Full wwPDB X-ray Structure Validation Report (i)

May 4, 2016 – 05:24 PM EDT

PDB ID	:	5I94
Title	:	Crystal structure of human glutaminase C in complex with the inhibitor UPGL-00019
Authors	:	Huang, Q.; Cerione, R.
Deposited on	:	2016-02-19
Resolution	:	2.98 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

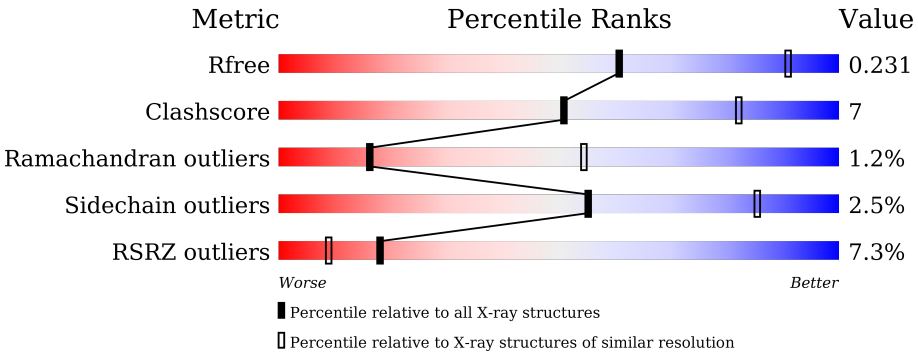
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.98 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}	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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 <=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	539	6% 63% 12% • 24%
1	B	539	4% 60% 15% 24%
1	C	539	7% 62% 12% • 24%
1	D	539	4% 62% 12% • 24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12850 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	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			
1	B	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			
1	C	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			
1	D	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	MET	-	initiating methionine	UNP O94925
A	60	ARG	-	expression tag	UNP O94925
A	61	GLY	-	expression tag	UNP O94925
A	62	SER	-	expression tag	UNP O94925
A	63	HIS	-	expression tag	UNP O94925
A	64	HIS	-	expression tag	UNP O94925
A	65	HIS	-	expression tag	UNP O94925
A	66	HIS	-	expression tag	UNP O94925
A	67	HIS	-	expression tag	UNP O94925
A	68	HIS	-	expression tag	UNP O94925
A	69	GLY	-	expression tag	UNP O94925
A	70	SER	-	expression tag	UNP O94925
A	267	ALA	VAL	conflict	UNP O94925
B	59	MET	-	initiating methionine	UNP O94925
B	60	ARG	-	expression tag	UNP O94925
B	61	GLY	-	expression tag	UNP O94925
B	62	SER	-	expression tag	UNP O94925
B	63	HIS	-	expression tag	UNP O94925
B	64	HIS	-	expression tag	UNP O94925
B	65	HIS	-	expression tag	UNP O94925
B	66	HIS	-	expression tag	UNP O94925

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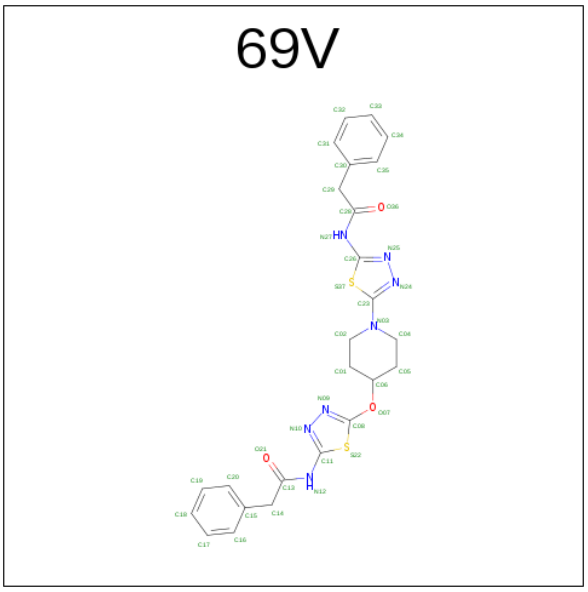
Chain	Residue	Modelled	Actual	Comment	Reference
B	67	HIS	-	expression tag	UNP O94925
B	68	HIS	-	expression tag	UNP O94925
B	69	GLY	-	expression tag	UNP O94925
B	70	SER	-	expression tag	UNP O94925
B	267	ALA	VAL	conflict	UNP O94925
C	59	MET	-	initiating methionine	UNP O94925
C	60	ARG	-	expression tag	UNP O94925
C	61	GLY	-	expression tag	UNP O94925
C	62	SER	-	expression tag	UNP O94925
C	63	HIS	-	expression tag	UNP O94925
C	64	HIS	-	expression tag	UNP O94925
C	65	HIS	-	expression tag	UNP O94925
C	66	HIS	-	expression tag	UNP O94925
C	67	HIS	-	expression tag	UNP O94925
C	68	HIS	-	expression tag	UNP O94925
C	69	GLY	-	expression tag	UNP O94925
C	70	SER	-	expression tag	UNP O94925
C	267	ALA	VAL	conflict	UNP O94925
D	59	MET	-	initiating methionine	UNP O94925
D	60	ARG	-	expression tag	UNP O94925
D	61	GLY	-	expression tag	UNP O94925
D	62	SER	-	expression tag	UNP O94925
D	63	HIS	-	expression tag	UNP O94925
D	64	HIS	-	expression tag	UNP O94925
D	65	HIS	-	expression tag	UNP O94925
D	66	HIS	-	expression tag	UNP O94925
D	67	HIS	-	expression tag	UNP O94925
D	68	HIS	-	expression tag	UNP O94925
D	69	GLY	-	expression tag	UNP O94925
D	70	SER	-	expression tag	UNP O94925
D	267	ALA	VAL	conflict	UNP O94925

