



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:16 PM GMT

PDB ID : 4HST  
Title : Crystal structure of a double mutant of a class III engineered cephalosporin acylase  
Authors : Vrieling, A.; Golden, E.; Patterson, R.; Tie, W.J.; Anandan, A.; Flematti, G.; Molla, G.; Rosini, E.; Pollegioni, L.  
Deposited on : 2012-10-30  
Resolution : 1.57 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

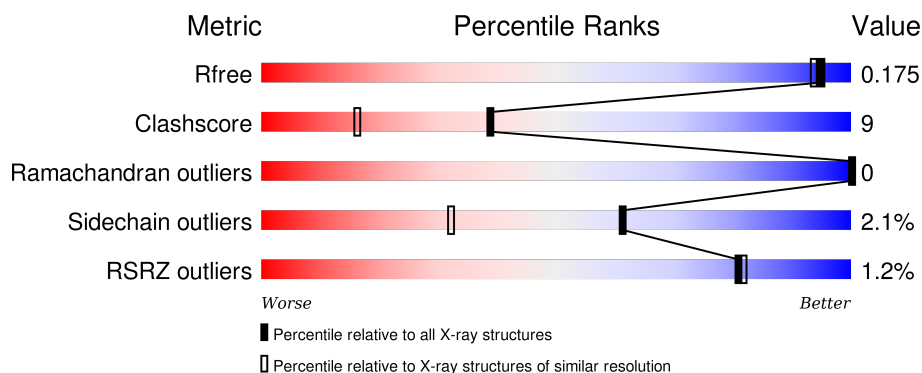
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.57 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	3815 (1.60-1.56)
Clashscore	102246	4131 (1.60-1.56)
Ramachandran outliers	100387	4021 (1.60-1.56)
Sidechain outliers	100360	4018 (1.60-1.56)
RSRZ outliers	91569	3823 (1.60-1.56)

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	229	<div> <div></div> <div>83% 9% • 6%</div> </div>
2	B	543	<div> <div></div> <div>81% 14% • •</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLJ	B	601	-	-	X	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6863 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.

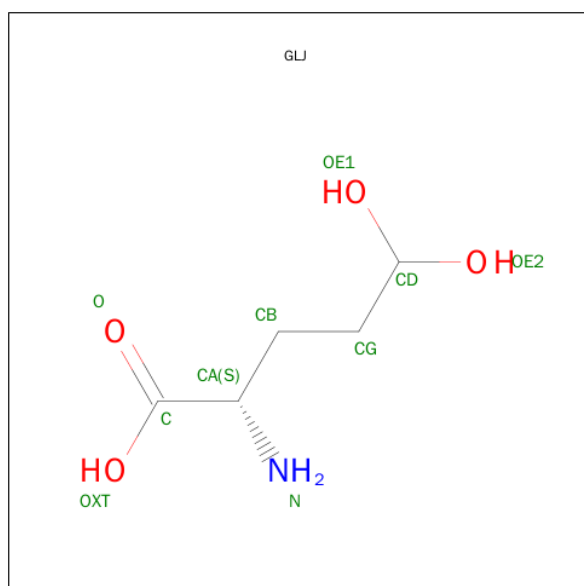
- Molecule 1 is a protein called glutaryl-7-aminocephalosporanic acid acylase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1686	1082	300	293	11	0	9	0

- Molecule 2 is a protein called glutaryl-7-aminocephalosporanic acid acylase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	535	4191	2647	765	763	16	0	17	0

- Molecule 3 is 5,5-DIHYDROXY-L-NORVALINE (three-letter code: GLJ) (formula:  $C_5H_{11}NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	B	1	10	5	1	4	0	0

