



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2025 – 02:06 PM EDT

PDB ID : 9PIA / pdb\_00009pia  
Title : Human glutaminase C mutant S482C  
Authors : Milano, S.K.; Ulrich, S.M.; Cerione, R.A.  
Deposited on : 2025-07-10  
Resolution : 2.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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>.

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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	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

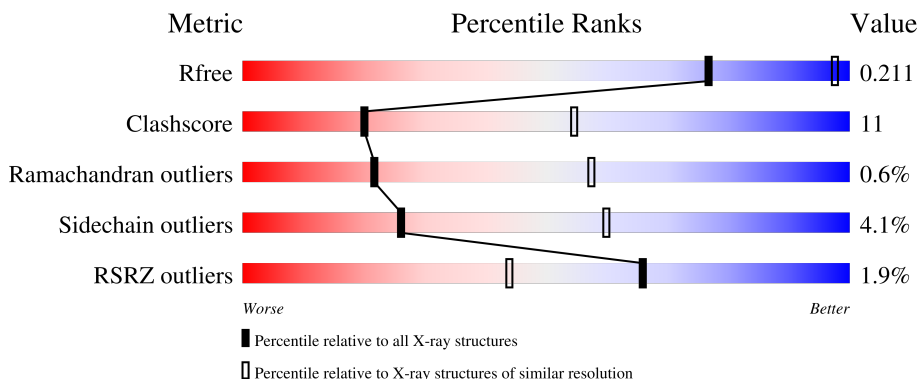
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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))
$R_{free}$	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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  $\geq 3$ , 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	598	<div> <div>%</div> <div> <div>48%</div> <div>17%</div> <div>•</div> <div>33%</div> </div> </div>
1	B	598	<div> <div>2%</div> <div> <div>50%</div> <div>16%</div> <div>•</div> <div>33%</div> </div> </div>
1	C	598	<div> <div>%</div> <div> <div>48%</div> <div>17%</div> <div>•</div> <div>33%</div> </div> </div>
1	D	598	<div> <div>%</div> <div> <div>50%</div> <div>15%</div> <div>•</div> <div>33%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12492 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 Isoform 3 of Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3099	1972	522	576	29			
1	B	398	Total	C	N	O	S	0	0	0
			3099	1972	522	576	29			
1	C	398	Total	C	N	O	S	0	0	0
			3099	1972	522	576	29			
1	D	398	Total	C	N	O	S	0	0	0
			3099	1972	522	576	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	482	CYS	SER	engineered mutation	UNP O94925
B	482	CYS	SER	engineered mutation	UNP O94925
C	482	CYS	SER	engineered mutation	UNP O94925
D	482	CYS	SER	engineered mutation	UNP O94925

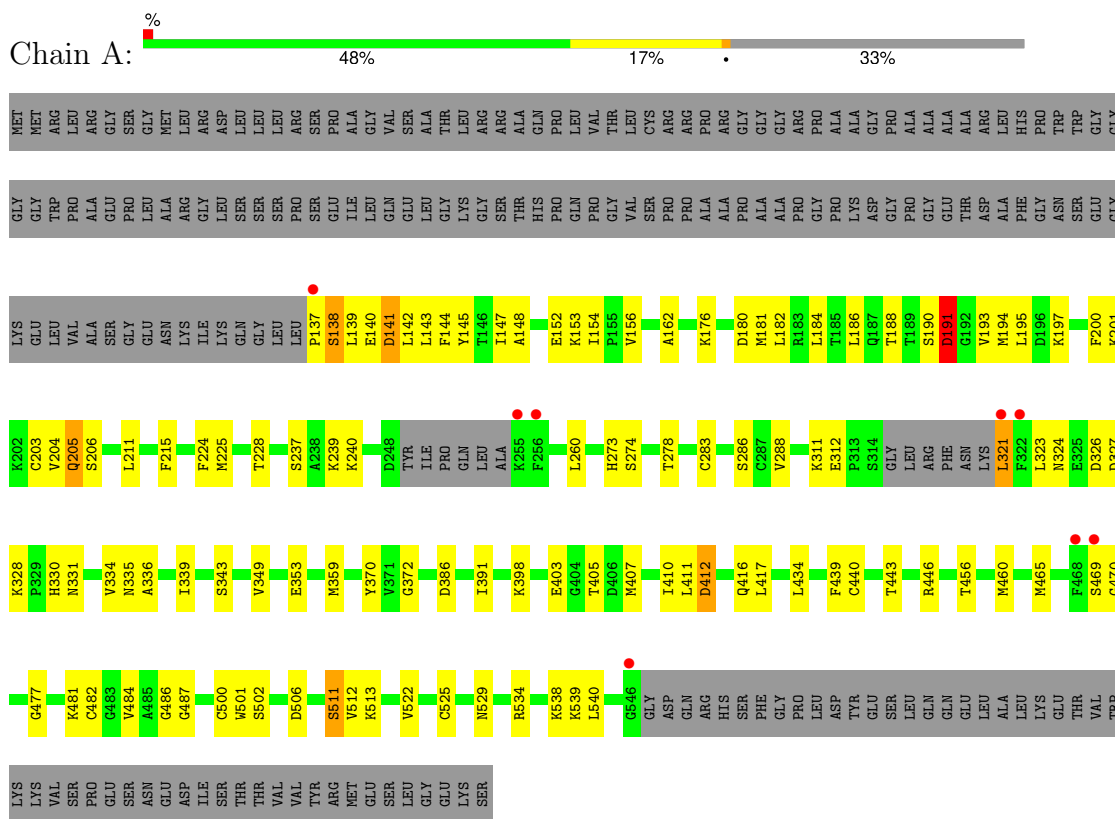
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	17	Total	O	0	0
			17	17		
2	B	29	Total	O	0	0
			29	29		
2	C	29	Total	O	0	0
			29	29		
2	D	21	Total	O	0	0
			21	21		