- Molecule 2 is 2-phenyl-N-{5-[4-({5-[(phenylacetyl)amino]-1,3,4-thiadiazol-2-yl}oxy)piperidin-1-yl]-1,3,4-thiadiazol-2-yl}acetamide (three-letter code: 69V) (formula: $C_{25}H_{25}N_7O_3S_2$).



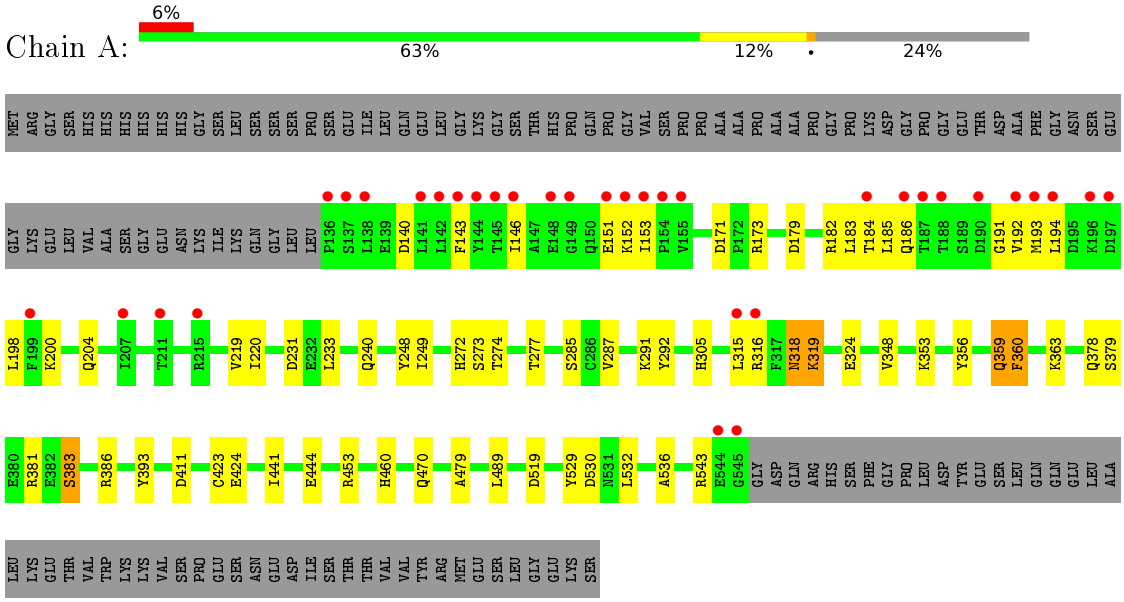
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			37	25	7	3	2		
2	B	1	Total	C	N	O	S	0	0
			37	25	7	3	2		

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.

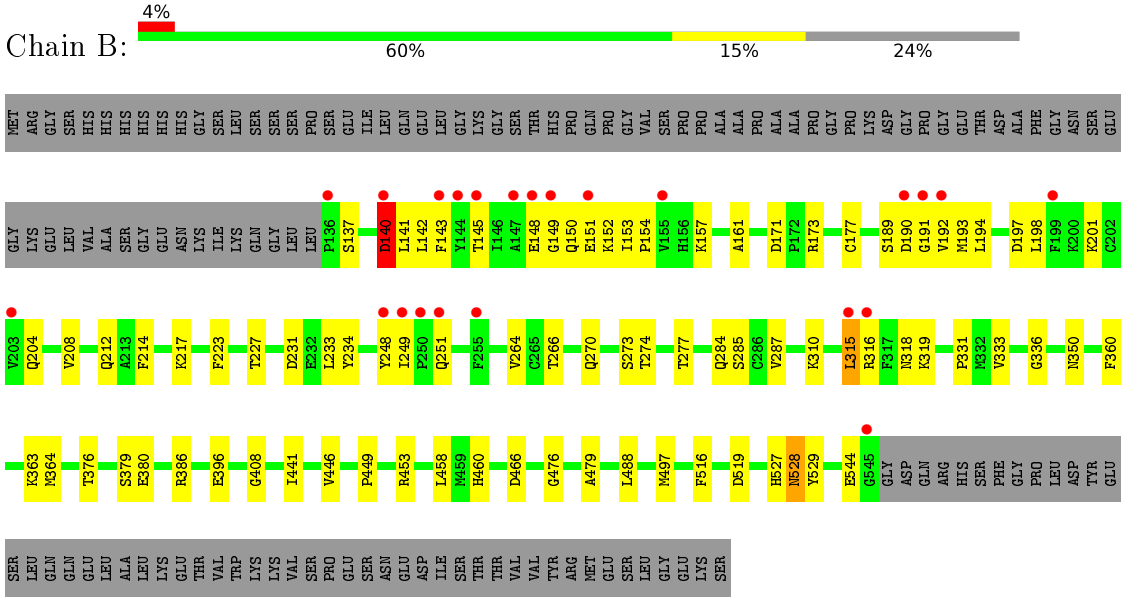
- Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain A:



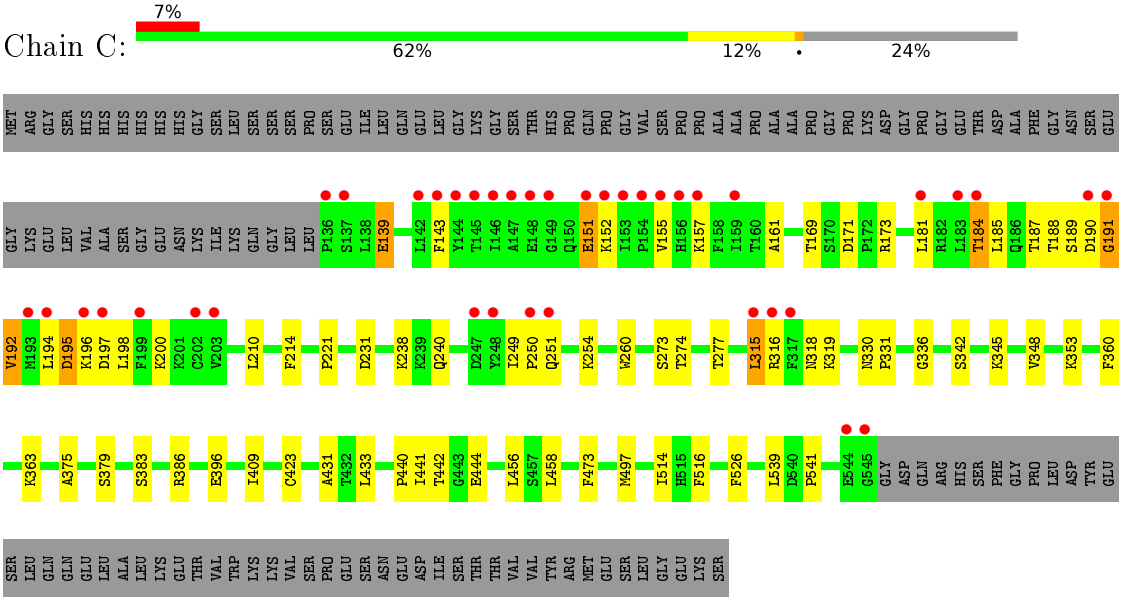
- Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain B:



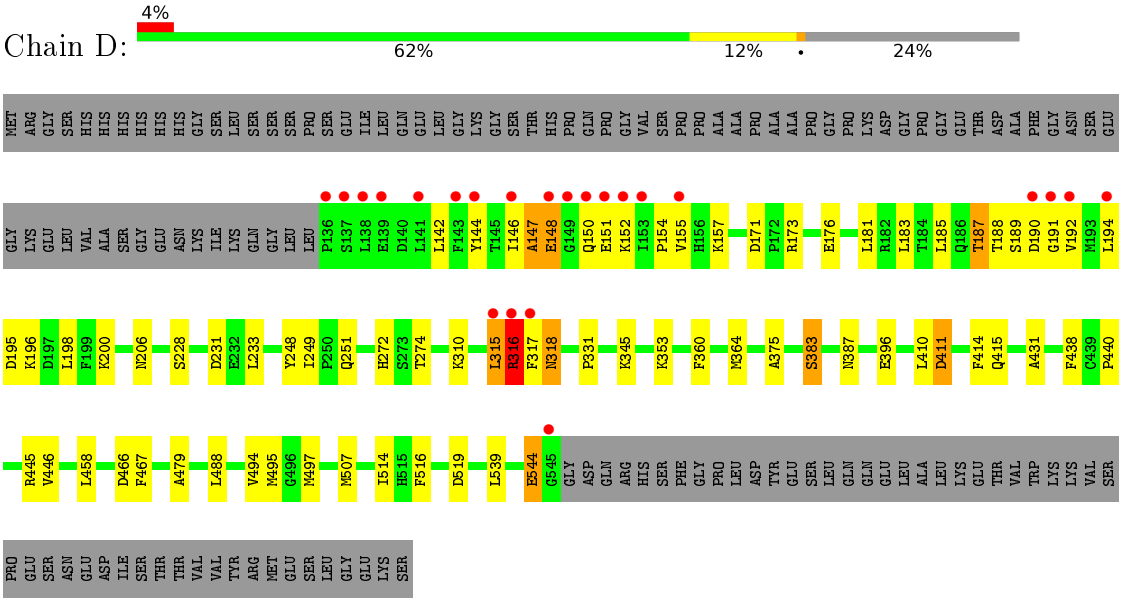
• Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain C:



• Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.44Å 137.79Å 175.75Å 90.00° 94.68° 90.00°	Depositor
Resolution (Å)	46.40 – 2.98 46.40 – 2.98	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.40-2.98) 98.8 (46.40-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.77 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.173 , 0.231 0.176 , 0.231	Depositor DCC
R_{free} test set	2012 reflections (4.26%)	DCC
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12850	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: 69V

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	0.47	0/3266	0.62	0/4408
1	B	0.46	0/3266	0.64	0/4408
1	C	0.47	0/3266	0.63	0/4408
1	D	0.48	0/3266	0.64	3/4408 (0.1%)
All	All	0.47	0/13064	0.63	3/17632 (0.0%)

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	B	0	2
1	C	0	2
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	315	LEU	CA-CB-CG	6.48	130.21	115.30
1	D	316	ARG	CB-CG-CD	5.40	125.63	111.60
1	D	316	ARG	CA-CB-CG	-5.20	101.96	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	140	ASP	Peptide
1	B	189	SER	Peptide
1	C	187	THR	Peptide
1	C	315	LEU	Peptide
1	D	315	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3194	0	3170	44	0
1	B	3194	0	3170	53	0
1	C	3194	0	3170	46	0
1	D	3194	0	3170	43	0
2	A	37	0	0	1	0
2	B	37	0	0	1	0
All	All	12850	0	12680	175	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 7.

