



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:20 AM UTC

PDB ID : 5W2J / pdb_00005w2j
Title : Crystal structure of dimeric form of mouse Glutaminase C
Authors : Cerione, R.A.; Li, Y.
Deposited on : 2017-06-06
Resolution : 2.50 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

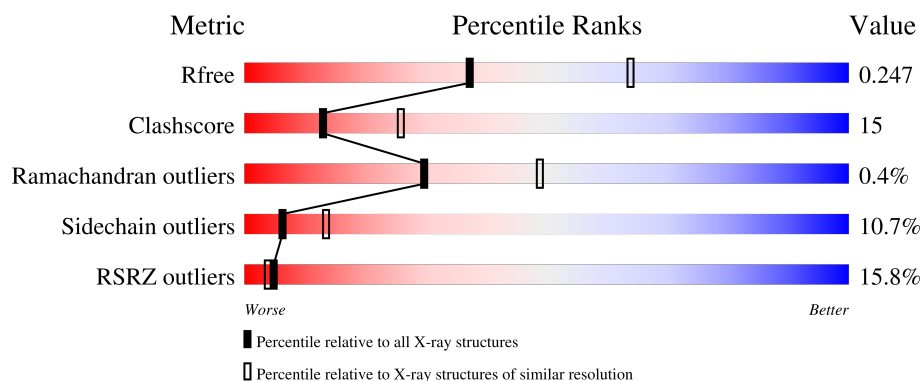
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	411	9% 74% 21% • •
1	B	411	20% 71% 24% 6%
2	F	14	100% 50% 36% 14%

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	CL	B	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6666 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 Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3190	2036	539	587	28			
1	B	411	Total	C	N	O	S	0	1	0
			3215	2053	543	591	28			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	391	LYS	ASP	engineered mutation	UNP D3Z7P3
B	391	LYS	ASP	engineered mutation	UNP D3Z7P3

- Molecule 2 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	14	Total	C	N	O	0	0	0
			90	56	16	18			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

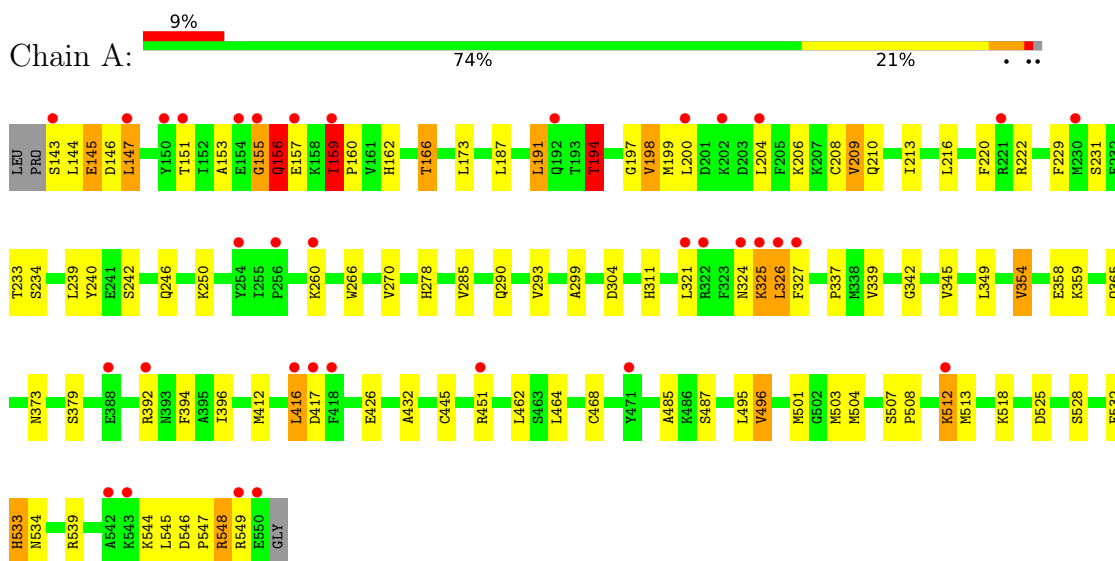
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	82	Total	O	0	0
			82	82		
4	B	87	Total	O	0	0
			87	87		