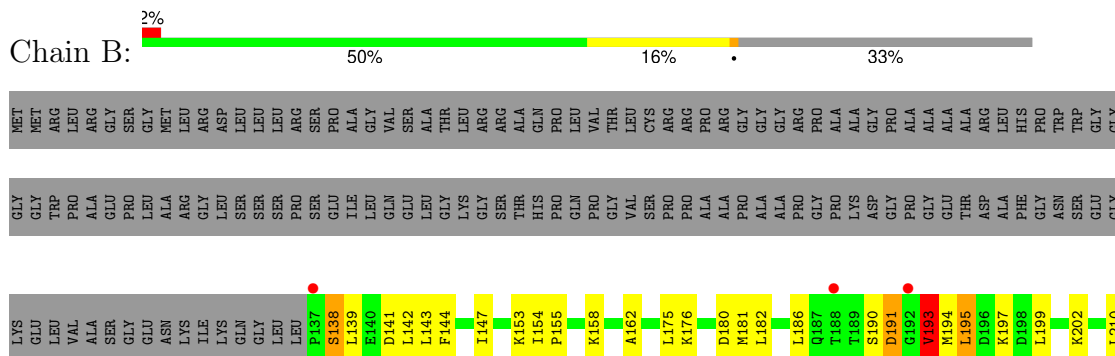
### 3 Residue-property plots

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.

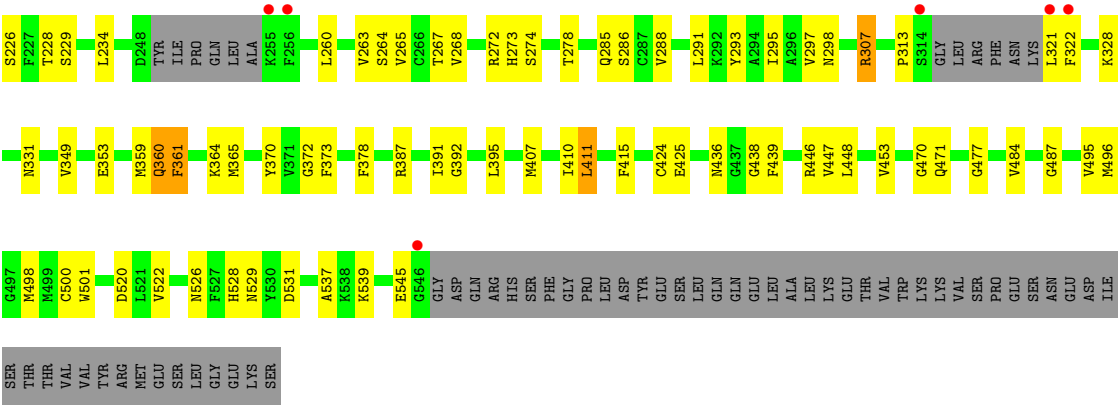
- Molecule 1: Isoform 3 of Glutaminase kidney isoform, mitochondrial



- Molecule 1: Isoform 3 of Glutaminase kidney isoform, mitochondrial







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.85Å 138.21Å 177.12Å 90.00° 93.58° 90.00°	Depositor
Resolution (Å)	49.61 – 2.99 49.61 – 2.99	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.61-2.99) 96.3 (49.61-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.188 , 0.209 0.188 , 0.211	Depositor DCC
$R_{free}$ test set	2012 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.2	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 34.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12492	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.42	0/3166	0.62	0/4270
1	B	0.41	0/3166	0.60	0/4270
1	C	0.43	0/3166	0.63	3/4270 (0.1%)
1	D	0.42	0/3166	0.62	0/4270
All	All	0.42	0/12664	0.62	3/17080 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	LYS	CD-CE-NZ	7.62	136.29	111.90
1	C	197	LYS	CD-CE-NZ	6.56	132.90	111.90
1	C	197	LYS	CB-CG-CD	-5.26	99.19	111.30

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	3099	0	3068	79	0
1	B	3099	0	3068	70	0
1	C	3099	0	3068	69	0
1	D	3099	0	3068	70	0
2	A	17	0	0	5	0
2	B	29	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	29	0	0	2	0
2	D	21	0	0	1	0
All	All	12492	0	12272	276	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 11.

