



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:18 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 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

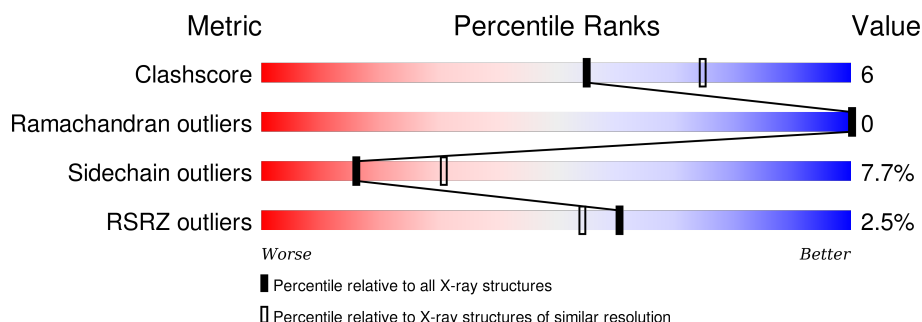
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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. 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	195	
1	C	195	
1	E	195	
1	G	195	
2	B	133	
2	D	133	
2	F	133	

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Mol	Chain	Length	Quality of chain
2	H	133	<div><div></div><div>2%</div><div>83%</div><div>15%</div><div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8815 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 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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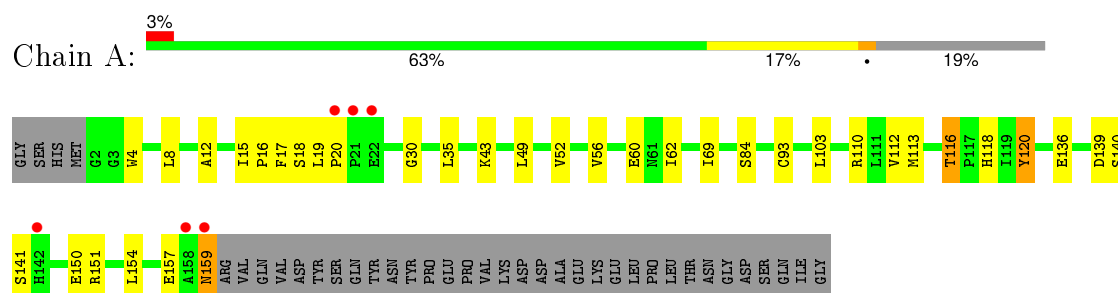
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	9	Total 9	O 9	0	0
5	G	9	Total 9	O 9	0	0
5	H	15	Total 15	O 15	0	0

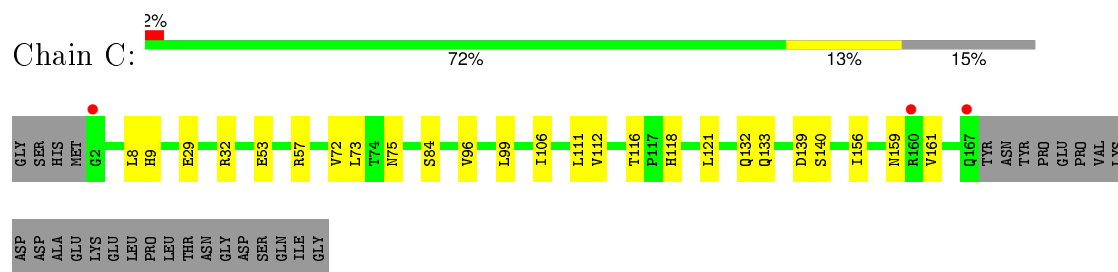
3 Residue-property plots [i](#)

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.