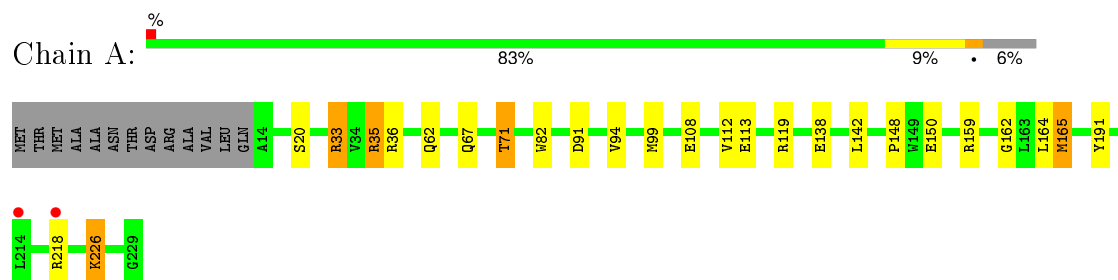
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	290	Total 290	O 290	0	0
4	B	686	Total 686	O 686	0	0

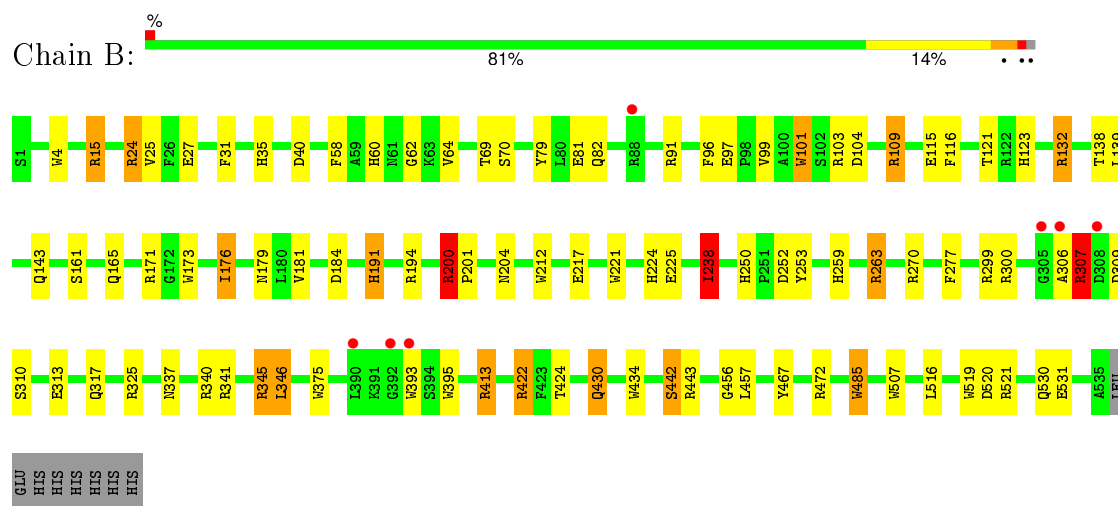
### 3 Residue-property plots [i](#)

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: glutaryl-7-aminocephalosporanic acid acylase alpha chain



- Molecule 2: glutaryl-7-aminocephalosporanic acid acylase beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.39Å 77.84Å 191.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.00 – 1.57 64.42 – 1.57	Depositor EDS
% Data completeness (in resolution range)	93.4 (96.00-1.57) 93.4 (64.42-1.57)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.51 (at 1.57Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.119 , 0.162 0.138 , 0.175	Depositor DCC
$R_{free}$ test set	6723 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.9	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 133826 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6863	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: GLJ

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	1.39	7/1753 (0.4%)	1.19	10/2375 (0.4%)
2	B	1.39	22/4366 (0.5%)	1.27	32/5968 (0.5%)
All	All	1.39	29/6119 (0.5%)	1.25	42/8343 (0.5%)