All (276) 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:B:392:GLY:HA3	1:B:407:MET:HE3	1.34	1.08
1:D:234:LEU:HD22	1:D:520:ASP:HB3	1.59	0.83
1:B:312:GLU:HG2	1:D:470:GLY:HA3	1.61	0.82
1:D:365:MET:HG2	1:D:447:VAL:HG11	1.61	0.82
1:B:392:GLY:CA	1:B:407:MET:HE3	2.09	0.82
1:A:283:CYS:HB2	2:A:601:HOH:O	1.79	0.80
1:D:274:SER:HB3	1:D:278:THR:HG21	1.64	0.79
1:C:148:ALA:HB2	1:C:154:ILE:HG12	1.64	0.78
1:A:143:LEU:HD23	1:A:200:PHE:HZ	1.50	0.76
1:C:138:SER:HB3	1:C:141:ASP:HB2	1.67	0.76
1:A:312:GLU:HG2	1:C:470:GLY:HA3	1.68	0.76
1:C:274:SER:HB3	1:C:278:THR:HG21	1.69	0.75
1:A:403:GLU:CD	1:A:403:GLU:H	1.95	0.73
1:C:524:LEU:HD23	1:C:525:CYS:SG	2.29	0.72
1:C:427:ALA:HB1	1:C:499:MET:HE3	1.71	0.72
1:A:456:THR:HG22	1:A:460:MET:HE2	1.72	0.70
1:C:265:VAL:HG22	1:C:498:MET:HE2	1.74	0.69
1:A:145:TYR:OH	1:A:197:LYS:HE3	1.93	0.69
1:D:285:GLN:O	1:D:288:VAL:HG12	1.93	0.68
1:A:274:SER:HB3	1:A:278:THR:HG21	1.74	0.68
1:D:268:VAL:HG23	1:D:495:VAL:C	2.18	0.68
1:C:443:THR:OG1	1:C:445:GLU:HG2	1.95	0.67
1:A:343:SER:HA	1:A:410:ILE:HD12	1.76	0.66
1:B:392:GLY:HA3	1:B:407:MET:CE	2.20	0.65
1:C:268:VAL:HG23	1:C:495:VAL:C	2.22	0.65
1:C:234:LEU:HD22	1:C:520:ASP:HB3	1.78	0.65
1:B:490:LEU:HB3	1:B:498:MET:HB2	1.80	0.64
1:C:155:PRO:HG2	1:C:158:LYS:HB2	1.79	0.64
1:C:286:SER:HA	1:C:289:LYS:HZ3	1.62	0.64
1:B:450:PRO:HG2	1:D:537:ALA:HB2	1.79	0.64
1:A:502:SER:O	1:A:511:SER:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:GLN:HG3	1:B:484:VAL:HG12	1.80	0.62
1:A:140:GLU:HB2	1:A:201:LYS:HD2	1.81	0.62
1:B:465:MET:HB3	1:B:468:PHE:HB3	1.81	0.62
1:C:224:PHE:O	1:C:228:THR:HG23	2.00	0.62
1:A:477:GLY:O	1:A:529:ASN:HB2	2.00	0.62
1:B:195:LEU:HD22	1:B:199:LEU:HD12	1.82	0.62
1:A:522:VAL:O	1:A:539:LYS:HE2	2.00	0.60
1:D:407:MET:HE2	1:D:411:LEU:HD23	1.83	0.60
1:A:349:VAL:CG1	1:A:353:GLU:HB2	2.32	0.60
1:A:156:VAL:HG21	1:A:186:LEU:HD21	1.84	0.60
1:C:490:LEU:HB3	1:C:498:MET:HB2	1.84	0.60
1:A:534:ARG:NH1	1:C:268:VAL:HG12	2.17	0.60
1:D:477:GLY:O	1:D:529:ASN:HB2	2.02	0.59
1:B:274:SER:HB3	1:B:278:THR:HG21	1.83	0.59
1:B:162:ALA:HB1	1:B:215:PHE:HE1	1.69	0.58
1:B:540:LEU:HG	1:B:542:PRO:HD3	1.87	0.57
1:A:139:LEU:HA	1:A:142:LEU:HD12	1.86	0.57
1:A:162:ALA:HB1	1:A:215:PHE:HE1	1.69	0.57
1:B:139:LEU:HA	1:B:142:LEU:HD12	1.86	0.57
1:B:495:VAL:HG12	1:B:496:MET:HG2	1.86	0.57
1:B:477:GLY:O	1:B:529:ASN:HB2	2.06	0.56
1:A:506:ASP:HB3	1:A:512:VAL:HG22	1.88	0.56
1:B:234:LEU:HD21	1:B:524:LEU:HD12	1.88	0.56
1:B:153:LYS:HB3	1:B:194:MET:HB3	1.88	0.56
1:D:143:LEU:HD22	1:D:147:ILE:HD11	1.87	0.56
1:C:427:ALA:HA	1:C:430:MET:HG3	1.88	0.56
1:A:283:CYS:CB	2:A:601:HOH:O	2.47	0.56
1:A:283:CYS:N	2:A:601:HOH:O	2.34	0.56
1:A:439:PHE:CE2	1:A:446:ARG:HB2	2.41	0.55
1:C:278:THR:HA	1:C:424:CYS:HB2	1.89	0.55
1:C:465:MET:HB2	1:C:469:SER:HA	1.89	0.55
1:B:199:LEU:HD22	1:B:202:LYS:HD3	1.89	0.55
1:B:465:MET:HB2	1:B:469:SER:HA	1.89	0.55
1:D:278:THR:HA	1:D:424:CYS:HB2	1.88	0.55
1:D:155:PRO:HD2	1:D:158:LYS:HE3	1.89	0.55
1:A:335:ASN:O	1:A:339:ILE:HG13	2.07	0.54
1:B:248:ASP:HA	1:B:255:LYS:NZ	2.23	0.54
1:C:151:GLN:HG2	1:C:152:GLU:H	1.73	0.54
1:D:360:GLN:HG3	1:D:361:PHE:N	2.21	0.54