All (175) 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:231:ASP:OD1	1:A:274:THR:HG21	1.13	1.27
1:B:231:ASP:OD1	1:B:274:THR:HG21	1.40	1.19
1:C:231:ASP:OD1	1:C:274:THR:HG21	1.49	1.12
1:D:231:ASP:OD1	1:D:274:THR:HG21	1.47	1.12
1:A:231:ASP:OD1	1:A:274:THR:CG2	2.06	1.02
1:B:249:ILE:HD12	1:B:379:SER:HB3	1.56	0.88
1:D:148:GLU:HB3	1:D:150:GLN:HB2	1.62	0.80
1:D:233:LEU:HD22	1:D:519:ASP:HB3	1.65	0.77
1:B:231:ASP:OD1	1:B:274:THR:CG2	2.29	0.76
1:B:273:SER:HB3	1:B:277:THR:HG21	1.67	0.76
1:C:194:LEU:HA	1:C:198:LEU:HD23	1.70	0.74
1:C:251:GLN:HA	1:C:254:LYS:HE3	1.68	0.74
1:B:194:LEU:HA	1:B:198:LEU:HD23	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ILE:HD12	1:A:379:SER:HB3	1.73	0.71
1:C:151:GLU:HG3	1:C:152:LYS:H	1.56	0.70
1:B:233:LEU:HD22	1:B:519:ASP:HB3	1.73	0.69
1:A:532:LEU:O	1:A:543:ARG:NH1	2.27	0.68
1:C:316:ARG:HD3	1:C:319:LYS:NZ	2.08	0.68
1:D:155:VAL:HG21	1:D:185:LEU:HD21	1.78	0.66
1:D:316:ARG:HG2	1:D:318:ASN:OD1	1.95	0.66
1:C:139:GLU:HG3	1:C:200:LYS:HG3	1.78	0.66
1:A:272:HIS:NE2	1:A:274:THR:HG23	2.10	0.65
1:B:140:ASP:HA	1:B:143:PHE:H	1.61	0.65
1:A:233:LEU:HD22	1:A:519:ASP:HB3	1.78	0.64
1:B:318:ASN:ND2	1:B:466:ASP:OD2	2.32	0.63
1:D:231:ASP:OD1	1:D:274:THR:CG2	2.37	0.61
1:D:316:ARG:HD3	1:D:466:ASP:OD2	2.01	0.61
1:D:467:PHE:HB2	1:D:507:MET:HG2	1.82	0.61
1:C:497:MET:HE1	1:C:516:PHE:CE1	2.35	0.60
1:A:272:HIS:NE2	1:A:274:THR:CG2	2.65	0.60
1:D:364:MET:HG2	1:D:446:VAL:HG11	1.84	0.59
1:D:154:PRO:HD2	1:D:157:LYS:HD2	1.84	0.57
1:D:316:ARG:HA	1:D:318:ASN:OD1	2.04	0.57
1:A:316:ARG:NH1	1:A:319:LYS:HD3	2.20	0.56
1:D:438:PHE:CE2	1:D:445:ARG:HB2	2.40	0.56
1:A:179:ASP:OD1	1:A:182:ARG:NH2	2.37	0.56
1:A:470:GLN:OE1	1:B:310:LYS:HE3	2.05	0.56
1:D:171:ASP:OD2	1:D:173:ARG:NH2	2.40	0.55
1:C:155:VAL:HG21	1:C:185:LEU:HD11	1.88	0.55
1:C:173:ARG:HD2	1:C:441:ILE:C	2.27	0.55
1:B:364:MET:HG3	1:B:446:VAL:HG11	1.89	0.54
1:D:147:ALA:O	1:D:148:GLU:HB2	2.07	0.54
1:A:460:HIS:HD1	1:B:529:TYR:HH	1.56	0.54
1:B:248:TYR:CE2	1:B:249:ILE:HG12	2.42	0.54
1:B:386:ARG:HB2	1:C:396:GLU:HG3	1.90	0.54
1:B:331:PRO:HD2	1:B:458:LEU:HD13	1.89	0.53
1:A:287:VAL:HG13	1:A:291:LYS:HE2	1.89	0.53
1:A:356:TYR:O	1:A:359:GLN:HG2	2.10	0.52
1:D:144:TYR:HA	1:D:147:ALA:HB2	1.92	0.52
1:A:248:TYR:CE2	1:A:249:ILE:HG12	2.45	0.51
1:A:378:GLN:O	1:A:381:ARG:HG2	2.10	0.51
1:A:383:SER:OG	1:A:383:SER:O	2.19	0.51
1:B:137:SER:O	1:B:141:LEU:HG	2.11	0.51
1:C:331:PRO:HD2	1:C:458:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ASP:OD1	1:D:173:ARG:HD3	2.11	0.51
1:C:342:SER:HA	1:C:409:ILE:HD12	1.93	0.51
1:B:476:GLY:O	1:B:528:ASN:HB2	2.12	0.50
1:C:195:ASP:HB2	1:C:197:ASP:HB3	1.93	0.50
1:A:363:LYS:HD3	1:A:444:GLU:OE2	2.12	0.50
1:C:189:SER:C	1:C:191:GLY:H	2.14	0.50
1:D:431:ALA:HB1	1:D:440:PRO:HG2	1.92	0.50
1:D:497:MET:HE1	1:D:516:PHE:CE2	2.47	0.50
1:B:316:ARG:O	1:B:316:ARG:HG2	2.12	0.50
1:A:536:ALA:HB2	1:B:449:PRO:HG2	1.93	0.49
1:B:497:MET:HE1	1:B:516:PHE:HE2	1.77	0.49
1:D:411:ASP:O	1:D:415:GLN:HG3	2.13	0.49
1:A:324:GLU:OE2	1:B:316:ARG:HB3	2.12	0.49
1:A:292:TYR:OH	1:A:305:HIS:NE2	2.34	0.49
1:C:345:LYS:HB3	1:C:353:LYS:HG2	1.94	0.49
1:D:387:ASN:HD22	1:D:414:PHE:HE1	1.61	0.49
1:B:273:SER:O	1:B:274:THR:CG2	2.61	0.49
1:A:140:ASP:O	1:A:143:PHE:HB3	2.13	0.49
1:A:393:TYR:OH	2:A:601:69V:S22	2.64	0.49
1:D:233:LEU:CD2	1:D:519:ASP:HB3	2.41	0.48
1:D:194:LEU:HA	1:D:198:LEU:HD23	1.96	0.48
1:A:479:ALA:HB2	1:A:489:LEU:HD12	1.96	0.48
1:D:142:LEU:HD11	1:D:146:ILE:HD11	1.96	0.48
1:B:154:PRO:HD2	1:B:157:LYS:HD2	1.95	0.48
1:C:363:LYS:HD3	1:C:444:GLU:OE2	2.14	0.48
1:D:248:TYR:CD1	1:D:249:ILE:HG23	2.49	0.47
1:D:345:LYS:HB3	1:D:353:LYS:HG2	1.94	0.47
1:B:152:LYS:HB2	1:B:193:MET:HE3	1.97	0.47
1:A:151:GLU:OE1	1:A:151:GLU:N	2.47	0.47
1:B:153:ILE:HG23	1:B:157:LYS:HD3	1.97	0.47
1:C:171:ASP:OD1	1:C:173:ARG:HD3	2.14	0.47
1:B:171:ASP:OD1	1:B:173:ARG:HD3	2.15	0.47
1:A:386:ARG:HB2	1:D:396:GLU:HG3	1.96	0.47
1:C:316:ARG:HD3	1:C:319:LYS:HZ2	1.78	0.46
1:D:191:GLY:HA3	1:D:192:VAL:HA	1.54	0.46
1:A:273:SER:HB3	1:A:277:THR:HG21	1.96	0.46
