Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 07:00 AM EDT

PDB ID	:	4HSR
Title	:	Crystal Structure of a class III engineered cephalosporin acylase
Authors	:	Vrielink, A.; Golden, E.; Patterson, R.; Tie, W.J.; Anandan, A.; Flematti, G.; Molla, G.; Rosini, E.; Pollegioni, L.
Deposited on	:	2012-10-30
Resolution	:	2.13 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

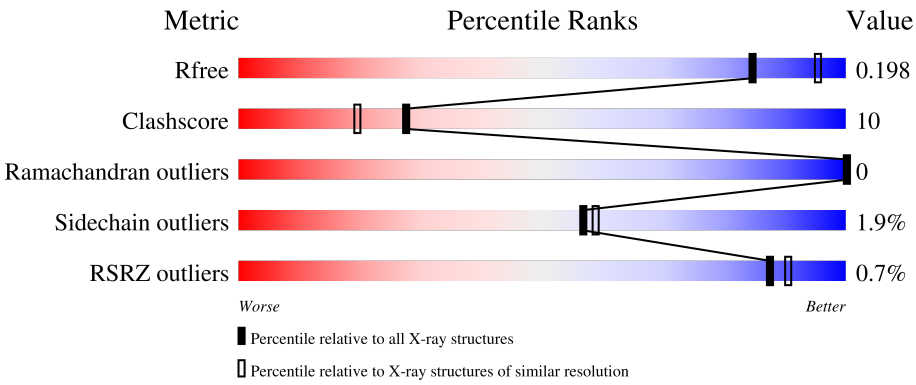
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 >=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 <=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	% 81% 12% • 6%
2	B	543	% 78% 18% ••

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 6401 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.

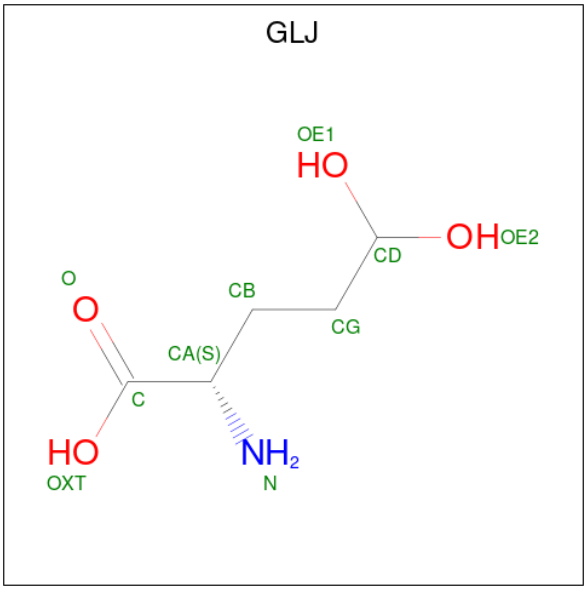
- Molecule 1 is a protein called glutaryl-7-aminocephalosporanic acid acylase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1655	1057	299	290	9	0	2	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	4175	2630	773	756	16	0	10	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.

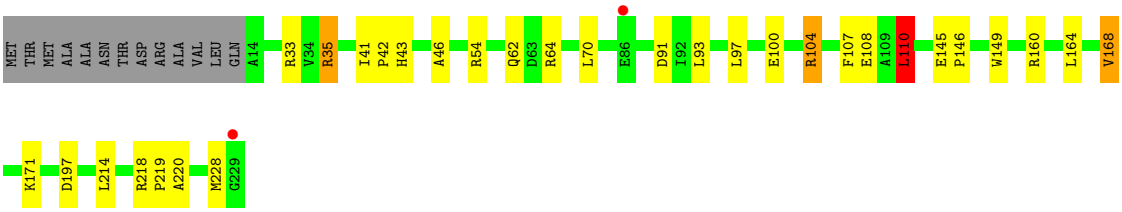
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	171	171	171	0	0
			Total	O		
4	B	390	390	390	0	0

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.