1:C:270:GLY:O	1:C:272:ARG:HG3	2.07	0.54
1:D:204:VAL:HG13	1:D:211:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:O	1:A:147:ILE:HD12	2.07	0.54
1:C:140:GLU:HB2	1:C:201:LYS:HG3	1.90	0.54
1:A:182:LEU:O	1:A:186:LEU:HG	2.07	0.54
1:D:313:PRO:HA	1:D:331:ASN:ND2	2.23	0.54
1:A:465:MET:HB2	1:A:469:SER:HA	1.89	0.53
1:D:139:LEU:HG	1:D:212:THR:HG21	1.90	0.53
1:A:204:VAL:HG13	1:A:211:LEU:HD12	1.91	0.53
1:B:181:MET:CE	1:B:202:LYS:HE2	2.39	0.53
1:C:166:THR:OG1	1:C:214:ALA:HB1	2.09	0.53
1:B:181:MET:HE1	1:B:202:LYS:HE2	1.90	0.53
1:D:522:VAL:O	1:D:539:LYS:HE2	2.08	0.53
1:C:191:ASP:O	1:C:192:GLY:C	2.52	0.52
1:D:162:ALA:HB1	1:D:215:PHE:HE1	1.74	0.52
1:C:392:GLY:HA3	1:C:407:MET:HE3	1.92	0.52
1:A:465:MET:HE1	1:A:482:CYS:SG	2.50	0.52
1:C:370:TYR:HB3	2:C:601:HOH:O	2.09	0.51
1:D:439:PHE:CE2	1:D:446:ARG:HB2	2.45	0.51
1:A:143:LEU:HD23	1:A:200:PHE:CZ	2.39	0.51
1:A:321:LEU:HD22	2:A:604:HOH:O	2.10	0.51
1:C:162:ALA:HB1	1:C:215:PHE:HE1	1.76	0.51
1:B:182:LEU:O	1:B:186:LEU:HG	2.10	0.51
1:B:228:THR:HB	1:B:273:HIS:ND1	2.26	0.51
1:A:138:SER:HB3	1:A:141:ASP:HB2	1.91	0.51
1:B:225:MET:HA	1:B:225:MET:HE3	1.93	0.51
1:C:220:VAL:HG21	1:C:495:VAL:HA	1.92	0.51
1:B:255:LYS:HD2	1:B:255:LYS:N	2.26	0.51
1:D:349:VAL:CG1	1:D:353:GLU:HB2	2.40	0.51
1:B:349:VAL:CG1	1:B:353:GLU:HB2	2.41	0.51
1:C:349:VAL:CG1	1:C:353:GLU:HB2	2.41	0.51
1:B:326:ASP:HB3	1:B:328:LYS:HG3	1.92	0.51
1:C:140:GLU:CB	1:C:201:LYS:HG3	2.41	0.51
1:B:286:SER:HA	1:B:289:LYS:HZ3	1.75	0.50
1:C:176:LYS:HE2	1:C:180:ASP:OD2	2.11	0.50
1:B:311:LYS:HE3	1:D:471:GLN:NE2	2.26	0.50
1:B:389:PHE:HA	1:B:411:LEU:HD11	1.93	0.50
1:D:392:GLY:HA3	1:D:407:MET:HE3	1.93	0.50
1:A:224:PHE:O	1:A:228:THR:HG23	2.10	0.50
1:C:387:ARG:O	1:C:391:ILE:HG13	2.12	0.50
1:A:470:GLY:HA3	1:C:312:GLU:HG2	1.93	0.50
1:B:228:THR:HB	1:B:273:HIS:CE1	2.46	0.50
1:A:156:VAL:HG23	1:A:195:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:PHE:CE1	1:C:446:ARG:HB2	2.46	0.50
1:A:487:GLY:HA2	1:A:500:CYS:O	2.12	0.49
1:B:498:MET:HE1	1:B:517:PHE:CE1	2.47	0.49
1:D:295:ILE:HG23	1:D:361:PHE:CE2	2.47	0.49
1:D:298:ASN:ND2	1:D:448:LEU:HA	2.27	0.49
1:A:336:ALA:HA	1:A:391:ILE:HG21	1.94	0.49
1:B:138:SER:HB3	1:B:141:ASP:HB2	1.93	0.49
1:A:225:MET:HE2	1:A:225:MET:HA	1.94	0.49
1:D:224:PHE:O	1:D:228:THR:HG23	2.12	0.49
1:B:265:VAL:HG22	1:B:498:MET:HG2	1.94	0.49
1:C:374:SER:HB2	1:C:421:GLU:OE2	2.12	0.49
1:D:496:MET:HE3	1:D:498:MET:CE	2.42	0.49
1:B:359:MET:HE1	1:B:371:VAL:HG12	1.94	0.49
1:A:237:SER:HA	1:A:240:LYS:HE2	1.94	0.49
1:B:144:PHE:CD1	1:B:154:ILE:HD11	2.48	0.49
1:B:278:THR:HA	1:B:424:CYS:HB2	1.94	0.49
1:A:260:LEU:HD13	1:A:501:TRP:CH2	2.48	0.48
1:B:224:PHE:O	1:B:228:THR:HG23	2.14	0.48
1:C:449:SER:O	1:C:453:VAL:HG23	2.13	0.48
1:C:484:VAL:HG22	2:C:618:HOH:O	2.13	0.48
1:A:331:ASN:O	1:A:334:VAL:HG22	2.13	0.48
1:D:392:GLY:C	1:D:407:MET:HE3	2.38	0.48
1:B:141:ASP:OD2	1:B:197:LYS:HD3	2.14	0.48
1:C:392:GLY:C	1:C:407:MET:HE3	2.37	0.48
1:A:176:LYS:HE2	1:A:180:ASP:OD2	2.13	0.48
1:A:143:LEU:HG	1:A:147:ILE:HD11	1.96	0.48
1:C:465:MET:HE1	1:C:482:CYS:SG	2.54	0.48
1:B:191:ASP:C	1:B:193:VAL:H	2.22	0.48