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
2	B	3	0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	101	TRP	CD2-CE2	11.66	1.55	1.41
2	B	225	GLU	CD-OE1	8.04	1.34	1.25
2	B	443	ARG	CZ-NH1	7.82	1.43	1.33
2	B	4	TRP	CG-CD1	7.46	1.47	1.36
2	B	485	TRP	CE3-CZ3	6.62	1.49	1.38
2	B	485	TRP	CD2-CE2	6.37	1.49	1.41
2	B	212	TRP	CD2-CE2	6.25	1.48	1.41
1	A	113	GLU	CD-OE1	6.14	1.32	1.25
1	A	91	ASP	CG-OD1	6.11	1.39	1.25
1	A	191	TYR	CG-CD1	5.95	1.46	1.39
1	A	138	GLU	CD-OE2	5.92	1.32	1.25
2	B	375	TRP	CD2-CE2	5.90	1.48	1.41
2	B	253	TYR	CG-CD1	5.77	1.46	1.39
2	B	531	GLU	CD-OE2	5.71	1.31	1.25
1	A	71[A]	THR	CB-CG2	-5.70	1.33	1.52
1	A	71[B]	THR	CB-CG2	-5.70	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	430	GLN	CD-OE1	5.69	1.36	1.24
2	B	97	GLU	CD-OE1	-5.69	1.19	1.25
2	B	277	PHE	CG-CD2	5.61	1.47	1.38
2	B	221	TRP	CD2-CE2	5.55	1.48	1.41
2	B	519	TRP	CG-CD1	5.44	1.44	1.36
1	A	82	TRP	CZ3-CH2	5.29	1.48	1.40
2	B	434	TRP	CD2-CE2	5.28	1.47	1.41
2	B	194	ARG	NE-CZ	5.26	1.39	1.33
2	B	395	TRP	CD2-CE2	5.23	1.47	1.41
2	B	442[A]	SER	CB-OG	-5.19	1.35	1.42
2	B	442[B]	SER	CB-OG	-5.19	1.35	1.42
2	B	15	ARG	CD-NE	5.18	1.55	1.46
2	B	507	TRP	CG-CD1	5.04	1.43	1.36

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	109[A]	ARG	NE-CZ-NH1	13.53	127.06	120.30
2	B	109[B]	ARG	NE-CZ-NH1	13.53	127.06	120.30
2	B	443	ARG	NE-CZ-NH2	-13.07	113.77	120.30
1	A	91	ASP	CB-CG-OD2	-12.24	107.28	118.30
2	B	109[A]	ARG	NE-CZ-NH2	-11.78	114.41	120.30
2	B	109[B]	ARG	NE-CZ-NH2	-11.78	114.41	120.30
2	B	307	ARG	NE-CZ-NH1	11.65	126.12	120.30
2	B	443	ARG	NE-CZ-NH1	11.59	126.10	120.30
2	B	422	ARG	NE-CZ-NH1	11.43	126.01	120.30
1	A	91	ASP	CB-CG-OD1	9.79	127.11	118.30
2	B	307	ARG	NE-CZ-NH2	-8.66	115.97	120.30
2	B	422	ARG	NE-CZ-NH2	-8.64	115.98	120.30
2	B	238[A]	ILE	CG1-CB-CG2	8.61	130.33	111.40
2	B	238[B]	ILE	CG1-CB-CG2	8.61	130.33	111.40
1	A	159	ARG	NE-CZ-NH1	8.01	124.30	120.30
2	B	345	ARG	NE-CZ-NH1	7.47	124.04	120.30
2	B	472	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	A	119	ARG	NE-CZ-NH2	-7.21	116.70	120.30
2	B	270	ARG	NE-CZ-NH1	-7.17	116.72	120.30
2	B	252	ASP	CB-CG-OD1	-7.06	111.95	118.30
1	A	35	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	165	MET	CG-SD-CE	-6.62	89.61	100.20
1	A	36	ARG	NE-CZ-NH2	-6.57	117.02	120.30
2	B	300	ARG	NE-CZ-NH1	6.49	123.54	120.30
2	B	200	ARG	NE-CZ-NH2	-6.40	117.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	442[A]	SER	N-CA-CB	-6.39	100.92	110.50
2	B	442[B]	SER	N-CA-CB	-6.39	100.92	110.50
2	B	176[A]	ILE	CB-CA-C	-6.10	99.40	111.60
2	B	176[B]	ILE	CB-CA-C	-6.10	99.40	111.60
1	A	159	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	33	ARG	NE-CZ-NH2	-5.85	117.37	120.30
2	B	24[A]	ARG	NE-CZ-NH1	5.85	123.22	120.30
2	B	24[B]	ARG	NE-CZ-NH1	5.85	123.22	120.30
2	B	132	ARG	NE-CZ-NH1	5.83	123.21	120.30
2	B	340	ARG	NE-CZ-NH2	-5.53	117.53	120.30
2	B	58	PHE	CB-CG-CD2	-5.46	116.98	120.80
1	A	36	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	B	413	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	B	263	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	B	346	LEU	CB-CG-CD1	-5.09	102.35	111.00
2	B	309	ASP	N-CA-CB	-5.06	101.49	110.60
2	B	300	ARG	NE-CZ-NH2	-5.03	117.79	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	121	THR	CB
2	B	138	THR	CB
2	B	238[A]	ILE	CB