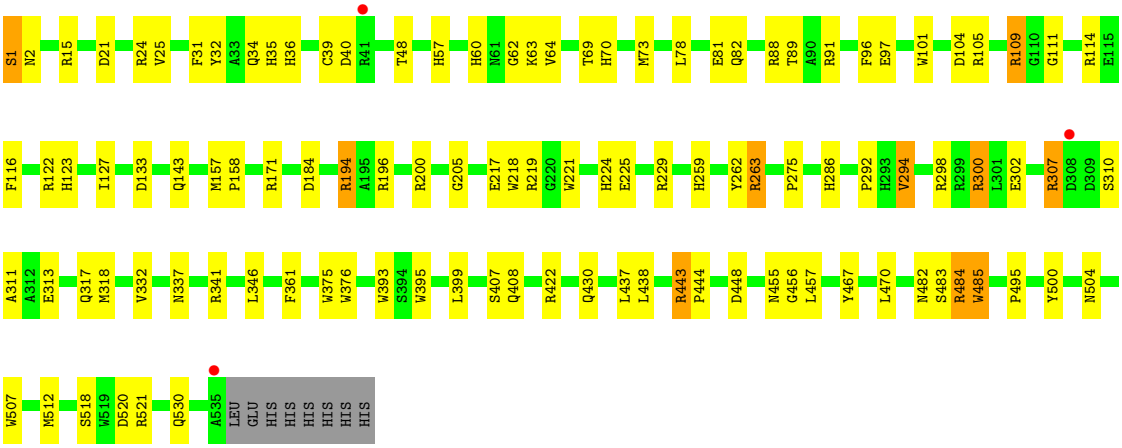
• Molecule 1: glutaryl-7-aminocephalosporanic acid acylase alpha chain

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.16Å 77.02Å 192.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.07 – 2.13 20.60 – 2.13	Depositor EDS
% Data completeness (in resolution range)	96.9 (96.07-2.13) 97.0 (20.60-2.13)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.13Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.152 , 0.198 0.152 , 0.198	Depositor DCC
R_{free} test set	2832 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6401	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	1.03	2/1698 (0.1%)	1.16	10/2303 (0.4%)
2	B	1.07	8/4318 (0.2%)	1.06	20/5900 (0.3%)
All	All	1.06	10/6016 (0.2%)	1.09	30/8203 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	SER	C-O	12.23	1.46	1.23
2	B	507	TRP	CD2-CE2	6.89	1.49	1.41
2	B	101	TRP	CD2-CE2	6.35	1.49	1.41
2	B	376	TRP	CD2-CE2	5.87	1.48	1.41
2	B	218	TRP	CD2-CE2	5.29	1.47	1.41
2	B	395	TRP	CD2-CE2	5.24	1.47	1.41
1	A	149	TRP	CD2-CE2	5.18	1.47	1.41
1	A	91	ASP	CB-CG	5.18	1.62	1.51
2	B	221	TRP	CD2-CE2	5.17	1.47	1.41
2	B	375	TRP	CD2-CE2	5.05	1.47	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	104	ARG	NE-CZ-NH1	-16.83	111.88	120.30
2	B	263	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	A	104	ARG	NE-CZ-NH2	9.09	124.84	120.30
2	B	263	ARG	NE-CZ-NH2	-7.87	116.37	120.30
2	B	307	ARG	NE-CZ-NH1	7.09	123.84	120.30
2	B	1	SER	CA-C-N	7.05	132.71	117.20
1	A	35	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	A	64	ARG	NE-CZ-NH1	7.03	123.81	120.30
2	B	194	ARG	NE-CZ-NH1	7.00	123.80	120.30
2	B	109	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	A	168	VAL	CB-CA-C	-6.79	98.50	111.40
2	B	422	ARG	NE-CZ-NH1	6.70	123.65	120.30
2	B	443	ARG	NE-CZ-NH2	-6.64	116.98	120.30
2	B	443	ARG	NE-CZ-NH1	6.60	123.60	120.30
2	B	294	VAL	CB-CA-C	-6.57	98.92	111.40
1	A	91	ASP	CB-CG-OD1	6.21	123.89	118.30
2	B	300	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	B	194	ARG	NE-CZ-NH2	-6.05	117.28	120.30
2	B	408	GLN	CB-CA-C	-5.99	98.43	110.40
1	A	168	VAL	CG1-CB-CG2	5.98	120.47	110.90
2	B	307	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	A	110	LEU	CB-CG-CD1	5.79	120.84	111.00
2	B	122	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	A	54	ARG	NE-CZ-NH2	-5.39	117.60	120.30
2	B	73	MET	CG-SD-CE	5.34	108.75	100.20
1	A	33	ARG	NE-CZ-NH1	5.17	122.88	120.30
2	B	1	SER	CA-C-O	-5.11	109.38	120.10
2	B	484[A]	ARG	NE-CZ-NH2	-5.09	117.75	120.30
2	B	484[B]	ARG	NE-CZ-NH2	-5.09	117.75	120.30
2	B	294	VAL	CG1-CB-CG2	5.05	118.98	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	ASP	Peptide
2	B	1	SER	Mainchain

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	1655	0	1688	21	0
2	B	4175	0	4003	96	1
3	B	10	0	9	12	0
4	A	171	0	0	6	0
4	B	390	0	0	29	0
All	All	6401	0	5700	115	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 10.