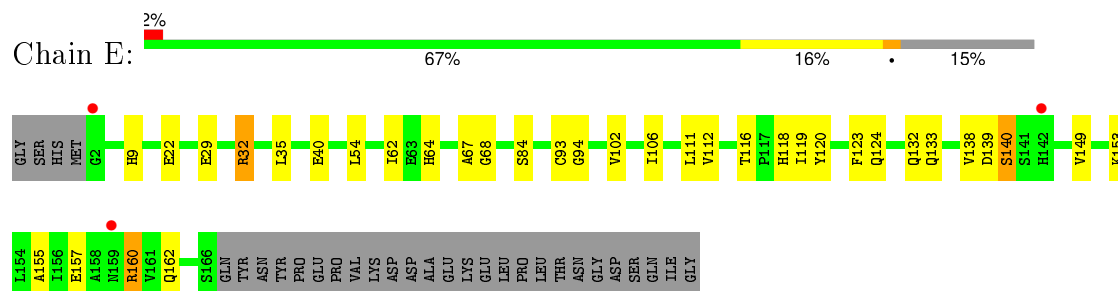
- Molecule 1: L-asparaginase alpha subunit



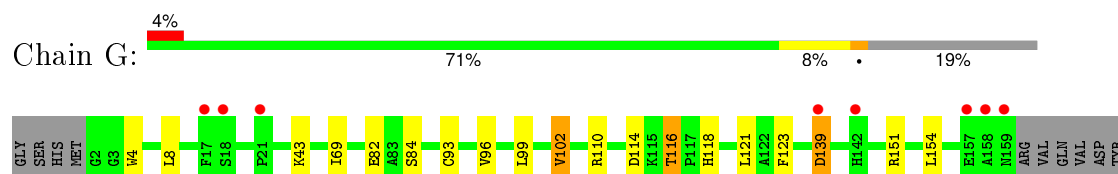
- Molecule 1: L-asparaginase alpha subunit



- Molecule 1: L-asparaginase alpha subunit

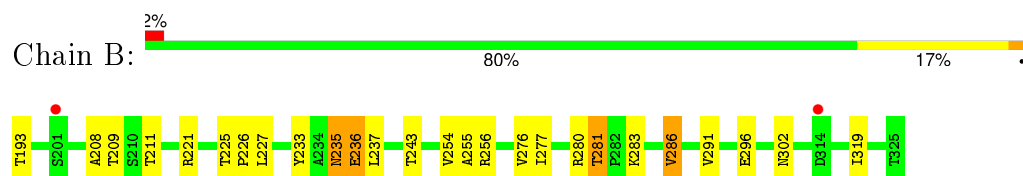


- Molecule 1: L-asparaginase alpha subunit

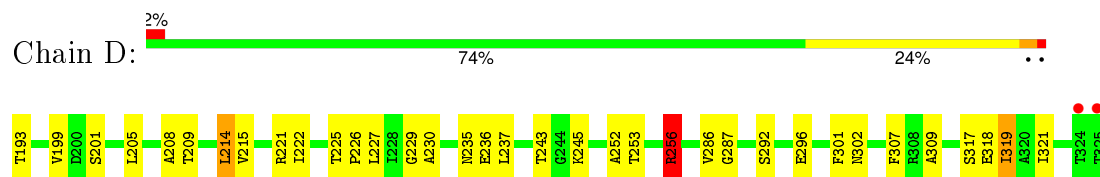


SER	GLN	TYR	ASN	TYR	PRO	GLU	PRO	VAL	LYS	ASP	ASP	ALA	GLU	LYS	LEU	PRO	LEU	THR	ASN	GLY	ASP	SER	GLN	ILE	GLY
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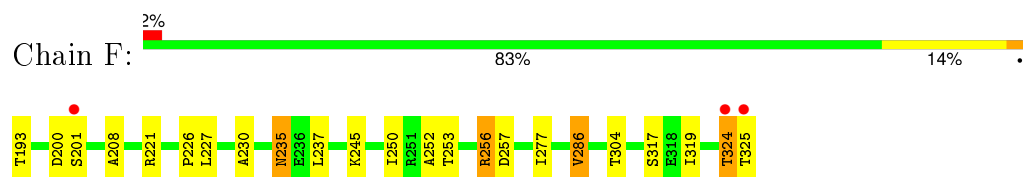
- Molecule 2: L-asparaginase beta subunit



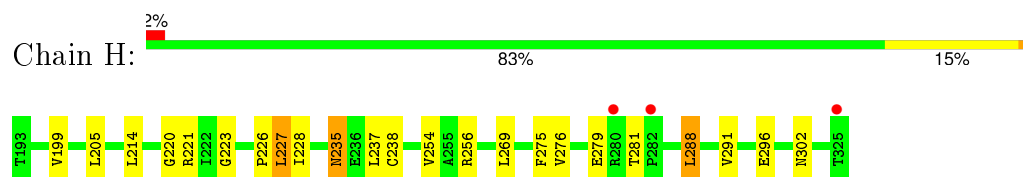
- Molecule 2: L-asparaginase beta subunit



- Molecule 2: L-asparaginase beta subunit



- Molecule 2: L-asparaginase beta subunit



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) 90.1 (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 0.202 , (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)	0.32 , 44.6	EDS
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.