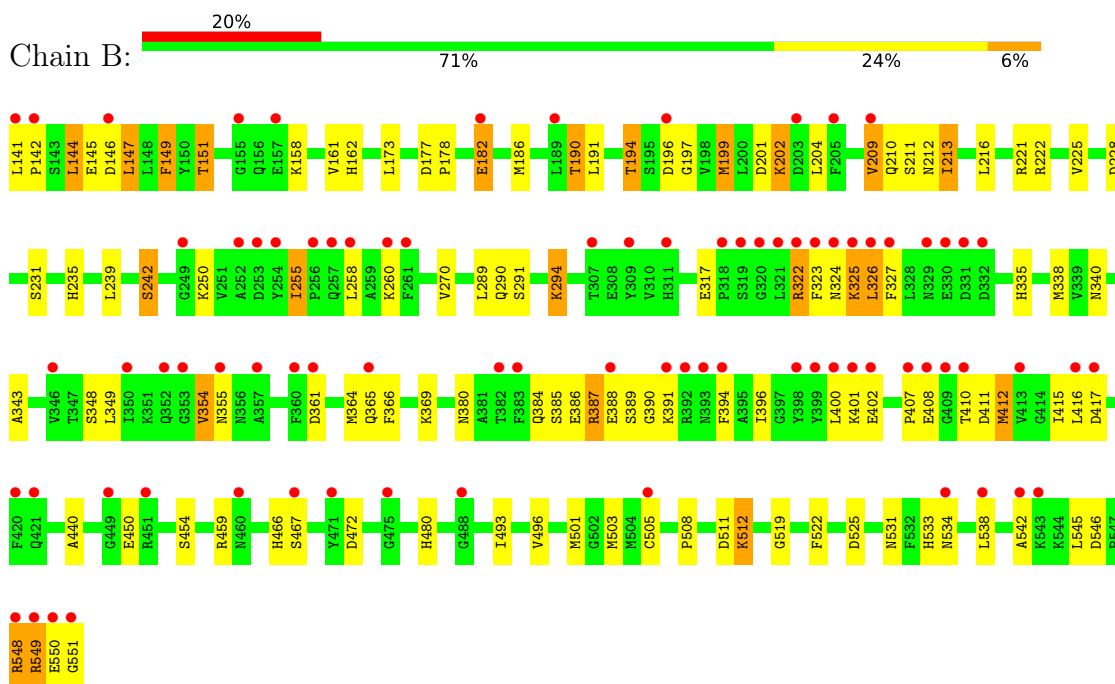
3 Residue-property plots

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.

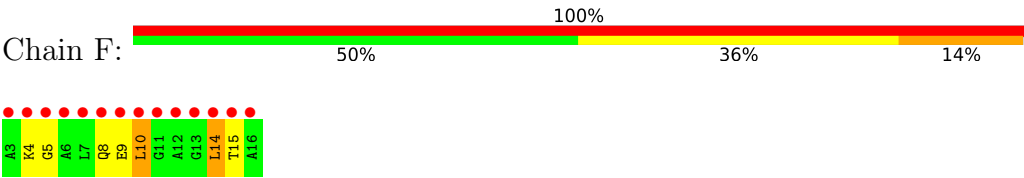
- Molecule 1: Glutaminase kidney isoform, mitochondrial



