Full wwPDB X-ray Structure Validation Report (i)

May 4, 2016 – 05:22 PM EDT

PDB ID	:	5FI6
Title	:	Crystal structure of human GAC in complex with inhibitor UPGL_00011: 2-phenyl- {N}-[5-[[(3 {S})-1-[5-(2-phenylethanoylamino)-1,3,4-thiadiazol-2-yl]pyrrolidin-3-yl]amino]-1,3,4-thiadiazol-2-yl]ethanamide
Authors	:	Huang, Q.; Cerione, R.
Deposited on	:	2015-12-22
Resolution	:	2.52 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:

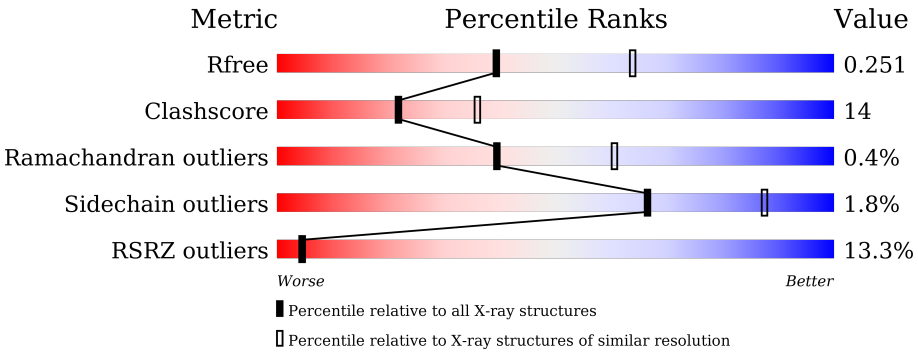
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.52 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	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (2.54-2.50)

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 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	10% 56% 18% · 24%
1	B	539	9% 55% 20% · 24%
1	C	539	10% 58% 17% · 24%
1	D	539	12% 57% 17% · 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13115 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 48 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
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
B	67	HIS	-	expression tag	UNP O94925

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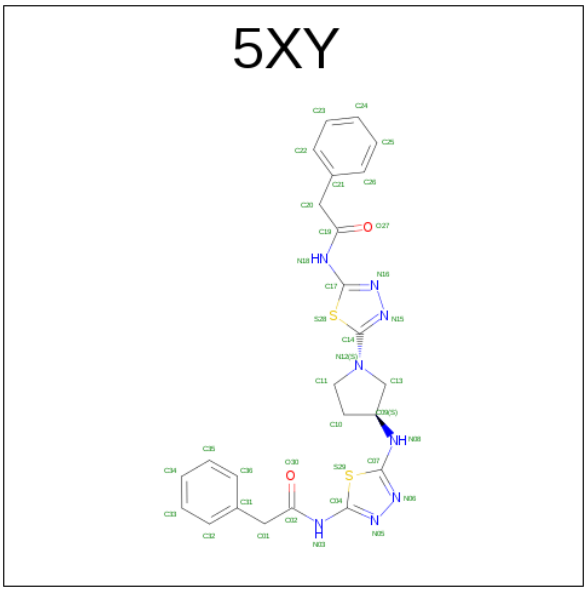
Chain	Residue	Modelled	Actual	Comment	Reference
B	68	HIS	-	expression tag	UNP O94925
B	69	GLY	-	expression tag	UNP O94925
B	70	SER	-	expression tag	UNP O94925
C	59	MET	-	initiating methionine	UNP O94925
C	60	ARG	-	expression tag	UNP O94925
C	61	GLY	-	expression tag	UNP O94925
C	62	SER	-	expression tag	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
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

- Molecule 2 is 2-phenyl- {N}-[5-[[(3 {S})-1-[5-(2-phenylethanoylamino)-1,3,4-thiadiazol-2-yl]pyrrolidin-3-yl]amino]-1,3,4-thiadiazol-2-yl]ethanamide (three-letter code: 5XY) (formula: $C_{24}H_{24}N_8O_2S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			36	24	8	2	2		
2	C	1	Total	C	N	O	S	0	0
			36	24	8	2	2		

- Molecule 3 is water.