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	1686	0	1753	19	0
2	B	4191	0	4056	89	0
3	B	10	0	9	10	0
4	A	290	0	0	9	1
4	B	686	0	0	25	1
All	All	6863	0	5818	105	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 9.

All (105) 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)
2:B:520:ASP:HB2	4:B:795:HOH:O	1.32	1.26
4:A:358:HOH:O	2:B:176[A]:ILE:HD11	1.34	1.26
2:B:109[B]:ARG:NH1	2:B:430:GLN:HE22	1.49	1.10
2:B:109[B]:ARG:CZ	2:B:430:GLN:HE22	1.64	1.09
2:B:109[B]:ARG:NH1	2:B:430:GLN:NE2	2.10	0.98
2:B:40:ASP:HB3	4:B:1274:HOH:O	1.65	0.95
1:A:142:LEU:HD23	2:B:109[B]:ARG:NH1	1.83	0.93
2:B:121:THR:HG23	2:B:123:HIS:H	1.35	0.91
2:B:15:ARG:NH2	4:B:1055:HOH:O	2.02	0.91
2:B:81:GLU:OE2	2:B:121:THR:HG21	1.69	0.91
1:A:62:GLN:HE22	2:B:530:GLN:HE22	1.20	0.90
2:B:60:HIS:HD2	2:B:62:GLY:H	1.18	0.88
2:B:346:LEU:HD21	2:B:393:TRP:HZ3	1.38	0.87
1:A:142:LEU:CD2	2:B:109[B]:ARG:NH1	2.37	0.86
2:B:109[B]:ARG:CZ	2:B:430:GLN:NE2	2.36	0.86
1:A:142:LEU:HD23	2:B:109[B]:ARG:HH12	1.40	0.85
2:B:99[B]:VAL:CG1	2:B:101:TRP:CD1	2.61	0.84
2:B:70[B]:SER:H	3:B:601:GLJ:HG3	1.43	0.83
1:A:67:GLN:O	1:A:71[A]:THR:HG22	1.79	0.83
2:B:70[A]:SER:H	3:B:601:GLJ:HG3	1.45	0.81
2:B:299:ARG:NH2	4:B:1119:HOH:O	2.13	0.81
2:B:413:ARG:NH2	4:B:1116:HOH:O	2.01	0.80
2:B:299:ARG:HD3	4:B:779:HOH:O	1.81	0.79
2:B:346:LEU:HD21	2:B:393:TRP:CZ3	2.17	0.79
1:A:164:LEU:H	2:B:143:GLN:HE22	1.30	0.79
2:B:132:ARG:HD2	4:B:1326:HOH:O	1.85	0.76
2:B:181:VAL:HG22	2:B:238[A]:ILE:HD11	1.68	0.76
2:B:345:ARG:HD2	4:B:1296:HOH:O	1.87	0.75
2:B:99[B]:VAL:HG11	2:B:101:TRP:NE1	2.03	0.73
2:B:346:LEU:CD2	2:B:393:TRP:HZ3	2.01	0.73
2:B:70[B]:SER:H	3:B:601:GLJ:CG	2.01	0.73
2:B:109[A]:ARG:HD3	2:B:430:GLN:HE22	1.55	0.71
2:B:70[A]:SER:H	3:B:601:GLJ:CG	2.03	0.71
1:A:150:GLU:HG2	4:A:442:HOH:O	1.90	0.70
2:B:250:HIS:HE1	4:B:794:HOH:O	1.76	0.68
2:B:99[B]:VAL:HG11	2:B:101:TRP:HE1	1.57	0.68
2:B:123:HIS:HE1	2:B:217:GLU:OE2	1.78	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:ARG:HD2	2:B:307:ARG:N	2.10	0.66
1:A:226:LYS:NZ	4:A:521:HOH:O	2.29	0.66
2:B:27[B]:GLU:OE2	2:B:31:PHE:HE1	1.78	0.65
2:B:337:ASN:ND2	2:B:341:ARG:HE	1.97	0.62
2:B:521:ARG:HD3	4:B:900:HOH:O	1.99	0.62
2:B:60:HIS:HD2	2:B:62:GLY:N	1.96	0.62
2:B:99[B]:VAL:CG1	2:B:101:TRP:HD1	2.13	0.61
2:B:99[B]:VAL:HG13	2:B:101:TRP:CD1	2.34	0.61
1:A:71[A]:THR:HG21	4:B:862:HOH:O	2.01	0.60
2:B:413:ARG:HD2	4:B:1176:HOH:O	2.00	0.60
2:B:24[B]:ARG:HE	3:B:601:GLJ:H	1.49	0.60
1:A:164:LEU:HD21	2:B:139:LEU:HD21	1.84	0.59
