



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:33 AM GMT

PDB ID : 2GEZ
Title : Crystal structure of potassium-independent plant asparaginase
Authors : Michalska, K.; Bujacz, G.; Jaskolski, M.
Deposited on : 2006-03-21
Resolution : 2.60 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

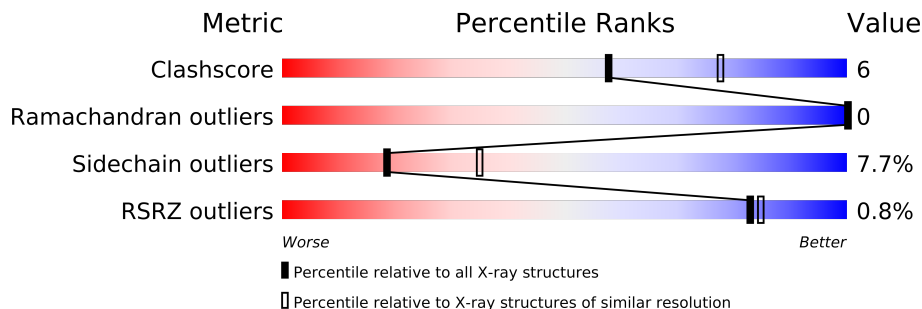
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	195	
1	C	195	
1	E	195	
1	G	195	
2	B	133	
2	D	133	
2	F	133	
2	H	133	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8815 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called L-asparaginase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1190	745	210	229	6			
1	C	166	Total	C	N	O	S	0	0	0
			1259	787	223	243	6			
1	E	165	Total	C	N	O	S	0	0	0
			1250	782	221	241	6			
1	G	158	Total	C	N	O	S	0	0	0
			1190	745	210	229	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP Q9ZSD6
A	-1	SER	-	CLONING ARTIFACT	UNP Q9ZSD6
A	0	HIS	-	CLONING ARTIFACT	UNP Q9ZSD6
C	-2	GLY	-	CLONING ARTIFACT	UNP Q9ZSD6
C	-1	SER	-	CLONING ARTIFACT	UNP Q9ZSD6
C	0	HIS	-	CLONING ARTIFACT	UNP Q9ZSD6
E	-2	GLY	-	CLONING ARTIFACT	UNP Q9ZSD6
E	-1	SER	-	CLONING ARTIFACT	UNP Q9ZSD6
E	0	HIS	-	CLONING ARTIFACT	UNP Q9ZSD6
G	-2	GLY	-	CLONING ARTIFACT	UNP Q9ZSD6
G	-1	SER	-	CLONING ARTIFACT	UNP Q9ZSD6
G	0	HIS	-	CLONING ARTIFACT	UNP Q9ZSD6

- Molecule 2 is a protein called L-asparaginase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			951	593	162	189	7			
2	D	133	Total	C	N	O	S	0	0	0
			951	593	162	189	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	133	Total	C	N	O	S	0	0	0
			951	593	162	189	7			
2	H	133	Total	C	N	O	S	0	0	0
			951	593	162	189	7			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	D	2	Total	Cl	0	0
			2	2		
4	F	2	Total	Cl	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total	O	0	0
			19	19		
5	B	15	Total	O	0	0
			15	15		
5	C	15	Total	O	0	0
			15	15		
5	D	13	Total	O	0	0
			13	13		
5	E	17	Total	O	0	0
			17	17		

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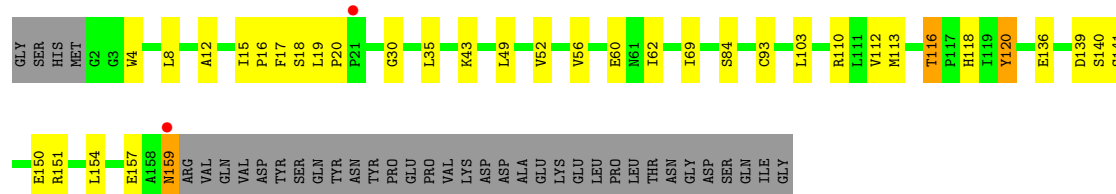
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	9	Total 9	O 9	0	0
5	G	9	Total 9	O 9	0	0
5	H	15	Total 15	O 15	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