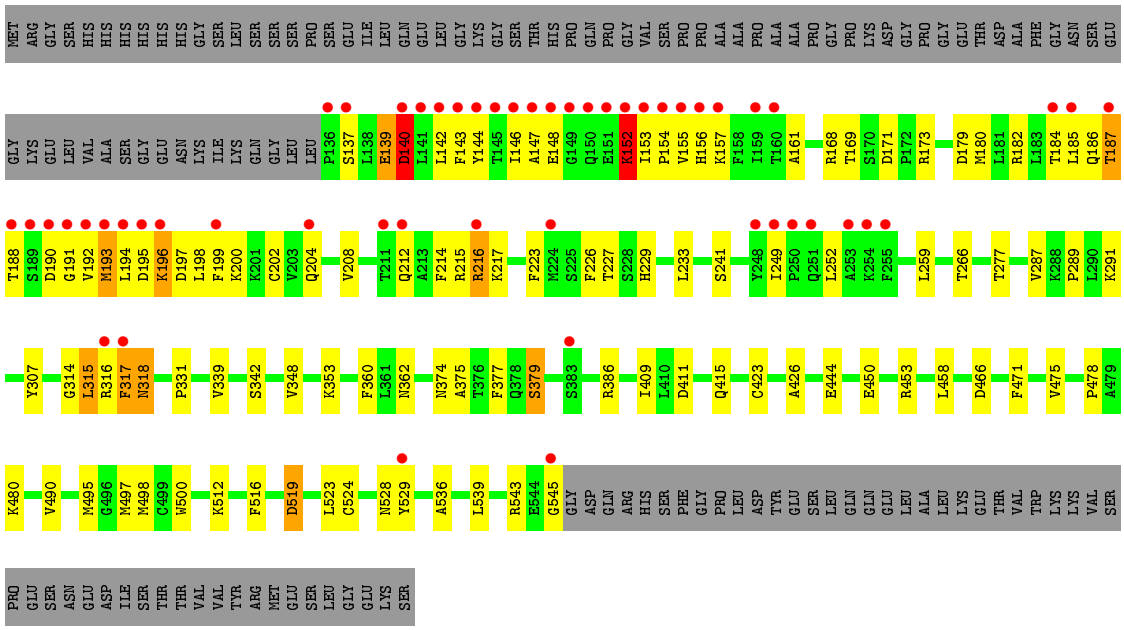
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total	O	0	0
			75	75		
3	B	56	Total	O	0	0
			56	56		
3	C	77	Total	O	0	0
			77	77		
3	D	59	Total	O	0	0
			59	59		

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.

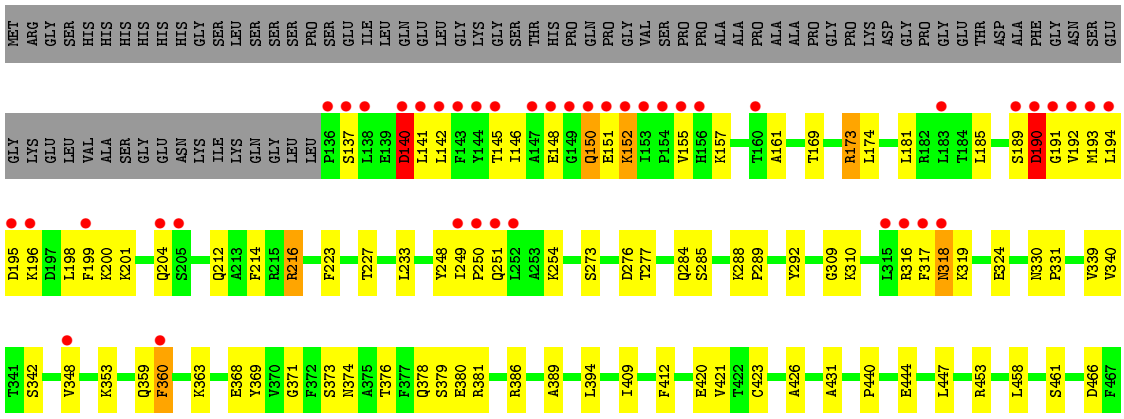
- Molecule 1: Glutaminase kidney isoform, mitochondrial