All (115) 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:160:ARG:HG3	4:A:435:HOH:O	1.11	1.25
1:A:228:MET:HE3	4:B:980:HOH:O	1.44	1.16
2:B:114:ARG:HD2	4:B:1029:HOH:O	1.47	1.14
3:B:601:GLJ:HA	3:B:601:GLJ:OE1	1.40	1.14
3:B:601:GLJ:OE1	3:B:601:GLJ:CA	1.95	1.14
1:A:70:LEU:CG	4:A:404:HOH:O	1.91	1.13
2:B:482:ASN:HB2	4:B:963:HOH:O	1.45	1.12
2:B:346[B]:LEU:HD12	2:B:346[B]:LEU:O	1.51	1.08
3:B:601:GLJ:OE1	3:B:601:GLJ:N	1.90	1.04
2:B:437:LEU:HB2	4:B:955:HOH:O	1.57	1.04
2:B:88:ARG:HG3	4:B:977:HOH:O	1.60	1.01
2:B:346[B]:LEU:HD12	2:B:346[B]:LEU:C	1.84	0.97
1:A:108:GLU:HG2	4:A:371:HOH:O	1.65	0.95
1:A:100:GLU:OE2	1:A:104:ARG:NH1	1.98	0.95
2:B:60:HIS:HD2	2:B:62:GLY:H	1.17	0.92
2:B:482:ASN:CB	4:B:963:HOH:O	2.10	0.88
2:B:57:HIS:ND1	4:B:981:HOH:O	2.06	0.88
1:A:62:GLN:HE22	2:B:530:GLN:HE22	1.16	0.88
2:B:346[B]:LEU:HD13	2:B:393:TRP:HZ3	1.43	0.83
2:B:482:ASN:CG	4:B:963:HOH:O	2.17	0.81
2:B:70:HIS:H	3:B:601:GLJ:CG	1.94	0.80
2:B:70:HIS:H	3:B:601:GLJ:HG2	1.46	0.80
2:B:69:THR:HA	3:B:601:GLJ:HG3	1.66	0.77
1:A:164:LEU:H	2:B:143:GLN:HE22	1.32	0.76
2:B:443:ARG:HH11	2:B:504:ASN:HD22	1.30	0.76
2:B:518:SER:HB2	2:B:521[B]:ARG:HG3	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317[B]:GLN:HE21	2:B:317[B]:GLN:HA	1.53	0.73
2:B:346[B]:LEU:CD1	2:B:393:TRP:HZ3	2.05	0.69
2:B:313:GLU:O	2:B:317[A]:GLN:HG3	1.93	0.68
2:B:111:GLY:HA3	4:B:972:HOH:O	1.92	0.68
2:B:70:HIS:N	3:B:601:GLJ:HG2	2.10	0.67
2:B:24:ARG:HB2	2:B:470:LEU:HD11	1.78	0.66
2:B:346[B]:LEU:C	2:B:346[B]:LEU:CD1	2.60	0.65
2:B:15:ARG:NH2	4:B:1053:HOH:O	2.17	0.65
1:A:35:ARG:HD3	4:A:382:HOH:O	1.97	0.64
2:B:109:ARG:HD3	2:B:430:GLN:HE22	1.61	0.64
2:B:60:HIS:HD2	2:B:62:GLY:N	1.92	0.64
2:B:82:GLN:HE22	2:B:91:ARG:HH11	1.46	0.64
2:B:224:HIS:HE1	4:B:907:HOH:O	1.81	0.63
2:B:337:ASN:ND2	2:B:341:ARG:HE	1.95	0.63
2:B:32:TYR:HE2	4:B:981:HOH:O	1.83	0.62
2:B:300:ARG:HD3	4:B:922:HOH:O	1.99	0.62
2:B:483:SER:C	2:B:484[A]:ARG:HG2	2.20	0.61
2:B:317[B]:GLN:HE21	2:B:317[B]:GLN:CA	2.13	0.61
2:B:57:HIS:HD2	2:B:194:ARG:HH22	1.47	0.60
2:B:60:HIS:CD2	2:B:62:GLY:H	2.08	0.58
2:B:40:ASP:HB3	4:B:946:HOH:O	2.04	0.58
2:B:109:ARG:HD3	2:B:430:GLN:NE2	2.19	0.57
2:B:317[B]:GLN:HA	2:B:317[B]:GLN:NE2	2.20	0.57
2:B:259:HIS:HD2	4:B:719:HOH:O	1.87	0.57
2:B:70:HIS:H	3:B:601:GLJ:HG3	1.69	0.57
2:B:109:ARG:CD	2:B:430:GLN:HE22	2.19	0.56
2:B:70:HIS:N	3:B:601:GLJ:CG	2.66	0.56
1:A:43:HIS:HA	2:B:36:HIS:HB3	1.87	0.56
2:B:196:ARG:HD2	4:B:851:HOH:O	2.06	0.55
2:B:31:PHE:HD2	2:B:470:LEU:HD11	1.72	0.55
2:B:298:ARG:O	2:B:302:GLU:HB2	2.08	0.54
2:B:60:HIS:HE1	4:B:707:HOH:O	1.89	0.54
