	0.84
1:A:92:ASP:OD1	1:A:94:ASP:HB2	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASN:N	1:A:378:ASN:ND2	2.21	0.81
1:A:214:LEU:HD13	1:A:434:THR:CG2	2.15	0.76
1:A:145:ALA:HB3	1:A:149:LEU:CD1	2.16	0.76
1:A:144:GLY:HA3	1:A:195:ASN:HA	1.68	0.75
1:A:301:GLU:HG3	1:A:302:VAL:N	2.01	0.75
1:A:159:GLU:O	1:A:171:ALA:HB2	1.86	0.75
1:A:378:ASN:HD22	1:A:378:ASN:H	1.35	0.75
1:A:145:ALA:HB2	4:A:2082:HOH:O	1.86	0.74
1:A:48:GLU:HB2	1:A:50:ARG:HG3	1.69	0.74
1:A:83:HIS:CD2	1:A:146:LEU:HD13	2.17	0.73
1:A:144:GLY:O	1:A:146:LEU:N	2.21	0.73
1:A:381:PHE:HB3	1:A:481:PHE:HE1	1.52	0.73
1:A:260:LEU:HD23	1:A:461:LEU:HD11	1.71	0.73
1:A:51:THR:HG22	1:A:66:ARG:HD3	1.73	0.70
1:A:476:ASP:HA	4:A:2171:HOH:O	1.91	0.70
1:A:214:LEU:HD13	1:A:434:THR:HG22	1.73	0.70
1:A:475:TYR:HE2	1:A:479:ARG:O	1.75	0.70
1:A:133:HIS:CD2	1:A:161:LYS:HE2	2.28	0.68
1:A:136:LEU:O	1:A:136:LEU:CD1	2.38	0.68
1:A:68:ALA:O	1:A:71:ASP:HB2	1.93	0.68
1:A:360:MET:HG3	1:A:385:GLN:HB2	1.75	0.67
1:A:260:LEU:HD23	1:A:461:LEU:CD1	2.25	0.67
1:A:144:GLY:HA2	1:A:196:GLY:H	1.59	0.67
1:A:21:ALA:HB1	1:A:22:PRO:HD2	1.76	0.67
1:A:447:GLN:O	1:A:450:ASP:HB2	1.94	0.67
1:A:409:THR:OG1	1:A:414:GLU:HB2	1.95	0.67
1:A:476:ASP:O	1:A:477:ARG:HB3	1.93	0.67
1:A:67:ILE:HG22	1:A:72:LEU:HD13	1.77	0.66
1:A:420:ALA:N	1:A:421:PRO:CD	2.58	0.66
1:A:317:PHE:CD2	1:A:324:ILE:HD12	2.30	0.66
1:A:471:GLU:OE1	1:A:487:LYS:CE	2.43	0.66
1:A:159:GLU:O	1:A:171:ALA:CB	2.43	0.66
1:A:51:THR:CG2	1:A:66:ARG:HD3	2.25	0.65
1:A:62:LEU:C	1:A:64:SER:H	1.99	0.65
1:A:144:GLY:CA	1:A:195:ASN:HA	2.27	0.65
1:A:11:THR:H	1:A:14:GLN:HE21	1.46	0.64
1:A:53:TYR:HA	1:A:57:THR:OG1	1.97	0.64
1:A:55:ILE:C	3:A:1511:GOL:H32	2.17	0.63
1:A:356:ILE:O	1:A:360:MET:HG2	1.99	0.63
1:A:410:SER:O	1:A:410:SER:OG	2.04	0.63
1:A:312:ASP:O	1:A:315:LEU:HD21	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:HA	1:A:171:ALA:HB1	1.81	0.63
1:A:379:SER:O	1:A:379:SER:OG	2.17	0.63
1:A:234:SER:N	1:A:235:PRO:CD	2.62	0.62
1:A:381:PHE:C	1:A:383:ILE:N	2.50	0.61
1:A:475:TYR:CE2	1:A:479:ARG:O	2.52	0.61
1:A:475:TYR:O	1:A:475:TYR:CG	2.54	0.60
1:A:410:SER:HB3	1:A:414:GLU:OE2	2.01	0.60
1:A:69:SER:HA	1:A:72:LEU:HD22	1.83	0.60
1:A:482:ALA:N	1:A:483:PRO:CD	2.65	0.59