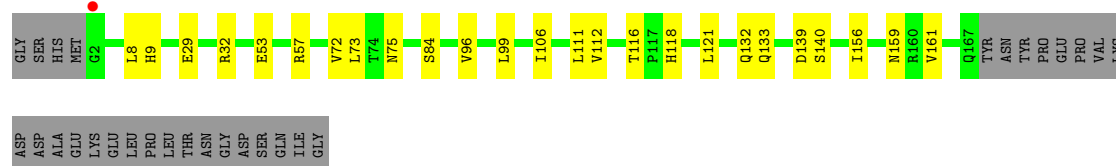
- Molecule 1: L-asparaginase alpha subunit

Chain A: 



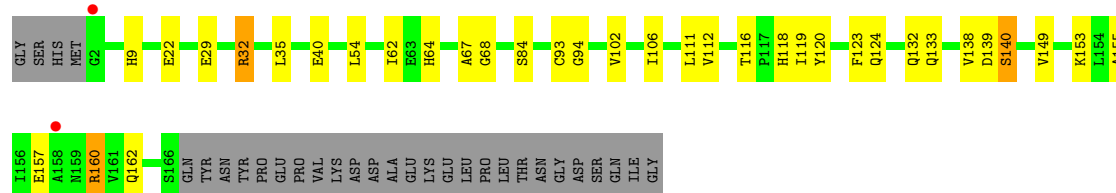
- Molecule 1: L-asparaginase alpha subunit

Chain C: 



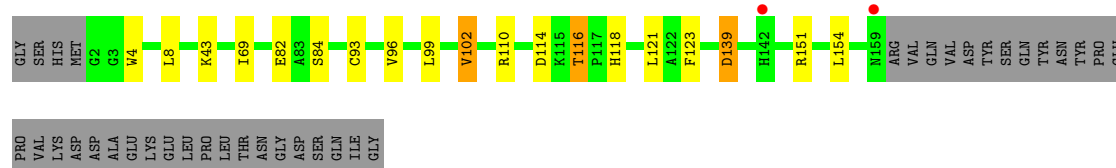
- Molecule 1: L-asparaginase alpha subunit

Chain E: 



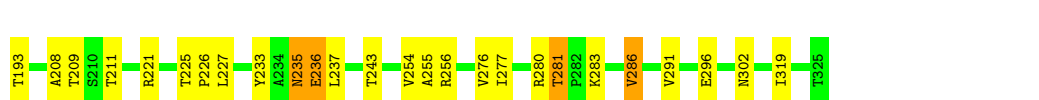
- Molecule 1: L-asparaginase alpha subunit

Chain G: 



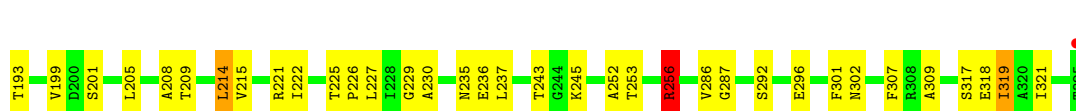
- Molecule 2: L-asparaginase beta subunit

Chain B:



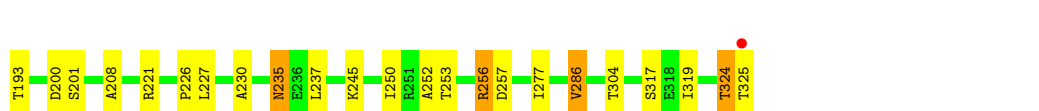
- Molecule 2: L-asparaginase beta subunit

Chain D:



- Molecule 2: L-asparaginase beta subunit

Chain F:



- Molecule 2: L-asparaginase beta subunit

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.68Å 60.20Å 114.63Å 100.60° 92.90° 113.40°	Depositor
Resolution (Å)	25.00 – 2.60 24.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (25.00-2.60) 97.4 (24.94-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.69 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.189 , 0.254 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.834	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.5	EDS
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 34621 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8815	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL

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	0.73	1/1209 (0.1%)	0.77	0/1637
1	C	0.73	0/1279	0.76	0/1732
1	E	0.79	1/1270 (0.1%)	0.84	1/1720 (0.1%)
1	G	0.72	1/1209 (0.1%)	0.77	0/1637
2	B	0.73	0/964	0.78	1/1307 (0.1%)
2	D	0.77	0/964	0.81	1/1307 (0.1%)
2	F	0.78	0/964	0.83	2/1307 (0.2%)
2	H	0.74	1/964 (0.1%)	0.81	1/1307 (0.1%)
All	All	0.75	4/8823 (0.0%)	0.79	6/11954 (0.1%)

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	G	0	1
2	F	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	CYS	CB-SG	-7.79	1.69	1.82
1	E	40	GLU	CG-CD	5.87	1.60	1.51
1	G	93	CYS	CB-SG	-5.70	1.72	1.81
2	H	238	CYS	CB-SG	-5.09	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	32	ARG	NE-CZ-NH1	7.26	123.93	120.30
2	D	256	ARG	NE-CZ-NH1	6.42	123.51	120.30
2	F	200	ASP	CB-CG-OD2	6.00	123.70	118.30
2	H	256	ARG	NE-CZ-NH2	5.98	123.29	120.30
2	F	256	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	B	280	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	324	THR	Peptide
1	G	139	ASP	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1190	0	1199	20	0
1	C	1259	0	1264	18	0
1	E	1250	0	1256	19	0
1	G	1190	0	1199	12	0
2	B	951	0	951	17	0
2	D	951	0	951	27	0
2	F	951	0	951	11	0
2	H	951	0	951	11	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	B	1	0	0	0	0
4	D	2	0	0	1	0
4	F	2	0	0	0	0
4	H	1	0	0	0	0
5	A	19	0	0	0	0
5	B	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	15	0	0	0	0
5	D	13	0	0	0	0
5	E	17	0	0	0	0
5	F	9	0	0	0	0
5	G	9	0	0	0	0
5	H	15	0	0	0	0
All	All	8815	0	8722	110	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (110) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:116:THR:HG22	1:E:118:HIS:H	1.34	0.92
1:C:116:THR:HG22	1:C:118:HIS:H	1.41	0.84
1:A:116:THR:HG22	1:A:118:HIS:H	1.49	0.77
2:D:319:ILE:HD13	2:D:319:ILE:H	1.51	0.75
1:E:112:VAL:O	1:E:116:THR:HB	1.88	0.73
1:G:116:THR:HG22	1:G:118:HIS:H	1.55	0.72
1:A:159:ASN:HD22	1:A:159:ASN:C	1.94	0.71
1:E:111:LEU:HD22	1:E:133:GLN:OE1	1.90	0.70
1:C:9:HIS:HE1	2:D:193:THR:HG22	1.59	0.66
2:B:227:LEU:HD22	2:D:227:LEU:HD22	1.82	0.62
2:H:254:VAL:HB	2:H:276:VAL:HG11	1.82	0.61
1:A:56:VAL:O	1:A:60:GLU:HG3	2.00	0.61
1:G:4:TRP:CH2	1:G:43:LYS:HG2	2.36	0.60
2:H:275:PHE:O	2:H:279:GLU:HB2	2.01	0.60
2:D:286:VAL:HG12	2:D:302:ASN:HD21	1.67	0.59
1:G:84:SER:HB3	2:H:226:PRO:HA	1.83	0.59
2:F:324:THR:OG1	2:F:325:THR:N	2.35	0.59
2:F:227:LEU:HD12	2:F:250:ILE:HG12	1.86	0.58
1:E:160:ARG:HB3	1:E:162:GLN:HG3	1.86	0.57