- Molecule 1: Glutaminase kidney isoform, mitochondrial



● Molecule 2: unidentified peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.94Å 100.88Å 145.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.0 (50.00-2.50) 99.2 (50.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.92 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.196 , 0.228 0.224 , 0.247	Depositor DCC
R_{free} test set	1070 reflections (1.91%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6666	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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, 0.333 respectively for untwinned datasets, and 0.375, 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:
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	1.35	11/3261 (0.3%)	1.19	9/4400 (0.2%)
1	B	1.29	18/3290 (0.5%)	1.15	8/4440 (0.2%)
2	F	0.72	0/89	0.87	0/118
All	All	1.31	29/6640 (0.4%)	1.16	17/8958 (0.2%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	480	HIS	ND1-CE1	7.05	1.39	1.32
1	A	311	HIS	ND1-CE1	6.78	1.39	1.32
1	A	299	ALA	C-O	-6.64	1.16	1.24
1	B	538	LEU	C-O	-6.57	1.15	1.24
1	B	505	CYS	N-CA	6.55	1.53	1.46
1	B	508	PRO	CA-C	6.52	1.58	1.52
1	A	304	ASP	C-O	-6.41	1.15	1.24
1	A	533	HIS	CG-CD2	6.09	1.42	1.35
1	B	177	ASP	CA-C	5.75	1.59	1.53
1	B	177	ASP	C-O	-5.70	1.17	1.24
1	B	235	HIS	CG-CD2	5.70	1.42	1.35
1	B	531	ASN	N-CA	-5.55	1.39	1.46
1	B	545	LEU	CA-C	5.38	1.59	1.52
1	B	466	HIS	CG-ND1	-5.35	1.32	1.38
1	A	496	VAL	C-O	-5.30	1.18	1.24
1	B	178	PRO	C-O	-5.26	1.17	1.24
1	B	149	PHE	N-CA	-5.25	1.40	1.46
1	B	199	MET	C-O	-5.25	1.17	1.24
1	A	242	SER	CA-C	5.25	1.59	1.52
1	A	468	CYS	N-CA	5.22	1.51	1.46
1	B	533	HIS	CE1-NE2	5.21	1.37	1.32
1	A	278	HIS	CG-ND1	-5.14	1.32	1.38
1	B	531	ASN	C-O	-5.14	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	225	VAL	CA-C	5.13	1.59	1.52
1	B	533	HIS	CG-CD2	5.12	1.41	1.35
1	A	345	VAL	CA-C	5.10	1.59	1.52
1	B	225	VAL	C-O	-5.08	1.18	1.24
1	A	194	THR	CA-C	5.03	1.59	1.52
1	A	544	LYS	N-CA	-5.01	1.39	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	508	PRO	N-CA-C	7.42	119.75	110.70
1	A	285	VAL	N-CA-C	7.39	116.77	108.05
1	A	198	VAL	N-CA-C	7.23	117.33	111.62
1	A	159	ILE	CB-CA-C	-7.03	103.08	110.53
1	B	508	PRO	N-CA-C	6.93	119.16	110.70
1	B	542	ALA	CB-CA-C	-6.52	109.06	116.63
1	B	213	ILE	N-CA-C	5.98	116.76	110.72
1	B	386	GLU	N-CA-C	-5.72	105.12	111.36
1	A	487	SER	CA-C-N	5.31	126.14	121.58
1	A	487	SER	C-N-CA	5.31	126.14	121.58
1	B	454	SER	CA-C-N	5.31	124.76	119.24
1	B	454	SER	C-N-CA	5.31	124.76	119.24
1	A	220	PHE	N-CA-C	5.26	117.76	111.71
1	A	445	CYS	CA-C-N	5.22	124.85	119.05
1	A	445	CYS	C-N-CA	5.22	124.85	119.05
1	B	146	ASP	N-CA-C	-5.21	105.68	111.36
1	B	242	SER	N-CA-C	-5.14	105.59	111.14

There are no chirality outliers.

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	3190	0	3178	95	0
1	B	3215	0	3207	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	90	0	95	12	0
3	A	1	0	0	0	0
3	B	1	0	0	2	0
4	A	82	0	0	2	0
4	B	87	0	0	3	0
All	All	6666	0	6480	194	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 15.