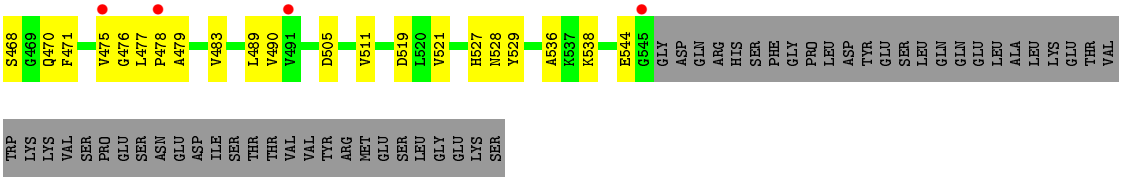
Chain A:



- Molecule 1: Glutaminase kidney isoform, mitochondrial

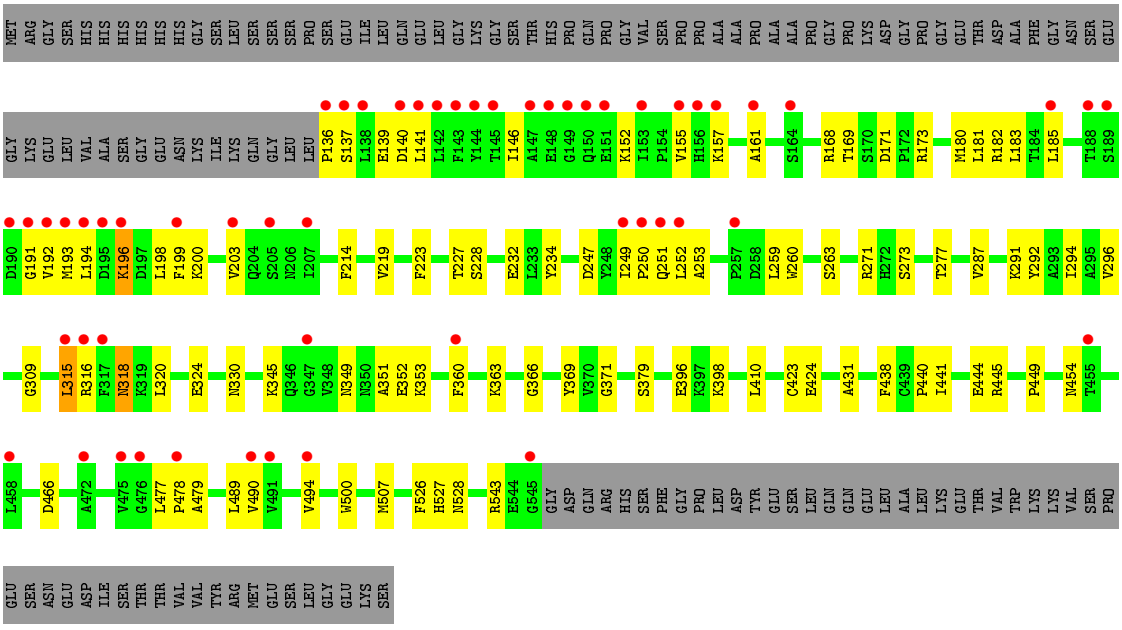
Chain B:





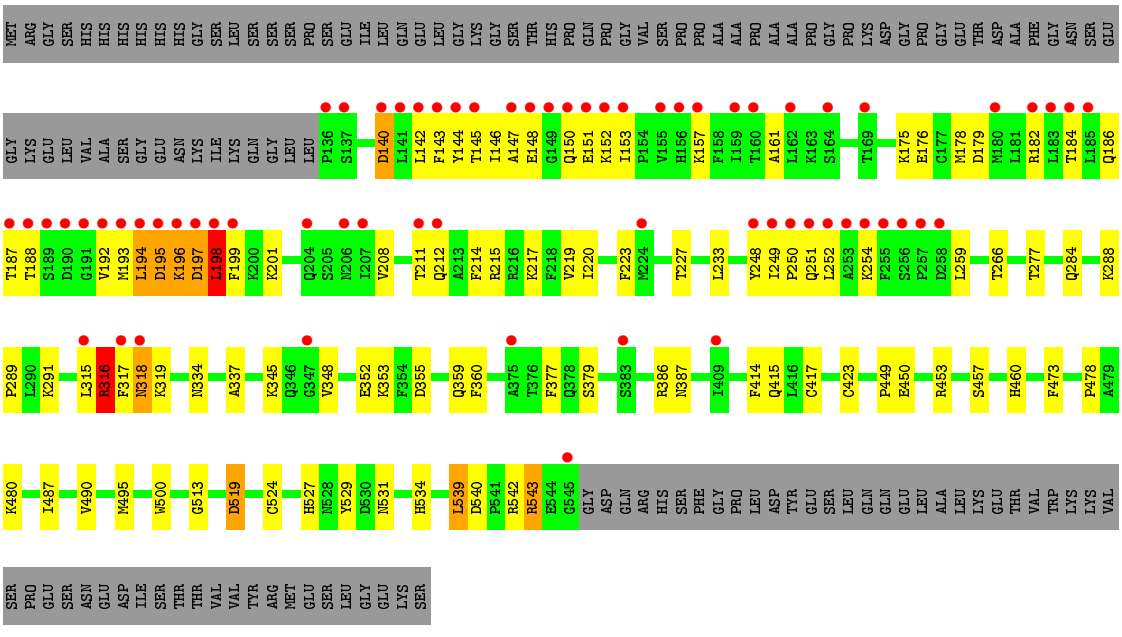
• Molecule 1: Glutaminase kidney isoform, mitochondrial

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	50.69Å 139.03Å 176.78Å 90.00° 95.56° 90.00°	Depositor
Resolution (Å)	47.30 – 2.52 47.43 – 2.52	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.30-2.52) 97.4 (47.43-2.52)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.209 , 0.253 0.206 , 0.251	Depositor DCC
R_{free} test set	1990 reflections (2.48%)	DCC
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13115	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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: 5XY

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	0.51	3/3266 (0.1%)	0.69	4/4408 (0.1%)
1	B	0.50	3/3266 (0.1%)	0.65	3/4408 (0.1%)
1	C	0.47	0/3266	0.62	1/4408 (0.0%)
1	D	0.57	6/3266 (0.2%)	0.65	4/4408 (0.1%)
All	All	0.51	12/13064 (0.1%)	0.65	12/17632 (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	A	0	1
1	C	0	2
1	D	0	1
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	316	ARG	CZ-NH1	-8.69	1.21	1.33
1	D	316	ARG	NE-CZ	-8.68	1.21	1.33
1	B	196	LYS	CD-CE	-7.38	1.32	1.51
1	D	316	ARG	CZ-NH2	-7.04	1.23	1.33
1	A	196	LYS	CD-CE	-6.71	1.34	1.51
1	D	176	GLU	CD-OE1	-6.16	1.18	1.25
1	D	176	GLU	CD-OE2	-6.13	1.19	1.25
1	B	196	LYS	CE-NZ	-5.62	1.35	1.49
1	D	316	ARG	CD-NE	-5.60	1.36	1.46
1	A	196	LYS	CB-CG	-5.29	1.38	1.52
1	B	190	ASP	CB-CG	-5.11	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	386	ARG	NE-CZ	5.09	1.39	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	140	ASP	CB-CG-OD1	9.44	126.80	118.30
1	A	193	MET	CG-SD-CE	7.77	112.63	100.20
1	A	193	MET	CB-CG-SD	7.55	135.05	112.40
1	C	196	LYS	CD-CE-NZ	-6.72	96.25	111.70
1	B	140	ASP	CB-CG-OD1	6.09	123.78	118.30
1	D	194	LEU	CA-CB-CG	5.90	128.88	115.30
1	D	539	LEU	CA-CB-CG	5.63	128.26	115.30
1	B	190	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	B	173	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	152	LYS	CB-CG-CD	-5.38	97.61	111.60
1	D	195	ASP	CB-CG-OD1	5.25	123.03	118.30
1	D	198	LEU	CB-CG-CD1	5.19	119.83	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	PHE	Peptide
1	C	315	LEU	Peptide
1	C	316	ARG	Peptide
1	D	140	ASP	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	3167	104	0
1	B	3194	0	3167	90	0
1	C	3194	0	3167	82	0
1	D	3194	0	3167	97	0
2	A	36	0	0	2	0
2	C	36	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	75	0	0	9	0
3	B	56	0	0	5	0
3	C	77	0	0	5	0
3	D	59	0	0	4	0
All	All	13115	0	12668	356	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 14.