1:D:145:TYR:OH	1:D:197:LYS:NZ	2.40	0.48
1:C:185:THR:HG21	1:C:199:LEU:HD11	1.95	0.48
1:D:163:LEU:HD21	1:D:175:LEU:HD13	1.96	0.48
1:A:141:ASP:OD1	1:A:141:ASP:N	2.47	0.47
1:D:387:ARG:O	1:D:391:ILE:HG13	2.14	0.47
1:A:538:LYS:HD2	1:A:538:LYS:N	2.30	0.47
1:D:370:TYR:CZ	1:D:372:GLY:HA3	2.50	0.47
1:A:312:GLU:OE2	1:C:471:GLN:HG2	2.15	0.47
1:D:147:ILE:HG22	1:D:158:LYS:NZ	2.30	0.47
1:A:144:PHE:CE1	1:A:154:ILE:HG13	2.49	0.47
1:C:155:PRO:HB2	1:C:157:HIS:CD2	2.50	0.47
1:C:291:LEU:O	1:C:295:ILE:HG13	2.14	0.47
1:A:386:ASP:OD2	1:B:396:LYS:HE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:GLY:O	1:A:501:TRP:HA	2.14	0.47
1:B:538:LYS:H	1:B:538:LYS:HG2	1.54	0.47
1:B:507:LYS:CE	1:B:507:LYS:H	2.28	0.46
1:D:407:MET:HE2	1:D:411:LEU:CD2	2.45	0.46
1:C:185:THR:HG22	1:C:193:VAL:HG11	1.97	0.46
1:D:264:SER:HB2	1:D:424:CYS:HB3	1.97	0.46
1:C:378:PHE:CE1	1:C:416:GLN:HG2	2.50	0.46
1:D:260:LEU:HD13	1:D:501:TRP:CH2	2.51	0.46
1:A:370:TYR:CZ	1:A:372:GLY:HA3	2.50	0.46
1:D:143:LEU:CD2	1:D:147:ILE:HD11	2.45	0.46
1:D:291:LEU:O	1:D:295:ILE:HG13	2.16	0.46
1:D:349:VAL:HG11	1:D:353:GLU:HB2	1.97	0.46
1:A:228:THR:HB	1:A:273:HIS:ND1	2.31	0.46
1:B:507:LYS:H	1:B:507:LYS:HE2	1.81	0.46
1:D:526:ASN:HA	1:D:531:ASP:OD2	2.16	0.46
1:B:379:GLN:OE1	1:B:382:ARG:HD3	2.16	0.45
1:B:432:ALA:HB1	1:B:441:PRO:HG3	1.96	0.45
1:A:153:LYS:HB3	1:A:194:MET:HG2	1.98	0.45
1:A:228:THR:HB	1:A:273:HIS:CE1	2.51	0.45
1:A:359:MET:HE1	1:A:372:GLY:O	2.17	0.45
1:B:465:MET:HE1	1:B:482:CYS:SG	2.55	0.45
1:A:434:LEU:HD13	1:A:460:MET:HE1	1.99	0.45
1:C:138:SER:O	1:C:139:LEU:C	2.59	0.45
1:D:169:ARG:HG3	1:D:272:ARG:HG3	1.99	0.45
1:D:378:PHE:HE1	1:D:415:PHE:HB2	1.82	0.45
1:D:365:MET:HG2	1:D:447:VAL:CG1	2.40	0.45
1:C:216:ARG:HB2	1:C:218:LYS:HD3	1.99	0.45
1:A:324:ASN:HB3	1:A:330:HIS:ND1	2.31	0.45
1:D:321:LEU:HD23	1:D:321:LEU:HA	1.81	0.45
1:D:487:GLY:HA2	1:D:500:CYS:O	2.17	0.45
1:B:175:LEU:HD21	1:B:210:LEU:HD23	1.99	0.45
1:D:211:LEU:HD23	1:D:211:LEU:HA	1.68	0.45
1:D:370:TYR:OH	1:D:372:GLY:HA3	2.17	0.45
1:B:248:ASP:HA	1:B:255:LYS:HZ1	1.81	0.44
1:C:337:GLY:O	1:C:341:VAL:HG23	2.17	0.44
1:C:268:VAL:HG13	1:C:436:ASN:CG	2.43	0.44
1:A:144:PHE:HZ	1:A:152:GLU:O	2.00	0.44
1:C:364:LYS:HB3	1:C:447:VAL:HG13	1.98	0.44
1:C:477:GLY:O	1:C:529:ASN:HB2	2.18	0.44
1:A:412:ASP:O	1:A:416:GLN:HG3	2.17	0.44
1:D:392:GLY:HA3	1:D:407:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:LYS:NZ	1:A:482:CYS:H	2.15	0.44
1:A:181:MET:HG2	1:A:203:CYS:HA	1.99	0.44
1:B:522:VAL:CG1	1:B:528:HIS:HB2	2.47	0.44
1:C:332:PRO:HB3	1:C:341:VAL:HG21	2.00	0.44
1:A:260:LEU:HB3	1:A:501:TRP:CZ3	2.53	0.43
1:A:311:LYS:HD3	1:C:474:PHE:CD1	2.53	0.43
1:C:151:GLN:CG	1:C:152:GLU:H	2.30	0.43
1:B:239:LYS:HE2	1:B:261:TRP:HD1	1.83	0.43
1:B:349:VAL:HG13	1:B:353:GLU:HB2	2.01	0.43
1:C:394:TYR:HE2	1:D:322:PHE:HZ	1.65	0.43
1:D:293:TYR:O	1:D:297:VAL:HG23	2.18	0.43
1:A:323:LEU:HD23	1:A:327:ASP:C	2.43	0.43
1:B:155:PRO:HG2	1:B:158:LYS:HB2	2.00	0.43
1:B:498:MET:HB3	1:B:498:MET:HE2	1.57	0.43
1:D:438:GLY:CA	1:D:453:VAL:HG21	2.48	0.43
1:C:153:LYS:HB3	1:C:194:MET:HB3	2.00	0.43
1:A:239:LYS:HA	1:A:513:LYS:HD3	2.00	0.43