All (194) 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:325:LYS:HB3	1:A:326:LEU:CA	1.40	1.46
1:A:325:LYS:CB	1:A:326:LEU:HA	1.38	1.41
1:A:325:LYS:HA	1:A:325:LYS:CE	1.44	1.26
1:A:324:ASN:O	1:A:325:LYS:HD2	1.43	1.15
1:A:325:LYS:HA	1:A:325:LYS:NZ	1.64	1.11
1:A:325:LYS:HA	1:A:325:LYS:HE3	1.28	1.09
1:B:194:THR:CG2	1:B:197:GLY:H	1.66	1.07
1:A:194:THR:HG22	1:A:197:GLY:H	1.19	1.07
1:A:325:LYS:CE	1:A:325:LYS:CA	2.30	1.07
1:A:354:VAL:HG13	1:A:358:GLU:CG	1.85	1.06
1:A:501:MET:HE3	1:A:503:MET:CE	1.85	1.06
1:A:354:VAL:CG1	1:A:358:GLU:HG3	1.88	1.03
1:A:325:LYS:HE3	1:A:325:LYS:CA	1.85	1.02
1:B:194:THR:HG22	1:B:197:GLY:H	1.21	1.01
1:B:412:MET:CE	1:B:416:LEU:HG	1.94	0.98
1:A:501:MET:HE3	1:A:503:MET:HE3	1.45	0.98
1:A:194:THR:CG2	1:A:197:GLY:H	1.76	0.97
1:A:326:LEU:CD2	1:A:396:ILE:HG12	2.01	0.91
1:B:412:MET:HE3	1:B:416:LEU:HG	1.52	0.88
1:A:354:VAL:HG11	1:A:358:GLU:HG3	1.54	0.88
1:A:155:GLY:HA2	1:A:156:GLN:O	1.73	0.88
1:A:512:LYS:HD2	1:A:512:LYS:H	1.37	0.88
1:A:354:VAL:HG13	1:A:358:GLU:HG2	1.58	0.85
1:A:198:VAL:HG12	1:A:199:MET:HE2	1.60	0.84
1:B:384:GLN:O	1:B:388:GLU:HG3	1.74	0.84
1:B:194:THR:HG22	1:B:197:GLY:N	1.92	0.83
1:A:325:LYS:HE2	1:A:327:PHE:CD1	2.13	0.83
1:A:191:LEU:HD13	1:A:200:LEU:HD21	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:THR:CG2	1:B:197:GLY:N	2.43	0.82
1:A:354:VAL:HG13	1:A:358:GLU:HG3	1.54	0.82
1:A:326:LEU:HD23	1:A:396:ILE:HG12	1.59	0.82
1:A:501:MET:CE	1:A:503:MET:CE	2.58	0.82
1:A:194:THR:HG22	1:A:197:GLY:N	1.95	0.81
1:A:546:ASP:OD1	1:A:548:ARG:HD2	1.80	0.81
1:A:512:LYS:H	1:A:512:LYS:CD	1.94	0.79
1:A:324:ASN:O	1:A:325:LYS:CD	2.30	0.79
1:B:239:LEU:HD22	1:B:525:ASP:HB3	1.63	0.78
1:B:385:SER:HA	1:B:388:GLU:HG3	1.66	0.77
1:B:503:MET:HE1	1:B:522:PHE:CE1	2.20	0.76
2:F:10:LEU:HD12	2:F:10:LEU:O	1.84	0.76
1:B:384:GLN:O	1:B:388:GLU:CG	2.36	0.73
1:B:503:MET:HE1	1:B:522:PHE:HE1	1.55	0.71
1:B:182:GLU:HG3	1:B:211:SER:OG	1.90	0.70
1:A:209:VAL:HG13	1:A:213:ILE:HD13	1.72	0.70
1:A:325:LYS:HD3	1:A:327:PHE:HE1	1.57	0.69
2:F:14:LEU:HD23	2:F:14:LEU:C	2.18	0.69
1:B:294:LYS:HE2	1:B:338:MET:O	1.93	0.68
1:B:348:SER:HA	1:B:415:ILE:HD12	1.75	0.68
1:B:270:VAL:HG22	1:B:503:MET:HG2	1.76	0.67
1:A:539:ARG:HG3	4:B:782:HOH:O	1.94	0.67
1:B:390:GLY:O	1:B:394:PHE:HD2	1.77	0.67
2:F:14:LEU:HD23	2:F:15:THR:N	2.10	0.66
1:A:209:VAL:HG22	1:A:216:LEU:CD1	2.26	0.66
1:B:325:LYS:O	1:B:327:PHE:CD1	2.49	0.65
1:A:155:GLY:HA2	1:A:156:GLN:CB	2.26	0.65
1:B:291:SER:HB2	3:B:601:CL:CL	2.33	0.65
1:A:501:MET:CE	1:A:503:MET:HE2	2.25	0.65
1:B:546:ASP:OD1	1:B:548:ARG:HD2	1.98	0.64
1:A:325:LYS:HA	1:A:325:LYS:HZ1	1.63	0.63
1:A:324:ASN:C	1:A:325:LYS:HD2	2.21	0.63
1:A:325:LYS:HD3	1:A:327:PHE:CE1	2.33	0.63
1:B:325:LYS:HB3	1:B:327:PHE:CE1	2.34	0.63
1:B:327:PHE:CE2	1:B:335:HIS:CE1	2.86	0.63
1:A:324:ASN:O	1:A:325:LYS:NZ	2.30	0.62