2:B:281:THR:HG23	2:B:302:ASN:HD21	1.69	0.57
1:A:84:SER:HB3	2:B:226:PRO:HA	1.87	0.56
2:F:221:ARG:HG3	1:G:118:HIS:CG	2.41	0.55
1:G:4:TRP:HH2	1:G:43:LYS:HG2	1.70	0.55
2:F:227:LEU:HB2	2:F:230:ALA:HB3	1.88	0.55
1:C:8:LEU:HD11	2:D:309:ALA:HB3	1.89	0.55
2:D:229:GLY:HA2	2:D:256:ARG:HB2	1.89	0.55
1:C:112:VAL:O	1:C:116:THR:HB	2.07	0.55
2:F:277:ILE:HD12	2:F:286:VAL:HG13	1.88	0.54
1:E:116:THR:HG22	1:E:118:HIS:N	2.14	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:8:LEU:C	1:A:8:LEU:HD12	2.28	0.54
2:B:254:VAL:HB	2:B:276:VAL:HG11	1.89	0.54
1:E:9:HIS:HE1	2:F:193:THR:HG22	1.73	0.53
2:B:209:THR:HG22	2:B:225:THR:HG23	1.92	0.52
2:D:214:LEU:HD13	4:D:407:CL:CL	2.47	0.52
1:C:111:LEU:HD22	1:C:133:GLN:OE1	2.10	0.51
1:A:118:HIS:CG	2:D:221:ARG:HG3	2.44	0.51
2:H:199:VAL:HB	2:H:205:LEU:HD23	1.92	0.50
1:G:116:THR:CG2	1:G:118:HIS:H	2.22	0.50
1:A:4:TRP:CH2	1:A:43:LYS:HG2	2.48	0.49
2:H:235:ASN:HB3	2:H:237:LEU:H	1.78	0.49
2:B:236:GLU:HA	2:B:236:GLU:OE2	2.12	0.48
1:A:120:TYR:CD1	2:D:222:ILE:HB	2.49	0.48
1:C:84:SER:HB3	2:D:226:PRO:HA	1.94	0.48
2:B:291:VAL:HA	2:B:296:GLU:O	2.13	0.48
1:C:96:VAL:HA	1:C:121:LEU:O	2.15	0.47
1:A:19:LEU:HD12	1:A:20:PRO:HD2	1.95	0.47
1:C:72:VAL:HB	2:D:215:VAL:HG22	1.96	0.47
1:G:4:TRP:CH2	1:G:43:LYS:CG	2.97	0.46
1:A:4:TRP:CH2	1:A:43:LYS:CG	2.98	0.46
1:E:84:SER:HB3	2:F:226:PRO:HA	1.98	0.46
1:G:8:LEU:C	1:G:8:LEU:HD12	2.36	0.46
2:B:235:ASN:HB3	2:B:237:LEU:N	2.31	0.46
1:C:75:ASN:O	1:E:153:LYS:HE2	2.16	0.46
2:D:209:THR:HG22	2:D:225:THR:HG23	1.97	0.46
2:F:277:ILE:CD1	2:F:286:VAL:HG13	2.46	0.45
1:G:99:LEU:HB3	1:G:102:VAL:HG13	1.98	0.45
2:B:256:ARG:HD3	2:D:253:THR:OG1	2.15	0.45
2:H:291:VAL:HA	2:H:296:GLU:O	2.15	0.45
1:A:159:ASN:ND2	1:A:159:ASN:C	2.63	0.45
1:C:116:THR:CG2	1:C:118:HIS:HB2	2.48	0.44
1:A:116:THR:CG2	1:A:118:HIS:H	2.27	0.44
1:C:161:VAL:HG12	2:D:214:LEU:HD23	1.99	0.44
2:F:235:ASN:HB3	2:F:237:LEU:H	1.82	0.44
1:C:106:ILE:HD11	2:D:208:ALA:HB1	1.99	0.44
1:E:106:ILE:HD11	2:F:208:ALA:HB1	1.99	0.44
2:B:193:THR:HG23	2:B:211:THR:HB	1.99	0.44
2:H:223:GLY:O	2:H:227:LEU:HD22	2.17	0.44
1:A:12:ALA:HB3	2:B:243:THR:HG23	1.99	0.44
1:A:112:VAL:O	1:A:116:THR:HB	2.18	0.44
2:D:319:ILE:H	2:D:319:ILE:CD1	2.26	0.44
1:G:96:VAL:HA	1:G:121:LEU:O	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:112:VAL:HG13	1:A:116:THR:HG21	1.99	0.44
2:B:235:ASN:HB3	2:B:237:LEU:H	1.83	0.44
1:E:62:ILE:HG22	1:E:64:HIS:H	1.83	0.44
1:E:67:ALA:O	1:E:68:GLY:C	2.57	0.44