1:B:276:GLY:O	1:B:278:THR:HG23	2.19	0.43
1:B:461:HIS:HD2	2:B:604:HOH:O	2.00	0.43
1:B:525:CYS:HA	1:B:540:LEU:O	2.18	0.43
1:A:349:VAL:HG12	1:A:353:GLU:HB2	2.00	0.43
1:A:144:PHE:CE2	1:A:197:LYS:HB2	2.54	0.42
1:A:286:SER:HB2	1:A:482:CYS:O	2.18	0.42
1:A:525:CYS:HA	1:A:540:LEU:O	2.19	0.42
1:D:359:MET:HE1	1:D:373:PHE:HB2	2.00	0.42
1:C:166:THR:HG22	1:C:168:LEU:H	1.84	0.42
1:D:529:ASN:HD22	1:D:529:ASN:C	2.27	0.42
1:B:413:PHE:O	1:B:416:GLN:HB2	2.20	0.42
1:D:365:MET:CE	1:D:448:LEU:HD11	2.50	0.42
1:A:440:CYS:SG	1:A:443:THR:HG23	2.60	0.42
1:B:312:GLU:CG	1:D:470:GLY:HA3	2.40	0.42
1:C:323:LEU:HD23	1:C:327:ASP:HA	2.01	0.42
1:D:265:VAL:HG12	1:D:273:HIS:O	2.20	0.42
1:A:191:ASP:O	1:A:193:VAL:N	2.53	0.42
1:A:260:LEU:HD13	1:A:501:TRP:HH2	1.84	0.42
1:A:370:TYR:OH	1:A:372:GLY:HA3	2.20	0.42
2:A:609:HOH:O	1:B:397:GLU:HA	2.19	0.42
1:C:260:LEU:HD13	1:C:501:TRP:CH2	2.55	0.42
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.75	0.42
1:A:201:LYS:O	1:A:205:GLN:HB3	2.19	0.42
1:A:405:THR:HG23	1:A:410:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:ARG:NH1	1:D:268:VAL:HG12	2.35	0.42
1:C:268:VAL:HG13	1:C:436:ASN:CB	2.50	0.42
1:B:182:LEU:HD23	1:B:182:LEU:HA	1.83	0.41
1:B:143:LEU:O	1:B:147:ILE:HD12	2.20	0.41
1:B:211:LEU:HD23	1:B:211:LEU:HA	1.91	0.41
1:C:138:SER:O	1:C:141:ASP:N	2.52	0.41
1:D:295:ILE:HG23	1:D:361:PHE:CD2	2.55	0.41
1:C:211:LEU:HA	1:C:211:LEU:HD23	1.82	0.41
1:C:349:VAL:HG12	1:C:353:GLU:HB2	2.02	0.41
1:B:244:GLY:HA2	1:B:505:LEU:O	2.20	0.41
1:C:413:PHE:HA	1:C:416:GLN:HG3	2.02	0.41
1:A:194:MET:HE3	1:A:194:MET:HB2	1.85	0.41
1:A:417:LEU:HD23	1:A:417:LEU:HA	1.92	0.41
1:B:422:VAL:HG21	1:B:427:ALA:HB2	2.03	0.41
1:D:145:TYR:HB2	2:D:601:HOH:O	2.21	0.41
1:B:426:SER:O	1:B:430:MET:HG3	2.21	0.41
1:D:226:SER:O	1:D:229:SER:HB2	2.20	0.41
1:D:264:SER:CB	1:D:424:CYS:HB3	2.51	0.41
1:D:410:ILE:HA	1:D:410:ILE:HD13	1.83	0.41
1:A:148:ALA:HB2	1:A:154:ILE:HG12	2.02	0.41
1:A:407:MET:SD	1:A:407:MET:C	3.04	0.41
1:B:176:LYS:HE2	1:B:180:ASP:OD2	2.21	0.41
1:C:268:VAL:HG21	1:C:494:ASN:C	2.46	0.41
1:C:457:LEU:HD23	1:C:457:LEU:HA	1.84	0.41
1:C:522:VAL:O	1:C:539:LYS:HE2	2.20	0.41
1:D:209:VAL:HG23	1:D:210:LEU:H	1.85	0.41
1:B:410:ILE:HD13	1:B:410:ILE:HA	1.82	0.41
1:C:522:VAL:CG1	1:C:528:HIS:HB2	2.51	0.41
1:D:268:VAL:HG13	1:D:436:ASN:CG	2.46	0.41
1:D:278:THR:O	1:D:425:GLU:HG3	2.21	0.41
1:C:410:ILE:HD13	1:C:410:ILE:HA	1.85	0.40
1:D:307:ARG:O	1:D:328:LYS:HD3	2.21	0.40
1:D:522:VAL:CG1	1:D:528:HIS:HB2	2.52	0.40
1:A:407:MET:SD	1:A:411:LEU:HD12	2.61	0.40
1:A:184:LEU:O	1:A:188:THR:HG23	2.21	0.40
1:D:313:PRO:HA	1:D:331:ASN:HD22	1.84	0.40
1:D:391:ILE:HG22	1:D:395:LEU:HD11	2.03	0.40
1:C:211:LEU:O	1:C:215:PHE:HD2	2.05	0.40
1:D:267:THR:HA	1:D:496:MET:CB	2.51	0.40
1:D:392:GLY:CA	1:D:407:MET:HE3	2.52	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	392/598 (66%)	374 (95%)	17 (4%)	1 (0%)	37	70
1	B	392/598 (66%)	372 (95%)	16 (4%)	4 (1%)	13	46
1	C	392/598 (66%)	375 (96%)	15 (4%)	2 (0%)	25	61
1	D	392/598 (66%)	368 (94%)	22 (6%)	2 (0%)	25	61
All	All	1568/2392 (66%)	1489 (95%)	70 (4%)	9 (1%)	22	57