1:A:169:LEU:HD22	1:A:173:GLU:OE2	2.02	0.59
1:A:181:GLU:O	1:A:183:LEU:HD23	2.02	0.59
1:A:382:MET:O	1:A:385:GLN:HB3	2.02	0.59
1:A:277:GLN:HG3	1:A:283:ARG:NH2	2.18	0.58
1:A:327:GLY:HA2	1:A:329:PHE:CE2	2.39	0.58
1:A:381:PHE:CD2	1:A:481:PHE:CE1	2.92	0.58
1:A:436:GLY:O	1:A:440:ILE:HD12	2.04	0.58
1:A:377:VAL:C	1:A:378:ASN:HD22	2.06	0.57
1:A:481:PHE:CD2	1:A:484:ASP:HB2	2.39	0.57
1:A:68:ALA:O	1:A:71:ASP:N	2.36	0.57
1:A:114:ILE:HD11	1:A:118:VAL:CG1	2.34	0.57
1:A:458:SER:OG	1:A:461:LEU:HG	2.05	0.57
1:A:469:ARG:NH2	1:A:474:HIS:HA	2.20	0.57
1:A:264:SER:HA	4:A:2105:HOH:O	2.04	0.57
1:A:317:PHE:HD2	1:A:324:ILE:HD12	1.68	0.57
1:A:332:GLU:N	1:A:333:PRO:HD2	2.19	0.57
1:A:476:ASP:O	1:A:477:ARG:CB	2.51	0.57
1:A:87:ILE:HG23	1:A:137:LYS:HB2	1.86	0.57
1:A:87:ILE:CG2	1:A:137:LYS:HB2	2.35	0.56
1:A:474:HIS:CD2	1:A:476:ASP:H	2.24	0.56
1:A:260:LEU:CD2	1:A:461:LEU:HD11	2.35	0.56
1:A:479:ARG:HG2	1:A:480:PHE:N	2.19	0.56
1:A:490:GLU:HG2	1:A:494:LYS:CD	2.36	0.56
1:A:143:SER:O	1:A:146:LEU:CD2	2.53	0.56
1:A:43:GLU:OE1	4:A:2029:HOH:O	2.17	0.56
1:A:474:HIS:NE2	1:A:476:ASP:CB	2.69	0.56
1:A:73:GLU:HG2	4:A:2038:HOH:O	2.05	0.56
1:A:209:PHE:HB3	4:A:2084:HOH:O	2.06	0.55
1:A:67:ILE:CG2	1:A:72:LEU:HD13	2.36	0.55
1:A:183:LEU:HD21	4:A:2078:HOH:O	2.05	0.55
1:A:412:ASN:N	1:A:412:ASN:ND2	2.54	0.55
1:A:114:ILE:HD11	1:A:118:VAL:HG11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:HIS:CD2	1:A:476:ASP:N	2.74	0.55
1:A:204:ALA:CB	1:A:303:LEU:HD21	2.36	0.55
1:A:75:LEU:O	1:A:76:GLN:C	2.46	0.54
1:A:169:LEU:HD13	1:A:173:GLU:OE2	2.07	0.54
1:A:2:GLU:HG3	1:A:2:GLU:O	2.03	0.54
1:A:48:GLU:HB2	1:A:50:ARG:CG	2.36	0.54
1:A:62:LEU:C	1:A:64:SER:N	2.61	0.54
1:A:190:GLY:O	1:A:194:LEU:HD22	2.08	0.54
1:A:32:ALA:N	1:A:33:PRO:CD	2.71	0.53
1:A:136:LEU:HD12	1:A:136:LEU:C	2.23	0.53
1:A:191:LEU:O	1:A:195:ASN:HB2	2.09	0.53
1:A:457:THR:OG1	1:A:458:SER:N	2.41	0.53
1:A:187:ALA:O	1:A:188:LYS:HB3	2.08	0.53
1:A:447:GLN:HE22	1:A:476:ASP:HA	1.72	0.53
1:A:52:ALA:N	1:A:56:ASN:OD1	2.38	0.53
1:A:145:ALA:O	1:A:148:PRO:HD2	2.09	0.53
1:A:264:SER:CA	4:A:2105:HOH:O	2.57	0.53
1:A:277:GLN:HG3	1:A:283:ARG:CZ	2.39	0.53
1:A:382:MET:HA	1:A:385:GLN:OE1	2.09	0.52
1:A:103:LYS:HD2	1:A:107:LEU:HD11	1.90	0.52