1:A:148:PRO:HB3	4:A:539:HOH:O	2.01	0.59
2:B:161:SER:H	2:B:165:GLN:NE2	2.00	0.59
2:B:81:GLU:OE2	2:B:138:THR:HG21	2.03	0.59
1:A:218:ARG:HD2	4:A:569:HOH:O	2.03	0.58
2:B:224:HIS:HE1	4:B:842:HOH:O	1.85	0.58
2:B:259:HIS:HD2	4:B:1146:HOH:O	1.87	0.58
2:B:99[B]:VAL:HG11	2:B:101:TRP:CD1	2.38	0.57
1:A:67:GLN:O	1:A:71[B]:THR:HG23	2.03	0.57
2:B:81:GLU:OE2	2:B:123:HIS:HD2	1.87	0.57
2:B:191:HIS:HB2	2:B:238[A]:ILE:CD1	2.34	0.57
2:B:109[B]:ARG:NH2	4:B:854:HOH:O	2.39	0.55
4:A:306:HOH:O	2:B:35:HIS:HE1	1.89	0.55
3:B:601:GLJ:HA	3:B:601:GLJ:OE1	2.06	0.55
2:B:121:THR:HG23	2:B:123:HIS:N	2.13	0.54
2:B:313:GLU:O	2:B:317:GLN:HG3	2.07	0.54
2:B:161:SER:H	2:B:165:GLN:HE21	1.55	0.54
1:A:112[A]:VAL:HG13	4:A:451:HOH:O	2.08	0.53
1:A:162:GLY:HA3	2:B:176[A]:ILE:CD1	2.38	0.53
2:B:60:HIS:HE1	4:B:707:HOH:O	1.90	0.53
2:B:173:TRP:NE1	4:B:1376:HOH:O	2.34	0.53
2:B:69:THR:HA	3:B:601:GLJ:HG3	1.91	0.52
2:B:171:ARG:HB2	2:B:171:ARG:NH1	2.25	0.51
2:B:179:ASN:OD1	2:B:191:HIS:HE1	1.94	0.49
2:B:82[A]:GLN:HE22	2:B:91:ARG:HH11	1.61	0.49
2:B:325:ARG:NH2	4:B:978:HOH:O	2.46	0.49
2:B:109[A]:ARG:NH2	4:B:917:HOH:O	2.42	0.48
1:A:33:ARG:HD2	1:A:35:ARG:NH2	2.29	0.47
2:B:103:ARG:HH21	2:B:115[B]:GLU:CD	2.17	0.47
2:B:456:GLY:HA3	2:B:467:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25[A]:VAL:HG13	2:B:27[A]:GLU:HG3	1.97	0.46
2:B:259:HIS:CD2	2:B:263:ARG:HH21	2.33	0.46
2:B:99[B]:VAL:HG13	2:B:101:TRP:HD1	1.79	0.46
3:B:601:GLJ:OE1	3:B:601:GLJ:CA	2.63	0.46
2:B:181:VAL:HG13	2:B:238[A]:ILE:HD13	1.99	0.45
2:B:191:HIS:HB2	2:B:238[A]:ILE:HD11	1.97	0.45
2:B:306:ALA:C	2:B:307:ARG:HD2	2.37	0.45
1:A:33:ARG:HD2	1:A:35:ARG:CZ	2.47	0.45
2:B:442[A]:SER:HB2	4:B:813:HOH:O	2.16	0.45
2:B:109[A]:ARG:HD3	2:B:430:GLN:NE2	2.28	0.44
2:B:346:LEU:C	2:B:346:LEU:HD23	2.38	0.44
4:A:313:HOH:O	2:B:191:HIS:HD2	2.00	0.44
2:B:64[B]:VAL:HG12	2:B:184:ASP:HB3	2.01	0.43
2:B:79:TYR:HB2	2:B:138:THR:CG2	2.49	0.43
2:B:299:ARG:HG3	4:B:1154:HOH:O	2.19	0.42
2:B:325:ARG:CZ	4:B:978:HOH:O	2.68	0.42
1:A:94:VAL:HB	1:A:99[B]:MET:HG3	2.02	0.42
2:B:104:ASP:HB3	2:B:116:PHE:CZ	2.54	0.41
2:B:516:LEU:HD23	2:B:516:LEU:HA	1.87	0.41
2:B:424[B]:THR:HG22	4:B:1198:HOH:O	2.20	0.41
2:B:176[A]:ILE:CD1	4:B:1378:HOH:O	2.68	0.41
2:B:200:ARG:HB2	2:B:201:PRO:CD	2.51	0.41
2:B:250:HIS:HD2	4:B:1113:HOH:O	2.04	0.40
1:A:20[C]:SER:OG	4:A:351:HOH:O	2.22	0.40
2:B:91:ARG:HB2	2:B:96:PHE:CZ	2.56	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)
4:A:578:HOH:O	4:B:835:HOH:O[3_656]	1.14	1.06