1:A:145[B]:GLU:OE1	1:A:146:PRO:HD2	2.07	0.54
2:B:346[B]:LEU:HD13	2:B:393:TRP:CZ3	2.33	0.53
2:B:91:ARG:HB2	2:B:96:PHE:CZ	2.44	0.53
1:A:228:MET:CE	4:B:980:HOH:O	2.25	0.52
2:B:313:GLU:O	2:B:317[B]:GLN:HG2	2.10	0.52
2:B:171:ARG:NH2	2:B:225:GLU:OE2	2.43	0.51
2:B:70:HIS:HB2	3:B:601:GLJ:HG2	1.94	0.50
2:B:69:THR:CA	3:B:601:GLJ:HG3	2.38	0.50
2:B:104:ASP:HB3	2:B:116:PHE:CZ	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:ARG:N	2:B:307:ARG:HD2	2.27	0.49
2:B:34:GLN:HB3	2:B:485:TRP:CH2	2.48	0.48
1:A:228:MET:HG2	4:B:980:HOH:O	2.12	0.48
2:B:275:PRO:HD2	4:B:1041:HOH:O	2.13	0.48
2:B:275:PRO:CD	4:B:1041:HOH:O	2.61	0.48
1:A:104:ARG:HH11	1:A:104:ARG:HD2	1.36	0.48
2:B:448:ASP:HA	2:B:455:ASN:O	2.15	0.47
1:A:107:PHE:HA	1:A:110:LEU:HD22	1.96	0.47
2:B:123:HIS:HE1	2:B:217:GLU:OE2	1.98	0.47
2:B:88:ARG:CG	4:B:977:HOH:O	2.35	0.46
1:A:218:ARG:HB3	1:A:219:PRO:HD3	1.98	0.46
2:B:259:HIS:CD2	2:B:263:ARG:HH21	2.33	0.46
2:B:317[B]:GLN:CA	2:B:317[B]:GLN:NE2	2.78	0.46
2:B:443:ARG:NH1	2:B:504:ASN:HD22	2.06	0.46
2:B:2:ASN:HB2	2:B:21:ASP:OD2	2.16	0.46
2:B:57:HIS:HB2	4:B:981:HOH:O	2.16	0.46
1:A:171:LYS:HE2	2:B:205:GLY:HA2	1.97	0.45
2:B:229:ARG:HD2	4:B:910:HOH:O	2.15	0.45
2:B:318:MET:HG2	2:B:332:VAL:HG13	1.98	0.45
2:B:63:LYS:HE3	2:B:63:LYS:HB2	1.81	0.44
2:B:35:HIS:CD2	2:B:48:THR:OG1	2.71	0.44
2:B:437:LEU:O	2:B:437:LEU:HG	2.15	0.44
2:B:484[B]:ARG:HB3	2:B:512:MET:HB3	2.00	0.43
1:A:93:LEU:O	1:A:97:LEU:HG	2.18	0.43
2:B:361:PHE:HB2	4:B:980:HOH:O	2.18	0.43
2:B:346[B]:LEU:CD1	2:B:393:TRP:CZ3	2.95	0.43
2:B:443:ARG:HB3	2:B:444:PRO:HD2	1.99	0.43
2:B:64[B]:VAL:HG12	2:B:184:ASP:HB3	2.00	0.43
2:B:275:PRO:N	4:B:1041:HOH:O	2.50	0.43
2:B:24:ARG:HB2	2:B:470:LEU:CD1	2.47	0.43
2:B:57:HIS:CG	4:B:981:HOH:O	2.65	0.43
1:A:41:ILE:HA	1:A:42:PRO:HD3	1.80	0.43
2:B:81:GLU:OE2	2:B:123:HIS:HD2	2.01	0.42
2:B:495:PRO:HA	2:B:500:TYR:CD2	2.54	0.42
1:A:46:ALA:O	2:B:39:CYS:HA	2.19	0.42
2:B:89:THR:HA	2:B:97:GLU:O	2.20	0.42
2:B:311:ALA:HB1	2:B:407:SER:HB2	2.01	0.42
1:A:220:ALA:HB2	4:A:408:HOH:O	2.20	0.42
2:B:456:GLY:HA3	2:B:467:TYR:CZ	2.54	0.42
2:B:25[B]:VAL:HG23	4:B:1063:HOH:O	2.19	0.41
2:B:70:HIS:CB	3:B:601:GLJ:HG2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:ARG:HA	2:B:114:ARG:O	2.20	0.41
2:B:262:TYR:CD2	2:B:292:PRO:HG3	2.56	0.41
1:A:145[A]:GLU:HB2	4:A:346:HOH:O	2.19	0.41
2:B:286:HIS:HD2	4:B:957:HOH:O	2.04	0.41
2:B:157:MET:N	2:B:158:PRO:CD	2.84	0.41
2:B:127:ILE:HG21	2:B:127:ILE:HD13	1.85	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)
2:B:133:ASP:OD1	2:B:219:ARG:NH2[4_566]	2.18	0.02