1:A:200:LYS:O	1:A:204:GLN:HG3	2.15	0.46
1:A:277:THR:O	1:A:424:GLU:HG3	2.15	0.46
1:B:315:LEU:H	1:B:315:LEU:HD12	1.80	0.46
1:B:231:ASP:O	1:B:234:TYR:HB3	2.16	0.46
1:D:152:LYS:HG2	1:D:195:ASP:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ALA:HB1	1:C:214:PHE:HE1	1.81	0.46
1:C:151:GLU:CG	1:C:152:LYS:H	2.26	0.45
1:A:194:LEU:HD23	1:A:198:LEU:HG	1.98	0.45
1:B:148:GLU:HB3	1:B:149:GLY:H	1.49	0.45
1:B:264:VAL:HG22	1:B:497:MET:HG2	1.98	0.45
1:D:544:GLU:N	1:D:544:GLU:OE1	2.48	0.45
1:A:146:ILE:HB	1:A:153:ILE:HD13	1.99	0.45
1:B:497:MET:HE1	1:B:516:PHE:CE2	2.51	0.45
1:D:410:LEU:HD23	1:D:410:LEU:HA	1.74	0.45
1:D:494:VAL:HG12	1:D:495:MET:HG2	1.99	0.45
1:B:284:GLN:O	1:B:287:VAL:HG12	2.17	0.45
1:C:238:LYS:HG3	1:C:260:TRP:HD1	1.81	0.45
1:A:171:ASP:OD1	1:A:173:ARG:HD3	2.17	0.45
1:C:441:ILE:HG13	1:C:442:THR:HG23	1.99	0.45
1:C:497:MET:HE1	1:C:516:PHE:HE1	1.80	0.45
1:B:201:LYS:HA	1:B:204:GLN:NE2	2.32	0.44
1:D:497:MET:HE1	1:D:516:PHE:HE2	1.82	0.44
1:A:152:LYS:HE3	1:A:193:MET:HB3	1.99	0.44
1:A:529:TYR:HH	1:B:460:HIS:HD1	1.62	0.44
1:C:348:VAL:O	1:C:353:LYS:HE3	2.18	0.44
1:B:161:ALA:HB1	1:B:214:PHE:HE1	1.82	0.44
1:C:251:GLN:HE21	1:C:375:ALA:HB1	1.82	0.44
1:C:195:ASP:HB2	1:C:198:LEU:H	1.83	0.44
1:C:315:LEU:HD12	1:C:315:LEU:HA	1.51	0.44
1:B:319:LYS:HB3	2:B:601:69V:N10	2.33	0.44
1:D:331:PRO:HD2	1:D:458:LEU:HD13	1.98	0.44
1:D:187:THR:O	1:D:189:SER:N	2.50	0.44
1:B:142:LEU:O	1:B:145:THR:HB	2.18	0.44
1:C:189:SER:O	1:C:191:GLY:N	2.50	0.44
1:C:473:PHE:CD2	1:D:310:LYS:HD2	2.53	0.44
1:B:191:GLY:HA3	1:B:192:VAL:HA	1.55	0.43
1:A:152:LYS:HB3	1:A:193:MET:HG3	2.00	0.43
1:A:530:ASP:OD1	1:B:453:ARG:HD3	2.18	0.43
1:A:348:VAL:O	1:A:353:LYS:HE3	2.18	0.43
1:B:350:ASN:ND2	1:B:408:GLY:O	2.45	0.43
1:B:396:GLU:HG3	1:C:386:ARG:HB2	1.99	0.43
1:D:272:HIS:NE2	1:D:274:THR:CG2	2.81	0.43
1:C:189:SER:C	1:C:191:GLY:N	2.72	0.43
1:B:363:LYS:HB3	1:B:446:VAL:HG22	2.01	0.43
1:B:479:ALA:HA	1:B:488:LEU:O	2.19	0.43
1:B:249:ILE:HG22	1:B:251:GLN:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:526:PHE:CZ	1:C:541:PRO:HG2	2.54	0.43
1:B:173:ARG:HD2	1:B:441:ILE:C	2.40	0.42
1:C:514:ILE:HA	1:C:514:ILE:HD13	1.89	0.42
1:C:191:GLY:HA3	1:C:192:VAL:HA	1.76	0.42
1:B:376:THR:O	1:B:380:GLU:HB2	2.19	0.42
1:C:157:LYS:HA	1:C:157:LYS:HD2	1.82	0.42
1:C:433:LEU:HB3	1:C:456:LEU:HD21	2.00	0.42
1:A:173:ARG:HD2	1:A:441:ILE:C	2.39	0.42
1:C:277:THR:HA	1:C:423:CYS:HB2	2.01	0.42
1:D:142:LEU:O	1:D:146:ILE:HG13	2.20	0.42
1:D:176:GLU:HG2	1:D:206:ASN:HD21	1.84	0.42
1:A:219:VAL:HG13	1:A:220:ILE:HG13	2.01	0.42
1:B:208:VAL:O	1:B:212:GLN:HG3	2.19	0.42
1:C:184:THR:HG22	1:C:185:LEU:HD23	2.02	0.42
1:A:191:GLY:HA3	1:A:192:VAL:HA	1.50	0.42
1:B:140:ASP:HB2	1:B:143:PHE:HB3	2.01	0.41
1:C:210:LEU:O	1:C:214:PHE:HD2	2.03	0.41
1:D:251:GLN:HE21	1:D:375:ALA:HB1	1.85	0.41
1:D:514:ILE:HA	1:D:514:ILE:HD13	1.80	0.41
1:B:266:THR:CG2	1:B:270:GLN:HB2	2.50	0.41
1:C:143:PHE:CE2	1:C:196:LYS:HB2	2.55	0.41
1:A:152:LYS:HB3	1:A:193:MET:CG	2.50	0.41
1:B:217:LYS:HA	1:B:217:LYS:HD3	1.85	0.41
1:C:273:SER:O	1:C:274:THR:CG2	2.67	0.41
1:B:333:VAL:HG23	1:B:336:GLY:H	1.85	0.41
1:A:184:THR:C	1:A:186:GLN:H	2.23	0.41
1:C:181:LEU:O	1:C:185:LEU:HG	2.20	0.41
1:A:277:THR:HA	1:A:423:CYS:HB2	2.03	0.41
1:B:223:PHE:O	1:B:227:THR:HG23	2.20	0.41
1:D:181:LEU:O	1:D:185:LEU:HG	2.21	0.41
1:B:273:SER:O	1:B:274:THR:HG23	2.22	0.40
1:D:479:ALA:HA	1:D:488:LEU:O	2.21	0.40
1:A:453:ARG:HD2	1:B:527:HIS:CG	2.56	0.40
1:D:183:LEU:HD12	1:D:183:LEU:HA	1.93	0.40
1:A:359:GLN:HG3	1:A:360:PHE:N	2.27	0.40
1:C:249:ILE:HA	1:C:250:PRO:HD2	1.87	0.40
1:C:330:ASN:O	1:C:336:GLY:HA3	2.22	0.40
1:C:249:ILE:HD13	1:C:379:SER:HB3	2.03	0.40
1:C:431:ALA:HB1	1:C:440:PRO:HG2	2.03	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	408/539 (76%)	385 (94%)	20 (5%)	3 (1%)	26	68
1	B	408/539 (76%)	369 (90%)	35 (9%)	4 (1%)	19	60
1	C	408/539 (76%)	373 (91%)	31 (8%)	4 (1%)	19	60
1	D	408/539 (76%)	379 (93%)	20 (5%)	9 (2%)	8	36
All	All	1632/2156 (76%)	1506 (92%)	106 (6%)	20 (1%)	16	54