1:B:142:PRO:O	2:F:8:GLN:NE2	2.28	0.62
1:A:191:LEU:CD1	1:A:200:LEU:HD21	2.30	0.62
1:B:354:VAL:HG13	1:B:355:ASN:N	2.12	0.62
2:F:10:LEU:HD12	2:F:10:LEU:C	2.24	0.62
1:A:354:VAL:CG1	1:A:358:GLU:CG	2.54	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:PHE:CD1	1:B:412:MET:HE1	2.35	0.61
1:A:155:GLY:HA2	1:A:156:GLN:C	2.22	0.61
1:B:141:LEU:N	1:B:142:PRO:CD	2.63	0.61
1:B:412:MET:HE3	1:B:416:LEU:CG	2.29	0.61
1:B:394:PHE:HD1	1:B:412:MET:HE1	1.65	0.61
1:B:186:MET:O	1:B:190:THR:HB	2.00	0.61
1:B:325:LYS:O	1:B:327:PHE:HD1	1.83	0.60
1:A:546:ASP:OD1	1:A:548:ARG:CD	2.50	0.60
1:A:145:GLU:HG3	1:A:206:LYS:HG3	1.83	0.60
1:A:533:HIS:CD2	1:B:459:ARG:HD2	2.37	0.60
1:A:325:LYS:HB3	1:A:326:LEU:CB	2.27	0.60
1:B:369:LYS:HD3	1:B:450:GLU:OE2	2.01	0.60
1:A:270:VAL:HG22	1:A:503:MET:HG2	1.84	0.59
1:B:209:VAL:HG13	1:B:213:ILE:HD13	1.85	0.59
1:A:143:SER:HA	1:A:146:ASP:HB2	1.86	0.58
1:B:396:ILE:HG22	1:B:400:LEU:CD1	2.34	0.58
1:A:359:LYS:HE2	4:A:720:HOH:O	2.05	0.57
1:A:512:LYS:HD2	1:A:512:LYS:N	2.11	0.57
1:B:291:SER:CB	3:B:601:CL:CL	2.90	0.57
1:A:240:TYR:CE1	1:A:266:TRP:CD1	2.93	0.57
1:B:407:PRO:O	1:B:410:THR:OG1	2.22	0.56
1:B:209:VAL:HG22	1:B:216:LEU:CD1	2.36	0.56
4:B:736:HOH:O	2:F:15:THR:HG21	2.06	0.56
1:B:385:SER:CA	1:B:388:GLU:HG3	2.35	0.56
1:B:144:LEU:CD2	2:F:4:LYS:HD2	2.37	0.55
1:B:412:MET:CE	1:B:416:LEU:CG	2.76	0.55
1:A:209:VAL:HG22	1:A:216:LEU:HD13	1.87	0.55
1:B:385:SER:HA	1:B:388:GLU:CG	2.37	0.55
1:A:394:PHE:CD1	1:A:416:LEU:HD22	2.42	0.54
1:A:160:PRO:HG3	1:A:199:MET:HE1	1.89	0.54
1:B:512:LYS:H	1:B:512:LYS:CD	2.19	0.54
1:A:147:LEU:O	1:A:151:THR:HG23	2.07	0.54
1:A:155:GLY:CA	1:A:156:GLN:O	2.53	0.54
1:B:512:LYS:H	1:B:512:LYS:HD2	1.73	0.53
1:B:380:ASN:O	1:B:384:GLN:HG2	2.09	0.53
1:B:390:GLY:O	1:B:394:PHE:CD2	2.61	0.53
1:B:144:LEU:HB2	2:F:4:LYS:HZ2	1.73	0.53
1:A:239:LEU:HD22	1:A:525:ASP:HB3	1.90	0.52
1:A:194:THR:CG2	1:A:197:GLY:N	2.58	0.52
1:A:325:LYS:CE	1:A:327:PHE:CD1	2.89	0.52
1:B:141:LEU:N	1:B:142:PRO:HD3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5:GLY:O	2:F:9:GLU:HG3	2.09	0.52
1:A:325:LYS:HE3	1:A:325:LYS:C	2.34	0.52
1:A:394:PHE:CE1	1:A:416:LEU:HD22	2.45	0.52
1:B:289:LEU:O	1:B:290:GLN:C	2.52	0.51
1:B:396:ILE:HG22	1:B:400:LEU:HD12	1.92	0.51
1:B:511:ASP:HA	1:B:512:LYS:HZ2	1.76	0.51
1:B:323:PHE:C	1:B:325:LYS:H	2.19	0.51
1:A:162:HIS:O	1:A:166:THR:CG2	2.59	0.51
1:B:387:ARG:CD	1:B:417:ASP:OD1	2.59	0.50
1:A:321:LEU:HD12	1:A:327:PHE:CZ	2.47	0.50
1:B:354:VAL:CG1	1:B:355:ASN:N	2.74	0.50
1:B:194:THR:HG22	1:B:197:GLY:CA	2.42	0.49
1:A:159:ILE:HG22	1:A:160:PRO:O	2.12	0.49
1:A:325:LYS:HE2	1:A:327:PHE:CE1	2.47	0.49
1:B:255:ILE:HG12	1:B:258:LEU:HD12	1.95	0.49
1:B:209:VAL:HG22	1:B:216:LEU:HD13	1.94	0.49
1:A:532:PHE:CZ	1:A:547:PRO:HG2	2.48	0.49
1:A:412:MET:SD	1:A:416:LEU:CD1	3.01	0.49
1:B:294:LYS:HG2	1:B:343:ALA:HB2	1.95	0.48