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	216/229 (94%)	212 (98%)	4 (2%)	0	100	100
2	B	542/543 (100%)	528 (97%)	14 (3%)	0	100	100
All	All	758/772 (98%)	740 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	163/171 (95%)	160 (98%)	3 (2%)	59	60
2	B	422/421 (100%)	414 (98%)	8 (2%)	57	59
All	All	585/592 (99%)	574 (98%)	11 (2%)	57	59

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LEU
1	A	168	VAL
1	A	214	LEU
2	B	78	LEU
2	B	200	ARG
2	B	294	VAL
2	B	310	SER
2	B	399	LEU
2	B	438	LEU
2	B	457	LEU
2	B	485	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	35	HIS
2	B	57	HIS
2	B	60	HIS
2	B	82	GLN
2	B	123	HIS
2	B	143	GLN
2	B	224	HIS
2	B	250	HIS
2	B	259	HIS
2	B	286	HIS
2	B	337	ASN
2	B	408	GLN
2	B	430	GLN
2	B	455	ASN
2	B	479	ASN
2	B	504	ASN
2	B	530	GLN

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)

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	-	8,9,9	1.68	3 (37%)	7,11,11	3.11	5 (71%)

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	-	-	5/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	GLJ	OE1-CD	2.77	1.50	1.39
3	B	601	GLJ	CG-CD	2.60	1.55	1.50
3	B	601	GLJ	O-C	2.10	1.28	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	GLJ	OXT-C-O	5.90	137.48	124.08
3	B	601	GLJ	CB-CA-N	3.28	118.68	110.12
3	B	601	GLJ	OE2-CD-CG	-2.57	102.40	109.33
3	B	601	GLJ	CB-CG-CD	-2.55	106.46	113.91
3	B	601	GLJ	CB-CA-C	-2.47	103.90	110.45

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	GLJ	N-CA-CB-CG
3	B	601	GLJ	C-CA-CB-CG
3	B	601	GLJ	O-C-CA-N
3	B	601	GLJ	OXT-C-CA-N
3	B	601	GLJ	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	GLJ	12	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, 95th 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^2)	Q<0.9
1	A	216/229 (94%)	-0.56	2 (0%)	84	87	14, 23, 38, 54	0
2	B	535/543 (98%)	-0.56	3 (0%)	89	91	12, 22, 40, 62	0
All	All	751/772 (97%)	-0.56	5 (0%)	87	90	12, 22, 40, 62	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	308	ASP	3.7
2	B	535[A]	ALA	2.8
1	A	86	GLU	2.8
2	B	41[A]	ARG	2.5
1	A	229	GLY	2.2

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, 95th 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(Å^2)	Q<0.9
3	GLJ	B	601	10/10	0.95	0.10	15,21,37,39	0

6.5 Other polymers (i)

There are no such residues in this entry.