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	LEU
1	B	190	ASP
1	B	544	GLU
1	C	190	ASP
1	D	147	ALA
1	D	148	GLU
1	D	187	THR
1	B	315	LEU
1	C	151	GLU
1	C	191	GLY
1	D	190	ASP
1	D	383	SER
1	D	196	LYS
1	D	316	ARG
1	D	544	GLU
1	A	185	LEU
1	A	318	ASN
1	B	150	GLN
1	D	188	THR
1	C	221	PRO

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	353/461 (77%)	344 (98%)	9 (2%)	55 85
1	B	353/461 (77%)	346 (98%)	7 (2%)	63 88
1	C	353/461 (77%)	342 (97%)	11 (3%)	47 82
1	D	353/461 (77%)	344 (98%)	9 (2%)	55 85
All	All	1412/1844 (77%)	1376 (98%)	36 (2%)	55 85

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	LEU
1	A	240	GLN
1	A	285	SER
1	A	318	ASN
1	A	319	LYS
1	A	359	GLN
1	A	360	PHE
1	A	383	SER
1	A	411	ASP
1	B	140	ASP
1	B	151	GLU
1	B	177	CYS
1	B	197	ASP
1	B	285	SER
1	B	360	PHE
1	B	528	ASN
1	C	139	GLU
1	C	169	THR
1	C	184	THR
1	C	188	THR
1	C	192	VAL
1	C	195	ASP
1	C	240	GLN
1	C	318	ASN

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Mol	Chain	Res	Type
1	C	360	PHE
1	C	383	SER
1	C	539	LEU
1	D	151	GLU
1	D	200	LYS
1	D	228	SER
1	D	317	PHE
1	D	318	ASN
1	D	360	PHE
1	D	383	SER
1	D	411	ASP
1	D	539	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	69V	A	601	-	33,41,41	1.96	8 (24%)	35,55,55	2.08	8 (22%)
2	69V	B	601	-	33,41,41	1.94	8 (24%)	35,55,55	1.86	5 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	69V	A	601	-	-	0/16/34/34	0/3/5/5
2	69V	B	601	-	-	0/16/34/34	0/3/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	69V	C02-N03	-3.45	1.41	1.46
2	A	601	69V	C04-N03	-3.18	1.42	1.46
2	B	601	69V	C04-N03	-3.17	1.42	1.46
2	A	601	69V	C02-N03	-3.09	1.42	1.46
2	A	601	69V	O07-C08	2.37	1.41	1.36
2	B	601	69V	O07-C08	2.56	1.42	1.36
2	A	601	69V	C28-N27	2.65	1.42	1.35
2	B	601	69V	C28-N27	2.94	1.42	1.35
2	A	601	69V	C13-N12	2.98	1.42	1.35
2	A	601	69V	C26-N27	2.99	1.41	1.36
2	B	601	69V	C13-N12	3.26	1.43	1.35
2	B	601	69V	C26-N27	3.31	1.42	1.36
2	B	601	69V	C11-N12	4.00	1.43	1.36
2	A	601	69V	C11-N12	4.44	1.43	1.36
2	B	601	69V	C23-N03	6.29	1.42	1.32
2	A	601	69V	C23-N03	7.03	1.43	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	69V	C08-O07-C06	-4.06	108.58	118.86
2	B	601	69V	C08-O07-C06	-3.51	109.97	118.86
2	A	601	69V	O21-C13-N12	-3.44	117.74	123.77
2	A	601	69V	C05-C06-C01	-3.26	106.18	111.56
2	B	601	69V	C05-C06-C01	-2.44	107.53	111.56
2	A	601	69V	C29-C28-N27	2.08	120.65	114.69
2	A	601	69V	C15-C14-C13	2.16	119.70	112.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	69V	C04-C05-C06	2.74	113.05	110.23
2	A	601	69V	C04-C05-C06	2.82	113.13	110.23
2	B	601	69V	C14-C13-N12	2.91	123.03	114.69
2	A	601	69V	C02-C01-C06	4.05	114.39	110.23
2	A	601	69V	C04-N03-C02	6.88	125.78	111.54
2	B	601	69V	C04-N03-C02	7.70	127.48	111.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	69V	1	0
2	B	601	69V	1	0