All (356) 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:152:LYS:NZ	1:A:193:MET:HB3	1.52	1.24
1:C:249:ILE:CG2	1:C:252:LEU:HD12	1.71	1.19
1:A:152:LYS:NZ	1:A:193:MET:CB	2.14	1.10
1:D:195:ASP:H	1:D:198:LEU:HD21	1.16	1.09
1:A:152:LYS:HZ3	1:A:193:MET:CB	1.65	1.08
1:C:249:ILE:HG22	1:C:252:LEU:HD12	1.36	1.03
1:A:152:LYS:HZ1	1:A:193:MET:CG	1.72	1.03
1:C:249:ILE:HD11	1:C:379:SER:HB2	1.38	1.01
1:C:249:ILE:HD11	1:C:379:SER:CB	1.92	1.00
1:A:152:LYS:HZ3	1:A:193:MET:HB3	1.14	0.96
1:B:544:GLU:O	3:B:601:HOH:O	1.82	0.96
1:A:152:LYS:CE	1:A:193:MET:HB3	1.97	0.94
1:D:195:ASP:H	1:D:198:LEU:CD2	1.82	0.92
1:C:249:ILE:HG21	1:C:252:LEU:HD12	1.52	0.90
1:B:185:LEU:HD22	1:B:192:VAL:HG11	1.57	0.87
1:D:233:LEU:HD22	1:D:519:ASP:HB3	1.57	0.86
1:B:444:GLU:OE1	3:B:602:HOH:O	1.91	0.86
1:B:152:LYS:HE2	1:B:193:MET:SD	2.16	0.85
1:A:152:LYS:NZ	1:A:193:MET:CG	2.40	0.84
1:B:276:ASP:O	3:B:603:HOH:O	1.95	0.84
1:B:470:GLN:HG2	3:D:608:HOH:O	1.78	0.83
1:D:386:ARG:NH2	1:D:387:ASN:OD1	2.11	0.82
1:D:152:LYS:HZ3	1:D:193:MET:HB2	1.45	0.81
1:A:185:LEU:HD23	1:A:192:VAL:HG23	1.65	0.79
1:A:362:ASN:OD1	3:A:701:HOH:O	2.00	0.78
1:D:195:ASP:N	1:D:198:LEU:HD21	1.95	0.78
1:A:197:ASP:OD2	3:A:702:HOH:O	2.01	0.77
1:D:143:PHE:CE2	1:D:153:ILE:HG13	2.20	0.76
1:B:146:ILE:O	1:B:157:LYS:NZ	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ILE:CD1	1:C:379:SER:HB2	2.16	0.75
1:B:216:ARG:NH2	1:B:544:GLU:OE2	2.18	0.75
1:A:233:LEU:HD22	1:A:519:ASP:HB3	1.69	0.74
1:C:351:ALA:O	3:C:701:HOH:O	2.05	0.74
1:A:450:GLU:OE1	3:A:703:HOH:O	2.05	0.73
1:C:140:ASP:HA	1:C:196:LYS:HZ1	1.54	0.72
1:A:249:ILE:HD11	1:A:379:SER:OG	1.91	0.70
1:A:444:GLU:OE1	3:A:704:HOH:O	2.07	0.70
1:C:139:GLU:HG3	1:C:200:LYS:HD2	1.74	0.69
1:D:186:GLN:O	3:D:602:HOH:O	2.10	0.69
1:C:140:ASP:HA	1:C:196:LYS:NZ	2.07	0.69
1:D:179:ASP:OD1	1:D:182:ARG:NH1	2.20	0.68
1:B:233:LEU:HD22	1:B:519:ASP:HB3	1.75	0.68
1:A:185:LEU:CD2	1:A:192:VAL:HG23	2.24	0.68
1:B:324:GLU:OE2	1:D:316:ARG:HB2	1.93	0.67
1:C:249:ILE:HG23	1:C:251:GLN:H	1.60	0.67
1:A:152:LYS:HZ3	1:A:193:MET:CA	2.07	0.66
1:C:161:ALA:HB1	1:C:214:PHE:HE1	1.61	0.66
1:B:368:GLU:OE1	3:B:604:HOH:O	2.13	0.66