1:A:143:SER:O	1:A:146:LEU:HG	2.09	0.52
1:A:279:PRO:HG2	1:A:358:LEU:CD1	2.40	0.52
1:A:381:PHE:N	1:A:381:PHE:CD1	2.76	0.52
1:A:381:PHE:HB3	1:A:481:PHE:CE1	2.40	0.52
1:A:119:ILE:HG22	1:A:123:ILE:HD12	1.90	0.52
1:A:214:LEU:CD1	1:A:434:THR:HB	2.40	0.52
1:A:381:PHE:HD1	1:A:381:PHE:H	1.58	0.52
1:A:75:LEU:CD1	1:A:75:LEU:C	2.78	0.51
1:A:209:PHE:O	1:A:212:GLU:HB2	2.10	0.51
1:A:301:GLU:HG3	1:A:302:VAL:H	1.74	0.51
1:A:418:SER:O	1:A:419:MET:HB2	2.09	0.51
1:A:145:ALA:HB3	1:A:149:LEU:HD12	1.92	0.51
1:A:360:MET:HG3	1:A:385:GLN:CD	2.30	0.51
1:A:378:ASN:O	1:A:379:SER:CB	2.58	0.51
1:A:68:ALA:HB3	1:A:71:ASP:OD1	2.10	0.51
1:A:96:VAL:HG11	1:A:131:TYR:HB3	1.91	0.51
1:A:46:ILE:HG22	1:A:47:ALA:N	2.26	0.50
1:A:76:GLN:O	1:A:79:LEU:HB2	2.11	0.50
1:A:204:ALA:HB3	1:A:303:LEU:HD21	1.94	0.50
1:A:301:GLU:CG	1:A:302:VAL:N	2.72	0.50
1:A:353:GLU:HA	1:A:356:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ALA:N	1:A:421:PRO:HD3	2.27	0.50
1:A:474:HIS:CD2	1:A:476:ASP:CA	2.94	0.50
1:A:506:LEU:HD13	1:A:509:LEU:HD12	1.94	0.49
1:A:142:ALA:O	1:A:143:SER:CB	2.61	0.49
1:A:51:THR:HG22	1:A:66:ARG:CD	2.41	0.48
1:A:136:LEU:HG	1:A:137:LYS:HG2	1.95	0.48
1:A:353:GLU:OE1	1:A:354:ARG:NE	2.31	0.48
1:A:381:PHE:O	1:A:384:ALA:N	2.35	0.48
1:A:147:ALA:O	1:A:151:HIS:HD2	1.97	0.48
1:A:381:PHE:C	1:A:383:ILE:H	2.17	0.48
1:A:506:LEU:CD1	1:A:509:LEU:HD12	2.43	0.48
1:A:23:VAL:HG13	1:A:97:ARG:HD2	1.94	0.48
1:A:146:LEU:O	1:A:147:ALA:C	2.53	0.48
1:A:481:PHE:C	1:A:483:PRO:HD2	2.34	0.47
1:A:143:SER:O	1:A:146:LEU:HD21	2.14	0.47
1:A:28:ASP:OD2	1:A:30:SER:OG	2.27	0.47
1:A:68:ALA:HB3	1:A:71:ASP:CG	2.35	0.47
1:A:106:SER:OG	1:A:309:ALA:O	2.31	0.47
1:A:475:TYR:O	1:A:477:ARG:N	2.48	0.47
1:A:360:MET:HG3	1:A:385:GLN:CB	2.44	0.47
1:A:270:HIS:O	1:A:271:LYS:C	2.52	0.47
1:A:478:ASP:HA	4:A:2172:HOH:O	2.14	0.47
3:A:1511:GOL:O3	3:A:1511:GOL:O1	2.31	0.47
1:A:59:PHE:HZ	3:A:1511:GOL:C1	2.14	0.47
1:A:19:HIS:ND1	1:A:209:PHE:HD2	2.13	0.47
1:A:381:PHE:CD2	1:A:481:PHE:HE1	2.33	0.47
1:A:421:PRO:HD2	4:A:2065:HOH:O	2.15	0.47
1:A:433:ASN:O	1:A:437:VAL:HG23	2.16	0.46
1:A:133:HIS:CD2	1:A:161:LYS:CE	2.98	0.46
1:A:412:ASN:N	1:A:412:ASN:HD22	2.13	0.46
1:A:62:LEU:O	1:A:64:SER:N	2.49	0.46