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, 95^{th} 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	410/539 (76%)	0.14	34 (8%) 14 6	19, 29, 78, 100	0
1	B	410/539 (76%)	0.04	23 (5%) 28 14	18, 31, 73, 92	0
1	C	410/539 (76%)	0.14	39 (9%) 10 5	16, 28, 78, 97	0
1	D	410/539 (76%)	0.01	23 (5%) 28 14	17, 30, 74, 95	0
All	All	1640/2156 (76%)	0.08	119 (7%) 18 9	16, 30, 77, 100	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	149	GLY	6.8
1	A	545	GLY	6.5
1	D	136	PRO	5.3
1	A	136	PRO	5.3
1	B	251	GLN	5.3
1	D	190	ASP	5.0
1	D	315	LEU	4.8
1	A	188	THR	4.6
1	A	152	LYS	4.6
1	A	149	GLY	4.6
1	B	316	ARG	4.6
1	A	151	GLU	4.5
1	C	148	GLU	4.4
1	B	250	PRO	4.4
1	C	545	GLY	4.4
1	A	148	GLU	4.3
1	D	316	ARG	4.2
1	C	145	THR	4.2
1	D	148	GLU	4.2
1	C	144	TYR	4.1
1	D	191	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	151	GLU	4.1
1	C	143	PHE	3.9
1	A	144	TYR	3.8
1	C	142	LEU	3.8
1	A	145	THR	3.8
1	C	147	ALA	3.7
1	B	149	GLY	3.7
1	C	251	GLN	3.7
1	C	315	LEU	3.7
1	C	194	LEU	3.7
1	C	184	THR	3.6
1	C	191	GLY	3.6
1	C	149	GLY	3.5
1	C	316	ARG	3.5
1	A	192	VAL	3.5
1	B	545	GLY	3.5
1	A	194	LEU	3.4
1	A	199	PHE	3.4
1	D	152	LYS	3.4
1	A	155	VAL	3.4
1	B	136	PRO	3.4
1	C	152	LYS	3.3
1	C	197	ASP	3.2
1	C	153	ILE	3.2
1	A	315	LEU	3.2
1	B	190	ASP	3.2
1	A	196	LYS	3.2
1	A	141	LEU	3.2
1	A	184	THR	3.2
1	B	199	PHE	3.1
1	B	248	TYR	3.1
1	B	192	VAL	3.0
1	C	196	LYS	3.0
1	C	151	GLU	3.0
1	B	255	PHE	3.0
1	D	144	TYR	3.0
1	C	250	PRO	3.0
1	A	137	SER	3.0
1	B	144	TYR	2.9
1	A	316	ARG	2.9
1	C	136	PRO	2.9
1	A	193	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	315	LEU	2.8
1	D	545	GLY	2.8
1	B	155	VAL	2.8
1	A	187	THR	2.7
1	A	154	PRO	2.7
1	B	140	ASP	2.7
1	A	142	LEU	2.7
1	C	190	ASP	2.7
1	A	544	GLU	2.7
1	D	317	PHE	2.7
1	A	143	PHE	2.6
1	A	153	ILE	2.6
1	C	155	VAL	2.6
1	A	211	THR	2.6
1	D	192	VAL	2.6
1	C	317	PHE	2.5
1	D	143	PHE	2.5
1	C	146	ILE	2.5
1	A	207	ILE	2.5
1	A	197	ASP	2.5
1	C	199	PHE	2.5
1	C	202	CYS	2.5
1	A	138	LEU	2.5
1	B	147	ALA	2.4
1	D	138	LEU	2.4
1	B	191	GLY	2.3
1	D	194	LEU	2.3
1	B	143	PHE	2.3
1	D	141	LEU	2.3
1	C	183	LEU	2.3
1	C	157	LYS	2.3
1	B	203	VAL	2.2
1	C	203	VAL	2.2
1	A	190	ASP	2.2
1	A	146	ILE	2.2
1	C	544	GLU	2.2
1	D	153	ILE	2.2
1	B	145	THR	2.2
1	D	146	ILE	2.2
1	D	150	GLN	2.2
1	C	247	ASP	2.2
1	C	154	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	151	GLU	2.2
1	A	215	ARG	2.1
1	B	148	GLU	2.1
1	D	155	VAL	2.1
1	C	137	SER	2.1
1	C	156	HIS	2.1
1	C	181	LEU	2.1
1	D	137	SER	2.1
1	B	249	ILE	2.1
1	D	139	GLU	2.1
1	C	159	ILE	2.0
1	A	186	GLN	2.0
1	C	193	MET	2.0
1	C	248	TYR	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, 95^{th} 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
2	69V	A	601	37/37	0.92	0.28	0.07	45,65,81,85	0
2	69V	B	601	37/37	0.92	0.27	-0.09	50,63,81,82	0

6.5 Other polymers (i)

There are no such residues in this entry.