1:D:143:PHE:O	1:D:153:ILE:HD11	1.96	0.65
1:D:540:ASP:O	1:D:543:ARG:HG3	1.96	0.65
1:A:152:LYS:HD2	1:A:153:ILE:N	2.12	0.65
1:A:188:THR:HG23	1:A:190:ASP:OD1	1.97	0.64
1:B:161:ALA:HB1	1:B:214:PHE:HE1	1.63	0.64
1:B:317:PHE:HE2	1:D:317:PHE:CD1	2.15	0.64
1:A:466:ASP:O	3:A:705:HOH:O	2.15	0.64
1:D:143:PHE:HB2	1:D:199:PHE:CD2	2.33	0.63
1:A:152:LYS:HB2	1:A:194:LEU:O	1.99	0.62
1:A:179:ASP:OD1	1:A:182:ARG:NH1	2.32	0.62
1:A:185:LEU:HD23	1:A:192:VAL:CG2	2.28	0.62
1:A:184:THR:O	1:A:187:THR:OG1	2.18	0.62
1:C:171:ASP:OD1	1:C:173:ARG:HD3	2.00	0.62
1:D:143:PHE:CD2	1:D:153:ILE:HD12	2.34	0.62
1:A:142:LEU:HD22	1:A:199:PHE:HZ	1.65	0.61
1:A:543:ARG:NH1	1:A:545:GLY:O	2.32	0.61
1:D:152:LYS:HZ3	1:D:193:MET:C	2.03	0.61
1:C:182:ARG:NH1	3:C:705:HOH:O	2.31	0.61
1:C:345:LYS:HB3	1:C:353:LYS:HG2	1.83	0.61
1:D:249:ILE:HB	1:D:252:LEU:HD12	1.83	0.60
1:B:479:ALA:HB2	1:B:489:LEU:HD12	1.84	0.60
1:B:316:ARG:HH22	1:B:319:LYS:HD3	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:LYS:NZ	1:D:193:MET:C	2.54	0.60
1:A:314:GLY:O	1:A:316:ARG:N	2.33	0.60
1:B:378:GLN:O	1:B:381:ARG:HG2	2.01	0.60
1:A:140:ASP:OD1	1:A:196:LYS:HE3	2.00	0.60
1:C:181:LEU:O	1:C:185:LEU:HG	2.02	0.60
1:C:277:THR:O	1:C:424:GLU:HG3	2.02	0.60
1:B:137:SER:OG	1:B:140:ASP:OD2	2.20	0.59
1:B:181:LEU:O	1:B:185:LEU:HG	2.01	0.59
1:B:374:ASN:N	3:B:606:HOH:O	2.35	0.59
1:C:137:SER:O	1:C:140:ASP:HB2	2.01	0.59
1:A:249:ILE:HG22	1:A:252:LEU:HB2	1.85	0.59
1:B:195:ASP:OD2	1:B:198:LEU:N	2.28	0.59
1:D:542:ARG:NH1	3:D:601:HOH:O	2.03	0.58
1:B:251:GLN:OE1	1:B:376:THR:HA	2.04	0.58
1:C:168:ARG:NH2	1:C:424:GLU:OE2	2.30	0.58
1:B:317:PHE:HE2	1:D:317:PHE:CG	2.21	0.58
1:D:377:PHE:CE1	1:D:415:GLN:HG3	2.37	0.58
1:C:155:VAL:HG21	1:C:185:LEU:HD21	1.85	0.58
1:A:316:ARG:HH22	2:A:601:5XY:C35	2.17	0.58
1:C:320:LEU:HD23	2:C:601:5XY:C17	2.32	0.58
1:D:387:ASN:HD22	1:D:414:PHE:HE1	1.52	0.58
1:B:141:LEU:O	1:B:145:THR:HG23	2.04	0.58
1:C:271:ARG:NH2	3:C:706:HOH:O	2.32	0.58
1:B:277:THR:HA	1:B:423:CYS:HB2	1.86	0.58
1:B:360:PHE:CE1	1:B:447:LEU:HD21	2.39	0.57
1:C:194:LEU:HD23	1:C:198:LEU:HD23	1.85	0.57
1:C:249:ILE:CG2	1:C:252:LEU:H	2.17	0.57