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	ASP
1	C	138	SER
1	C	192	GLY
1	D	193	VAL
1	B	138	SER
1	D	194	MET
1	B	193	VAL
1	B	256	PHE
1	B	222	PRO

### 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	345/500 (69%)	330 (96%)	15 (4%)	25	58
1	B	345/500 (69%)	337 (98%)	8 (2%)	45	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	345/500 (69%)	330 (96%)	15 (4%)	25	58
1	D	345/500 (69%)	327 (95%)	18 (5%)	19	52
All	All	1380/2000 (69%)	1324 (96%)	56 (4%)	26	60

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	PRO
1	A	138	SER
1	A	141	ASP
1	A	190	SER
1	A	191	ASP
1	A	205	GLN
1	A	206	SER
1	A	288	VAL
1	A	321	LEU
1	A	326	ASP
1	A	328	LYS
1	A	398	LYS
1	A	412	ASP
1	A	484	VAL
1	A	511	SER
1	B	190	SER
1	B	191	ASP
1	B	193	VAL
1	B	195	LEU
1	B	311	LYS
1	B	326	ASP
1	B	412	ASP
1	B	467	ASP
1	C	166	THR
1	C	191	ASP
1	C	193	VAL
1	C	195	LEU
1	C	209	VAL
1	C	248	ASP
1	C	275	THR
1	C	326	ASP
1	C	364	LYS
1	C	397	GLU
1	C	408	VAL