1:A:145:ALA:CB	4:A:2082:HOH:O	2.54	0.46
1:A:317:PHE:CE2	1:A:324:ILE:HD12	2.50	0.46
1:A:28:ASP:O	1:A:31:ALA:HB3	2.16	0.46
1:A:69:SER:O	1:A:72:LEU:HB2	2.16	0.46
1:A:230:LEU:HA	4:A:2087:HOH:O	2.16	0.46
1:A:48:GLU:OE1	1:A:50:ARG:NE	2.49	0.46
1:A:317:PHE:CD2	1:A:324:ILE:CD1	2.99	0.45
1:A:67:ILE:O	1:A:68:ALA:C	2.54	0.45
1:A:381:PHE:O	1:A:382:MET:C	2.51	0.45
1:A:182:PRO:C	1:A:183:LEU:HD23	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:GLU:CD	1:A:487:LYS:HE2	2.35	0.45
1:A:288:VAL:CG1	1:A:351:LEU:HD22	2.47	0.45
1:A:317:PHE:CE2	1:A:324:ILE:CD1	3.00	0.45
1:A:482:ALA:N	1:A:483:PRO:HD3	2.32	0.45
1:A:10:LEU:HD23	1:A:10:LEU:HA	1.79	0.44
1:A:481:PHE:HD2	1:A:484:ASP:HB2	1.79	0.44
1:A:67:ILE:N	1:A:67:ILE:HD13	2.32	0.44
1:A:149:LEU:HD13	1:A:193:LEU:O	2.17	0.44
1:A:32:ALA:N	1:A:33:PRO:HD3	2.32	0.44
1:A:279:PRO:HG2	1:A:358:LEU:HD11	2.00	0.44
1:A:347:GLU:OE2	1:A:347:GLU:HA	2.17	0.44
1:A:360:MET:CG	1:A:385:GLN:HB2	2.45	0.44
1:A:59:PHE:HE2	1:A:75:LEU:HD11	1.82	0.44
1:A:155:VAL:HA	1:A:171:ALA:CB	2.47	0.44
1:A:95:LEU:HD12	1:A:95:LEU:HA	1.89	0.44
1:A:145:ALA:O	1:A:148:PRO:CD	2.66	0.44
1:A:378:ASN:HB2	1:A:379:SER:H	1.63	0.43
1:A:492:LEU:HD23	1:A:492:LEU:HA	1.84	0.43
1:A:54:GLY:O	3:A:1511:GOL:H12	2.17	0.43
1:A:67:ILE:CG2	1:A:72:LEU:CD1	2.96	0.43
1:A:188:LYS:N	3:A:1511:GOL:O3	2.42	0.43
1:A:458:SER:OG	1:A:461:LEU:CG	2.66	0.43
1:A:146:LEU:CD1	4:A:2015:HOH:O	2.66	0.43
1:A:284:CYS:HA	1:A:287:GLN:OE1	2.18	0.43
1:A:279:PRO:HG2	1:A:358:LEU:HD13	2.01	0.42
1:A:306:GLU:HG2	1:A:334:VAL:CG2	2.48	0.42
1:A:139:SER:O	1:A:421:PRO:HG2	2.19	0.42
1:A:381:PHE:HD2	1:A:481:PHE:CE1	2.34	0.42
1:A:51:THR:HG21	1:A:66:ARG:HD3	2.01	0.42
1:A:72:LEU:HD12	1:A:72:LEU:HA	1.82	0.42
1:A:143:SER:O	1:A:146:LEU:CG	2.68	0.42
1:A:481:PHE:C	1:A:483:PRO:CD	2.87	0.42
1:A:105:ASN:ND2	1:A:308:ASN:HA	2.34	0.42
1:A:148:PRO:HB3	4:A:2062:HOH:O	2.20	0.42
1:A:262:ASP:OD1	1:A:262:ASP:N	2.52	0.42
1:A:481:PHE:O	1:A:482:ALA:C	2.57	0.42
1:A:205:LEU:HD23	1:A:205:LEU:HA	1.86	0.42
1:A:104:ILE:HD13	1:A:123:ILE:HG13	2.02	0.42
1:A:423:ALA:O	1:A:426:ARG:NH1	2.49	0.42
1:A:146:LEU:HD12	4:A:2015:HOH:O	2.20	0.42
1:A:155:VAL:HA	1:A:159:GLU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ASN:ND2	2:A:1510:SO4:O3	2.39	0.42