1:B:387:ARG:HD3	1:B:417:ASP:OD1	2.13	0.48
1:B:493:ILE:HD12	1:B:519:GLY:HA3	1.96	0.48
1:A:191:LEU:O	1:A:194:THR:HB	2.13	0.48
1:A:373:ASN:ND2	4:A:701:HOH:O	2.35	0.48
1:B:546:ASP:HB3	1:B:549:ARG:HD2	1.96	0.48
1:A:155:GLY:CA	1:A:156:GLN:HB2	2.44	0.48
1:A:143:SER:CA	1:A:146:ASP:HB2	2.43	0.47
1:B:384:GLN:C	1:B:388:GLU:HG3	2.40	0.47
1:A:462:LEU:HD21	1:A:496:VAL:HG11	1.96	0.47
1:A:155:GLY:CA	1:A:156:GLN:CB	2.89	0.47
1:B:144:LEU:HD22	2:F:4:LYS:HD2	1.97	0.47
1:B:412:MET:HE2	1:B:416:LEU:HG	1.91	0.47
1:B:294:LYS:HE3	1:B:343:ALA:HB2	1.97	0.47
1:A:160:PRO:CB	1:A:199:MET:HE1	2.45	0.46
1:A:266:TRP:CE3	1:A:507:SER:HB2	2.51	0.46
1:B:411:ASP:OD1	1:B:411:ASP:C	2.58	0.46
1:B:327:PHE:CD2	1:B:335:HIS:HE1	2.33	0.46
1:B:327:PHE:CD2	1:B:335:HIS:CE1	3.04	0.46
1:B:270:VAL:HG22	1:B:503:MET:CG	2.46	0.46
1:A:240:TYR:CZ	1:A:266:TRP:CD1	3.04	0.46
1:A:209:VAL:CG1	1:A:213:ILE:HD13	2.43	0.45
1:B:144:LEU:HD23	2:F:4:LYS:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:PHE:CG	1:B:202:LYS:HG2	2.51	0.45
1:B:501:MET:HE3	1:B:503:MET:SD	2.57	0.45
1:A:153:ALA:O	1:A:156:GLN:CB	2.65	0.45
1:B:294:LYS:NZ	1:B:340:ASN:OD1	2.47	0.45
1:B:384:GLN:O	1:B:388:GLU:HG2	2.15	0.44
1:A:325:LYS:NZ	1:A:325:LYS:CA	2.58	0.44
1:A:160:PRO:HB3	1:A:199:MET:HE1	2.00	0.44
1:B:228:ASP:CG	1:B:231:SER:HB2	2.42	0.44
1:A:229:PHE:O	1:A:233:THR:HG23	2.17	0.44
1:A:162:HIS:O	1:A:166:THR:HG22	2.17	0.44
1:A:432:ALA:HB1	1:A:504:MET:HE2	2.00	0.44
1:A:501:MET:SD	1:A:503:MET:HE2	2.58	0.44
1:B:196:ASP:OD2	1:B:199:MET:HG2	2.17	0.44
1:A:339:VAL:HG23	1:A:342:GLY:H	1.82	0.44
1:B:327:PHE:CD1	1:B:327:PHE:N	2.86	0.44
1:B:144:LEU:HD12	1:B:144:LEU:HA	1.85	0.43
1:B:194:THR:CG2	1:B:197:GLY:CA	2.95	0.43
1:B:147:LEU:O	1:B:151:THR:CG2	2.66	0.43
1:B:325:LYS:O	1:B:327:PHE:CE1	2.71	0.43
1:B:161:VAL:HG13	1:B:162:HIS:N	2.34	0.43
1:B:147:LEU:O	1:B:151:THR:HG22	2.18	0.42
1:B:396:ILE:HG22	1:B:400:LEU:HD11	2.00	0.42
1:A:187:LEU:HD23	1:A:208:CYS:SG	2.59	0.42
1:B:222:ARG:HA	4:B:757:HOH:O	2.19	0.42
1:B:326:LEU:C	1:B:326:LEU:HD12	2.45	0.42
1:B:389:SER:O	1:B:389:SER:OG	2.19	0.42
1:A:290:GLN:O	1:A:293:VAL:HG12	2.20	0.42
1:B:550:GLU:O	1:B:551:GLY:C	2.62	0.42
1:A:160:PRO:CG	1:A:199:MET:HE1	2.50	0.42
1:A:325:LYS:CE	1:A:327:PHE:HD1	2.29	0.41
1:A:337:PRO:HG2	1:A:464:LEU:HD13	2.01	0.41
1:B:182:GLU:HG2	1:B:212:ASN:OD1	2.21	0.41
1:B:322:ARG:HG2	1:B:472:ASP:OD2	2.20	0.41
1:A:246:GLN:O	1:A:518:LYS:HE3	2.20	0.41
2:F:14:LEU:C	2:F:14:LEU:CD2	2.88	0.41
1:A:532:PHE:CZ	1:A:547:PRO:CG	3.03	0.41
1:B:201:ASP:OD1	1:B:201:ASP:C	2.62	0.41
1:B:387:ARG:HD2	1:B:417:ASP:OD1	2.21	0.41
1:A:485:ALA:HB2	1:A:495:LEU:HD12	2.03	0.41
1:A:501:MET:HE3	1:A:503:MET:HE2	1.79	0.41
1:B:322:ARG:HH11	1:B:322:ARG:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:SER:HB2	1:A:426:GLU:OE2	2.22	0.40
1:B:440:ALA:HB2	1:B:496:VAL:HG13	2.04	0.40