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Mol	Chain	Res	Type
1	C	467	ASP
1	C	520	ASP
1	C	529	ASN
1	C	545	GLU
1	D	137	PRO
1	D	139	LEU
1	D	143	LEU
1	D	153	LYS
1	D	189	THR
1	D	191	ASP
1	D	193	VAL
1	D	195	LEU
1	D	209	VAL
1	D	263	VAL
1	D	286	SER
1	D	307	ARG
1	D	360	GLN
1	D	361	PHE
1	D	364	LYS
1	D	411	LEU
1	D	484	VAL
1	D	545	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	A	471	GLN
1	A	510	ASN
1	B	213	GLN
1	B	347	GLN
1	B	379	GLN
1	B	516	HIS
1	C	535	HIS
1	D	230	HIS
1	D	298	ASN
1	D	368	ASN
1	D	436	ASN
1	D	510	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	398/598 (66%)	-0.40	8 (2%) 64 43	40, 65, 108, 157	0
1	B	398/598 (66%)	-0.41	10 (2%) 58 36	38, 65, 116, 169	0
1	C	398/598 (66%)	-0.40	5 (1%) 74 54	39, 67, 121, 170	0
1	D	398/598 (66%)	-0.39	8 (2%) 64 43	41, 67, 118, 193	0
All	All	1592/2392 (66%)	-0.40	31 (1%) 66 44	38, 66, 116, 193	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	321	LEU	4.7
1	A	255	LYS	4.7
1	B	255	LYS	4.2
1	D	321	LEU	4.1
1	A	321	LEU	4.1
1	C	325	GLU	3.9
1	D	255	LYS	3.9
1	C	321	LEU	3.8
1	C	256	PHE	3.6
1	D	137	PRO	3.3
1	D	322	PHE	3.2
1	C	137	PRO	3.1
1	B	137	PRO	2.9
1	A	546	GLY	2.8
1	A	137	PRO	2.8
1	B	322	PHE	2.6
1	C	322	PHE	2.6
1	D	314	SER	2.6
1	D	256	PHE	2.5
1	A	256	PHE	2.5
1	D	546	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	348	GLY	2.4
1	B	325	GLU	2.4
1	D	193	VAL	2.4
1	B	188	THR	2.3
1	B	468	PHE	2.2
1	B	256	PHE	2.2
1	A	468	PHE	2.1
1	A	469	SER	2.1
1	B	192	GLY	2.1
1	A	322	PHE	2.1

## 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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.