1:A:490:GLU:HG2	1:A:494:LYS:NZ	2.35	0.42
1:A:76:GLN:OE1	4:A:2039:HOH:O	2.22	0.41
1:A:381:PHE:CD2	1:A:481:PHE:CZ	3.08	0.41
1:A:490:GLU:HG2	1:A:494:LYS:HZ2	1.85	0.41
1:A:55:ILE:CD1	1:A:188:LYS:HB2	2.50	0.41
1:A:74:ASN:HD22	1:A:74:ASN:HA	1.60	0.41
1:A:11:THR:HG1	1:A:14:GLN:HG3	1.80	0.41
1:A:312:ASP:O	1:A:315:LEU:CD2	2.67	0.41
1:A:171:ALA:O	1:A:175:LEU:HG	2.21	0.41
1:A:270:HIS:O	1:A:270:HIS:CD2	2.74	0.41
1:A:145:ALA:O	1:A:146:LEU:C	2.58	0.41
1:A:76:GLN:CB	1:A:185:LEU:HB2	2.51	0.40
1:A:97:ARG:HB2	1:A:131:TYR:CE1	2.56	0.40
1:A:246:GLN:HB2	4:A:2093:HOH:O	2.21	0.40
1:A:131:TYR:HA	1:A:132:PRO:HD3	1.89	0.40
1:A:136:LEU:HD21	1:A:425:LYS:HD2	2.04	0.40
1:A:337:ALA:O	1:A:340:ASN:HB2	2.21	0.40
1:A:475:TYR:O	1:A:475:TYR:HD1	1.93	0.40
1:A:28:ASP:O	1:A:31:ALA:CB	2.69	0.40
1:A:136:LEU:CD1	1:A:136:LEU:C	2.88	0.40
1:A:265:GLU:N	4:A:2105:HOH:O	2.29	0.40
1:A:381:PHE:O	1:A:383:ILE:N	2.55	0.40
1:A:385:GLN:NE2	4:A:2139:HOH:O	2.51	0.40
1:A:119:ILE:HG22	1:A:123:ILE:CD1	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:SER:OG	1:A:405:ASP:OD2[4_555]	2.19	0.01

## 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	507/509 (100%)	455 (90%)	31 (6%)	21 (4%)	<b>3</b> <b>1</b>

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	SER
1	A	145	ALA
1	A	146	LEU
1	A	271	LYS
1	A	275	LYS
1	A	363	HIS
1	A	364	MET
1	A	371	LEU
1	A	373	GLU
1	A	374	ASN
1	A	379	SER
1	A	372	VAL
1	A	476	ASP
1	A	411	ALA
1	A	478	ASP
1	A	479	ARG
1	A	366	GLN
1	A	370	PHE
1	A	367	LEU
1	A	477	ARG
1	A	369	PRO

### 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	387/387 (100%)	325 (84%)	62 (16%)	<b>2</b> <b>1</b>

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	2	GLU
1	A	23	VAL
1	A	24	ARG
1	A	25	LEU
1	A	26	GLN
1	A	44	GLN
1	A	45	ILE
1	A	50	ARG
1	A	66	ARG
1	A	67	ILE
1	A	72	LEU
1	A	73	GLU
1	A	75	LEU
1	A	77	ARG
1	A	106	SER
1	A	146	LEU
1	A	157	LEU
1	A	167	GLN
1	A	170	SER
1	A	172	THR
1	A	183	LEU
1	A	184	THR
1	A	194	LEU
1	A	195	ASN
1	A	200	SER
1	A	262	ASP
1	A	271	LYS
1	A	272	ASN
1	A	275	LYS
1	A	277	GLN
1	A	301	GLU
1	A	345	ILE
1	A	360	MET
1	A	362	LYS
1	A	363	HIS
1	A	366	GLN
1	A	367	LEU
1	A	371	LEU
1	A	372	VAL
1	A	373	GLU
1	A	374	ASN