There are no symmetry-related clashes.

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	406/411 (99%)	392 (97%)	12 (3%)	2 (0%)	24	43
1	B	410/411 (100%)	396 (97%)	13 (3%)	1 (0%)	43	63
2	F	12/14 (86%)	12 (100%)	0	0	100	100
All	All	828/836 (99%)	800 (97%)	25 (3%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	GLY
1	B	324	ASN
1	A	156	GLN

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	354/356 (99%)	320 (90%)	34 (10%)	8	17
1	B	357/356 (100%)	316 (88%)	41 (12%)	5	11
2	F	7/7 (100%)	5 (71%)	2 (29%)	0	0
All	All	718/719 (100%)	641 (89%)	77 (11%)	6	13

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	LEU
1	A	145	GLU
1	A	147	LEU
1	A	156	GLN
1	A	157	GLU
1	A	159	ILE
1	A	166	THR
1	A	173	LEU
1	A	191	LEU
1	A	194	THR
1	A	204	LEU
1	A	209	VAL
1	A	210	GLN
1	A	222	ARG
1	A	231	SER
1	A	234	SER
1	A	250	LYS
1	A	260	LYS
1	A	325	LYS
1	A	326	LEU
1	A	349	LEU
1	A	354	VAL
1	A	365	GLN
1	A	392	ARG
1	A	416	LEU
1	A	417	ASP
1	A	451	ARG
1	A	512	LYS
1	A	513	MET
1	A	528	SER
1	A	534	ASN
1	A	545	LEU
1	A	548	ARG
1	A	549	ARG

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Mol	Chain	Res	Type
1	B	144	LEU
1	B	145	GLU
1	B	147	LEU
1	B	151	THR
1	B	158	LYS
1	B	173	LEU
1	B	182	GLU
1	B	190	THR
1	B	191	LEU
1	B	194	THR
1	B	202	LYS
1	B	204	LEU
1	B	209	VAL
1	B	210	GLN
1	B	221	ARG
1	B	242	SER
1	B	250	LYS
1	B	255	ILE
1	B	260	LYS
1	B	294	LYS
1	B	317	GLU
1	B	322	ARG
1	B	325	LYS
1	B	326	LEU
1	B	349	LEU
1	B	354	VAL
1	B	361	ASP
1	B	364	MET
1	B	365	GLN
1	B	366	PHE
1	B	387	ARG
1	B	391	LYS
1	B	401	LYS
1	B	402	GLU
1	B	408	GLU
1	B	412	MET
1	B	467	SER
1	B	512	LYS
1	B	534	ASN
1	B	548	ARG
1	B	549	ARG
2	F	10	LEU