1:C:53:GLU:O	1:C:57:ARG:HG3	2.18	0.43
2:D:309:ALA:HA	2:D:318:GLU:O	2.18	0.43
2:D:286:VAL:HG12	2:D:302:ASN:ND2	2.31	0.43
2:D:287:GLY:HA2	2:D:301:PHE:HA	2.01	0.43
1:G:123:PHE:CZ	2:H:220:GLY:HA2	2.53	0.43
1:E:118:HIS:CG	2:H:221:ARG:HG3	2.53	0.42
1:C:73:LEU:HD13	1:E:149:VAL:HG11	2.01	0.42
1:C:139:ASP:OD2	1:C:140:SER:N	2.52	0.42
1:A:52:VAL:HG23	2:B:208:ALA:HB2	2.00	0.42
2:B:277:ILE:CD1	2:B:286:VAL:HG22	2.50	0.42
2:H:288:LEU:C	2:H:288:LEU:HD12	2.40	0.42
1:A:110:ARG:O	1:A:113:MET:HB3	2.19	0.42
1:C:116:THR:HG22	1:C:118:HIS:N	2.21	0.42
1:G:110:ARG:NE	1:G:114:ASP:OD1	2.51	0.42
1:E:160:ARG:HD2	1:E:162:GLN:HE21	1.85	0.42
2:D:229:GLY:CA	2:D:256:ARG:HB2	2.49	0.42
2:H:281:THR:HG23	2:H:302:ASN:HD21	1.84	0.42
2:B:221:ARG:HG3	1:C:118:HIS:CG	2.56	0.41
2:F:252:ALA:O	2:F:253:THR:C	2.57	0.41
2:D:236:GLU:HB2	2:D:237:LEU:HD12	2.02	0.41
2:D:227:LEU:HB2	2:D:230:ALA:HB3	2.01	0.41
2:D:292:SER:OG	2:D:296:GLU:HB2	2.20	0.41
1:E:94:GLY:HA2	1:E:119:ILE:O	2.19	0.41
1:E:139:ASP:OD2	1:E:140:SER:N	2.53	0.41
1:C:161:VAL:CG1	2:D:214:LEU:HD23	2.51	0.41
1:E:155:ALA:HB2	1:E:162:GLN:OE1	2.21	0.41
1:A:15:ILE:HA	1:A:16:PRO:HD3	1.92	0.41
1:A:30:GLY:CA	1:A:62:ILE:HD13	2.51	0.41
1:A:12:ALA:CB	2:B:243:THR:HG23	2.50	0.41
2:D:252:ALA:O	2:D:253:THR:C	2.59	0.40
2:D:307:PHE:CD2	2:D:321:ILE:HG12	2.55	0.40
1:E:123:PHE:O	1:E:124:GLN:C	2.58	0.40
1:E:153:LYS:NZ	1:E:157:GLU:OE2	2.53	0.40
2:D:199:VAL:HB	2:D:205:LEU:HD23	2.04	0.40
2:B:233:TYR:CB	2:B:255:ALA:HB1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	156/195 (80%)	149 (96%)	7 (4%)	0	100	100
1	C	164/195 (84%)	155 (94%)	9 (6%)	0	100	100
1	E	163/195 (84%)	156 (96%)	7 (4%)	0	100	100
1	G	156/195 (80%)	151 (97%)	5 (3%)	0	100	100
2	B	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
2	D	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
2	F	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
2	H	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
All	All	1163/1312 (89%)	1113 (96%)	50 (4%)	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	129/162 (80%)	112 (87%)	17 (13%)	6	10
1	C	137/162 (85%)	131 (96%)	6 (4%)	39	68
1	E	136/162 (84%)	124 (91%)	12 (9%)	14	27
1	G	129/162 (80%)	122 (95%)	7 (5%)	31	57
2	B	97/97 (100%)	91 (94%)	6 (6%)	26	49
2	D	97/97 (100%)	89 (92%)	8 (8%)	17	31
2	F	97/97 (100%)	88 (91%)	9 (9%)	13	24
2	H	97/97 (100%)	91 (94%)	6 (6%)	26	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	919/1036 (89%)	848 (92%)	71 (8%)	18	35