1	A	377	VAL

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Mol	Chain	Res	Type
1	A	378	ASN
1	A	381	PHE
1	A	382	MET
1	A	410	SER
1	A	412	ASN
1	A	413	GLN
1	A	425	LYS
1	A	426	ARG
1	A	429	GLU
1	A	453	LYS
1	A	468	LEU
1	A	476	ASP
1	A	477	ARG
1	A	478	ASP
1	A	479	ARG
1	A	481	PHE
1	A	487	LYS
1	A	494	LYS
1	A	508	SER

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	14	GLN
1	A	26	GLN
1	A	74	ASN
1	A	83	HIS
1	A	270	HIS
1	A	277	GLN
1	A	378	ASN
1	A	412	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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
3	GOL	A	1511	-	5,5,5	0.63	0	5,5,5	0.39	0
2	SO4	A	1510	-	4,4,4	0.69	0	6,6,6	0.04	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1511	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1511	GOL	C1-C2-C3-O3
3	A	1511	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1511	GOL	8	0
2	A	1510	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	493/509 (96%)	0.75	52 (10%) <b>6</b>   <b>6</b>	12, 23, 55, 105	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	THR	7.9
1	A	382	MET	7.5
1	A	271	LYS	7.4
1	A	145	ALA	6.5
1	A	477	ARG	6.4
1	A	476	ASP	6.1
1	A	360	MET	5.3
1	A	64	SER	5.0
1	A	146	LEU	5.0
1	A	381	PHE	4.6
1	A	2	GLU	4.5
1	A	70	HIS	4.1
1	A	411	ALA	4.1
1	A	377	VAL	3.7
1	A	378	ASN	3.5
1	A	362	LYS	3.3
1	A	143	SER	3.1
1	A	147	ALA	3.1
1	A	479	ARG	3.1
1	A	89	ALA	3.1
1	A	478	ASP	3.0
1	A	270	HIS	3.0
1	A	383	ILE	3.0
1	A	276	VAL	3.0
1	A	179	GLY	3.0
1	A	466	GLN	2.9
1	A	144	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	413	GLN	2.7
1	A	176	ALA	2.6
1	A	47	ALA	2.5
1	A	268	LEU	2.5
1	A	65	THR	2.5
1	A	155	VAL	2.5
1	A	174	ALA	2.4
1	A	156	LEU	2.4
1	A	361	ASP	2.3
1	A	21	ALA	2.3
1	A	68	ALA	2.3
1	A	50	ARG	2.2
1	A	59	PHE	2.2
1	A	375	GLY	2.2
1	A	69	SER	2.2
1	A	122	LEU	2.2
1	A	45	ILE	2.2
1	A	48	GLU	2.1
1	A	380	GLY	2.1
1	A	480	PHE	2.1
1	A	489	VAL	2.1
1	A	148	PRO	2.1
1	A	481	PHE	2.0
1	A	75	LEU	2.0
1	A	49	ASP	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 monosaccharides 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
2	SO4	A	1510	5/5	0.85	0.23	99,101,109,112	0
3	GOL	A	1511	6/6	0.85	0.21	37,48,54,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.