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Mol	Chain	Res	Type
2	F	14	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	162	HIS
1	A	235	HIS
1	A	352	GLN
1	A	393	ASN
1	A	476	GLN
1	B	246	GLN
1	B	335	HIS
1	B	355	ASN
1	B	393	ASN
1	B	466	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	408/411 (99%)	0.37	35 (8%) 16 14	30, 49, 85, 122	0
1	B	411/411 (100%)	1.17	83 (20%) 3 2	30, 52, 100, 119	1 (0%)
2	F	14/14 (100%)	4.40	14 (100%) 0 0	77, 108, 123, 126	0
All	All	833/836 (99%)	0.83	132 (15%) 5 4	30, 50, 98, 126	1 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	3	ALA	7.6
1	B	550	GLU	6.8
2	F	14	LEU	6.4
1	B	321	LEU	6.3
2	F	16	ALA	6.2
1	B	327	PHE	5.9
1	B	324	ASN	5.6
2	F	5	GLY	5.2
1	B	543	LYS	4.9
1	A	325	LYS	4.8
1	B	542	ALA	4.8
1	B	551	GLY	4.8
2	F	4	LYS	4.6
2	F	13	GLY	4.5
1	A	550	GLU	4.4
1	B	323	PHE	4.3
1	B	322	ARG	4.3
2	F	10	LEU	4.3
1	B	141	LEU	4.3
1	B	319	SER	4.2
2	F	15	THR	4.0
1	B	549	ARG	4.0
1	B	256	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
2	F	7	LEU	3.9
1	B	142	PRO	3.9
1	B	329	ASN	3.9
1	B	182	GLU	3.9
1	B	393	ASN	3.8
1	B	391	LYS	3.8
1	A	416	LEU	3.8
1	B	325	LYS	3.7
1	B	401	LYS	3.7
1	B	155	GLY	3.6
1	B	258	LEU	3.6
1	B	365	GLN	3.5
1	B	388	GLU	3.5
1	A	155	GLY	3.5
2	F	11	GLY	3.5
1	B	402	GLU	3.5
1	B	398	TYR	3.5
1	B	399	TYR	3.4
1	B	318	PRO	3.4
1	B	408	GLU	3.4
2	F	9	GLU	3.4
1	A	321	LEU	3.4
1	B	409	GLY	3.4
1	B	417	ASP	3.3
1	A	326	LEU	3.2
1	B	357	ALA	3.1
2	F	8	GLN	3.1
1	A	324	ASN	3.1
1	B	400	LEU	3.0
1	B	254	TYR	3.0
1	B	253	ASP	3.0
1	B	350	ILE	3.0
1	A	388	GLU	3.0
1	B	548	ARG	3.0
1	B	392	ARG	2.9
1	B	407	PRO	2.9
1	A	543	LYS	2.9
1	B	332	ASP	2.9
1	B	320	GLY	2.9
1	B	353	GLY	2.9
1	B	157	GLU	2.9
1	B	538	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	361	ASP	2.8
1	B	355	ASN	2.8
1	A	260	LYS	2.8
1	B	252	ALA	2.8
1	B	416	LEU	2.8
1	A	157	GLU	2.8
1	A	221	ARG	2.8
1	A	549	ARG	2.8
1	A	322	ARG	2.7
1	B	257	GLN	2.7
1	B	203	ASP	2.6
1	B	467	SER	2.6
1	A	151	THR	2.6
1	B	309	TYR	2.6
1	B	471	TYR	2.6
2	F	12	ALA	2.6
1	A	327	PHE	2.6
1	B	383	PHE	2.6
1	B	410	THR	2.6
1	B	331	ASP	2.5
1	A	159	ILE	2.5
1	A	154	GLU	2.5
1	B	475	GLY	2.5
1	B	261	PHE	2.5
1	A	143	SER	2.5
1	A	202	LYS	2.5
1	B	249	GLY	2.4
1	B	196	ASP	2.4
1	B	326	LEU	2.4
1	B	394	PHE	2.4
1	B	352	GLN	2.4
1	B	449	GLY	2.4
1	B	205	PHE	2.4
1	A	512	LYS	2.4
1	B	534	ASN	2.3
1	B	311	HIS	2.3
1	A	230	MET	2.3
1	A	392	ARG	2.3
1	A	417	ASP	2.3
1	B	209	VAL	2.3
1	B	346	VAL	2.2
1	B	505	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	260	LYS	2.2
1	B	360	PHE	2.2
1	B	413	VAL	2.2
1	A	542	ALA	2.2
1	A	204	LEU	2.2
1	A	256	PRO	2.2
1	A	418	PHE	2.2
1	B	460	ASN	2.2
2	F	6	ALA	2.2
1	B	307	THR	2.2
1	B	421	GLN	2.1
1	A	200	LEU	2.1
1	B	488	GLY	2.1
1	A	451	ARG	2.1
1	B	330	GLU	2.1
1	A	147	LEU	2.1
1	A	150	TYR	2.1
1	A	254	TYR	2.1
1	B	146	ASP	2.1
1	A	192	GLN	2.0
1	B	451	ARG	2.0
1	B	189	LEU	2.0
1	B	382	THR	2.0
1	A	471	TYR	2.0
1	B	420	PHE	2.0

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 oligosaccharides 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. 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($\text{\AA}^2$)	Q<0.9
3	CL	B	601	1/1	0.83	0.17	81,81,81,81	0
3	CL	A	601	1/1	0.94	0.33	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.