²Theoretical 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: 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 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	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
5	C	15	0	0	0	0
5	D	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 6.

All (110) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:96:VAL:HA	1:G:121:LEU:O	2.18	0.44
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%)	5	9
1	C	137/162 (85%)	131 (96%)	6 (4%)	35	63
1	E	136/162 (84%)	124 (91%)	12 (9%)	12	24
1	G	129/162 (80%)	122 (95%)	7 (5%)	27	52
2	B	97/97 (100%)	91 (94%)	6 (6%)	23	45
2	D	97/97 (100%)	89 (92%)	8 (8%)	14	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	97/97 (100%)	88 (91%)	9 (9%)	11	21
2	H	97/97 (100%)	91 (94%)	6 (6%)	23	45
All	All	919/1036 (89%)	848 (92%)	71 (8%)	16	31

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

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Mol	Chain	Res	Type
2	D	256	ARG
2	D	317	SER
2	D	319	ILE
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

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Mol	Chain	Res	Type
1	A	132	GLN
1	A	159	ASN
2	B	235	ASN
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 [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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.14	6 (3%)	44 36	21, 26, 32, 36	0
1	C	166/195 (85%)	-0.19	3 (1%)	71 66	18, 25, 33, 37	0
1	E	165/195 (84%)	-0.20	3 (1%)	71 66	18, 25, 33, 36	0
1	G	158/195 (81%)	0.05	8 (5%)	32 25	21, 26, 32, 34	0
2	B	133/133 (100%)	-0.12	2 (1%)	76 71	22, 25, 30, 36	1 (0%)
2	D	133/133 (100%)	-0.10	2 (1%)	76 71	20, 26, 32, 38	0
2	F	133/133 (100%)	-0.06	3 (2%)	64 57	21, 26, 32, 39	1 (0%)
2	H	133/133 (100%)	-0.00	3 (2%)	64 57	21, 26, 31, 36	0
All	All	1179/1312 (89%)	-0.06	30 (2%)	61 54	18, 26, 32, 39	2 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	325	THR	8.3
1	A	21	PRO	5.8
2	H	325	THR	5.1
2	D	325	THR	5.0
1	C	2	GLY	4.1
1	G	159	ASN	3.6
1	A	159	ASN	3.2
1	A	142	HIS	3.0
1	G	142	HIS	3.0
1	G	139	ASP	2.7
1	E	2	GLY	2.5
2	F	324	THR	2.5
1	G	21	PRO	2.4
2	D	324	THR	2.4
2	H	282	PRO	2.3
1	G	158	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	280	ARG	2.3
1	G	17	PHE	2.3
1	G	18	SER	2.3
1	C	160	ARG	2.3
1	E	159	ASN	2.2
1	G	157	GLU	2.2
2	B	314	ASP	2.2
1	A	22	GLU	2.1
1	C	167	GLN	2.1
1	A	20	PRO	2.1
1	A	158	ALA	2.1
2	F	201	SER	2.1
1	E	142	HIS	2.0
2	B	201	SER	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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	CL	D	407	1/1	0.97	0.14	-0.01	26,26,26,26	0
4	CL	H	409	1/1	0.98	0.15	-0.29	30,30,30,30	0
4	CL	B	406	1/1	0.97	0.13	-1.26	39,39,39,39	0
3	NA	A	401	1/1	0.94	0.11	-1.41	28,28,28,28	0
3	NA	C	400	1/1	0.98	0.05	-2.47	16,16,16,16	0
4	CL	F	408	1/1	0.97	0.06	-2.49	29,29,29,29	0
3	NA	G	403	1/1	0.93	0.10	-3.12	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NA	E	402	1/1	0.98	0.03	-3.92	16,16,16,16	0
4	CL	D	405	1/1	0.94	0.15	-	28,28,28,28	0
4	CL	F	404	1/1	0.95	0.15	-	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.