## 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	224/229 (98%)	221 (99%)	3 (1%)	0	100	100
2	B	550/543 (101%)	537 (98%)	13 (2%)	0	100	100
All	All	774/772 (100%)	758 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	171/171 (100%)	168 (98%)	3 (2%)	66	40
2	B	430/421 (102%)	420 (98%)	10 (2%)	58	28
All	All	601/592 (102%)	588 (98%)	13 (2%)	61	30

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	GLU
1	A	165	MET
1	A	226	LYS
2	B	191	HIS
2	B	200	ARG
2	B	204	ASN
2	B	238[A]	ILE
2	B	238[B]	ILE
2	B	307	ARG
2	B	310	SER
2	B	422	ARG
2	B	457	LEU
2	B	485	TRP

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

Mol	Chain	Res	Type
2	B	35	HIS
2	B	60	HIS
2	B	94	ASN
2	B	123	HIS
2	B	143	GLN
2	B	165	GLN
2	B	191	HIS
2	B	204	ASN
2	B	224	HIS
2	B	250	HIS
2	B	259	HIS
2	B	286	HIS
2	B	337	ASN
2	B	430	GLN
2	B	479	ASN
2	B	530	GLN

### 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 ⓘ

1 ligand is 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	GLJ	B	601	-	3,9,9	1.55	1 (33%)	2,11,11	2.37	1 (50%)

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	GLJ	B	601	-	-	0/3/9/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	GLJ	CB-CG	-2.16	1.42	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	GLJ	CB-CA-N	3.29	119.86	110.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	GLJ	10	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 [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	216/229 (94%)	-0.45	2 (0%) 85 86	4, 10, 22, 42	0
2	B	535/543 (98%)	-0.27	7 (1%) 79 80	4, 9, 22, 40	0
All	All	751/772 (97%)	-0.32	9 (1%) 81 82	4, 10, 22, 42	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	393	TRP	4.5
2	B	306	ALA	2.8
2	B	308	ASP	2.6
2	B	392	GLY	2.6
1	A	214	LEU	2.5
1	A	218	ARG	2.3
2	B	305	GLY	2.2
2	B	390	LEU	2.0
2	B	88	ARG	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GLJ	B	601	10/10	0.92	0.13	2.29	6,14,29,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.