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	PHE
1	A	18	SER
1	A	35	LEU
1	A	49	LEU
1	A	69	ILE
1	A	103	LEU
1	A	116	THR
1	A	120	TYR
1	A	136	GLU
1	A	139	ASP
1	A	140	SER
1	A	141	SER
1	A	150	GLU
1	A	151	ARG
1	A	154	LEU
1	A	157	GLU
1	A	159	ASN
2	B	235	ASN
2	B	236	GLU
2	B	281	THR
2	B	283	LYS
2	B	286	VAL
2	B	319	ILE
1	C	29	GLU
1	C	32	ARG
1	C	99	LEU
1	C	132	GLN
1	C	156	ILE
1	C	159	ASN
2	D	201	SER
2	D	214	LEU
2	D	235	ASN
2	D	243	THR
2	D	245	LYS
2	D	256	ARG
2	D	317	SER
2	D	319	ILE

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Mol	Chain	Res	Type
1	E	22	GLU
1	E	29	GLU
1	E	32	ARG
1	E	35	LEU
1	E	54	LEU
1	E	93	CYS
1	E	102	VAL
1	E	120	TYR
1	E	132	GLN
1	E	138	VAL
1	E	140	SER
1	E	160	ARG
2	F	201	SER
2	F	235	ASN
2	F	245	LYS
2	F	256	ARG
2	F	257	ASP
2	F	286	VAL
2	F	304	THR
2	F	317	SER
2	F	319	ILE
1	G	69	ILE
1	G	82	GLU
1	G	102	VAL
1	G	116	THR
1	G	139	ASP
1	G	151	ARG
1	G	154	LEU
2	H	214	LEU
2	H	227	LEU
2	H	228	ILE
2	H	235	ASN
2	H	269	LEU
2	H	288	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	132	GLN
1	A	159	ASN
2	B	235	ASN

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Mol	Chain	Res	Type
1	C	167	GLN
2	D	235	ASN
2	F	235	ASN
1	G	89	ASN
1	G	132	GLN
2	H	235	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	158/195 (81%)	-0.15	2 (1%) 74 75	21, 26, 32, 36	0
1	C	166/195 (85%)	-0.44	1 (0%) 86 89	18, 25, 33, 37	0
1	E	165/195 (84%)	-0.48	2 (1%) 75 77	18, 25, 33, 36	0
1	G	158/195 (81%)	-0.22	2 (1%) 74 75	21, 26, 32, 34	0
2	B	133/133 (100%)	-0.38	0 100 100	22, 25, 30, 36	1 (0%)
2	D	133/133 (100%)	-0.36	1 (0%) 83 85	20, 26, 32, 38	0
2	F	133/133 (100%)	-0.32	1 (0%) 83 85	21, 26, 32, 39	1 (0%)
2	H	133/133 (100%)	-0.29	1 (0%) 83 85	21, 26, 31, 36	0
All	All	1179/1312 (89%)	-0.33	10 (0%) 83 85	18, 26, 32, 39	2 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	325	THR	6.9
2	D	325	THR	5.8
2	H	325	THR	4.1
1	A	21	PRO	3.9
1	C	2	GLY	3.2
1	G	159	ASN	2.6
1	A	159	ASN	2.5
1	E	2	GLY	2.5
1	G	142	HIS	2.1
1	E	158	ALA	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CL	D	405	1/1	0.13	0.63	28,28,28,28	0
4	CL	D	407	1/1	0.13	-0.02	26,26,26,26	0
4	CL	F	404	1/1	0.10	-0.76	27,27,27,27	0
4	CL	H	409	1/1	0.10	-0.91	30,30,30,30	0
4	CL	B	406	1/1	0.10	-1.36	39,39,39,39	0
4	CL	F	408	1/1	0.05	-1.79	29,29,29,29	0
3	NA	A	401	1/1	0.09	-1.88	28,28,28,28	0
3	NA	G	403	1/1	0.10	-2.27	36,36,36,36	0
3	NA	C	400	1/1	0.06	-2.33	16,16,16,16	0
3	NA	E	402	1/1	0.06	-2.58	16,16,16,16	0

6.5 Other polymers

There are no such residues in this entry.