1:D:188:THR:HG22	1:D:192:VAL:HG12	1.85	0.57
1:A:374:ASN:OD1	3:A:706:HOH:O	2.17	0.57
1:C:152:LYS:HB2	1:C:193:MET:HE1	1.86	0.57
1:B:198:LEU:HD12	1:B:201:LYS:HD3	1.85	0.57
1:C:180:MET:HE3	1:C:183:LEU:HD23	1.87	0.57
1:A:137:SER:OG	1:A:140:ASP:OD2	2.18	0.57
1:A:152:LYS:HZ1	1:A:193:MET:CE	2.18	0.57
1:C:146:ILE:O	1:C:157:LYS:NZ	2.37	0.57
1:D:143:PHE:CD2	1:D:153:ILE:CD1	2.88	0.56
1:D:178:MET:O	1:D:182:ARG:HG3	2.04	0.56
1:D:140:ASP:OD1	1:D:143:PHE:HD1	1.88	0.56
1:A:215:ARG:O	1:A:216:ARG:HB2	2.05	0.56
1:A:528:ASN:HD21	1:C:528:ASN:ND2	2.04	0.56
1:D:318:ASN:N	1:D:318:ASN:OD1	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:TYR:HA	1:A:147:ALA:HB3	1.86	0.56
1:C:223:PHE:O	1:C:227:THR:HG23	2.06	0.56
1:B:273:SER:HB3	1:B:277:THR:HG21	1.87	0.56
1:D:140:ASP:OD2	1:D:144:TYR:N	2.39	0.56
1:B:527:HIS:CD2	1:D:453:ARG:HD2	2.40	0.56
1:C:431:ALA:HB1	1:C:440:PRO:HG2	1.88	0.56
1:D:147:ALA:HB1	1:D:150:GLN:O	2.05	0.56
1:D:161:ALA:HB1	1:D:214:PHE:HE1	1.70	0.56
1:C:249:ILE:HG21	1:C:252:LEU:CD1	2.32	0.55
1:A:536:ALA:HB2	1:C:449:PRO:HG2	1.87	0.55
1:D:184:THR:O	1:D:187:THR:HG22	2.07	0.55
1:D:152:LYS:HZ3	1:D:193:MET:CB	2.15	0.55
1:D:142:LEU:O	1:D:145:THR:HB	2.07	0.55
1:D:143:PHE:HB2	1:D:199:PHE:CE2	2.42	0.55
1:B:318:ASN:ND2	1:B:466:ASP:OD1	2.39	0.55
1:B:536:ALA:HB2	1:D:449:PRO:HG2	1.87	0.55
1:C:249:ILE:HG22	1:C:252:LEU:CD1	2.24	0.54
1:D:194:LEU:HD23	1:D:198:LEU:HG	1.89	0.54
1:A:226:PHE:CE2	1:A:495:MET:HE1	2.42	0.54
1:A:478:PRO:HD2	1:A:490:VAL:O	2.07	0.54
1:A:249:ILE:CD1	1:A:379:SER:OG	2.55	0.54
1:C:478:PRO:HD2	1:C:490:VAL:O	2.08	0.54
1:D:348:VAL:O	1:D:353:LYS:HE3	2.07	0.54
1:A:266:THR:HA	1:A:495:MET:HA	1.89	0.54
1:A:154:PRO:HB2	1:A:156:HIS:CD2	2.43	0.53
1:B:248:TYR:OH	1:B:380:GLU:OE2	2.23	0.53
1:C:318:ASN:N	1:C:318:ASN:OD1	2.40	0.53
1:A:194:LEU:HD23	1:A:198:LEU:HG	1.90	0.53
1:A:524:CYS:HA	1:A:539:LEU:O	2.09	0.53
1:A:226:PHE:HE2	1:A:495:MET:HE1	1.74	0.53
1:D:146:ILE:O	1:D:157:LYS:NZ	2.42	0.53
1:D:249:ILE:HD12	1:D:379:SER:HB3	1.90	0.53
1:B:155:VAL:HG21	1:B:185:LEU:HD21	1.88	0.53
1:B:331:PRO:HD2	1:B:458:LEU:HD13	1.90	0.53
1:A:289:PRO:HD3	1:A:480:LYS:HG2	1.90	0.53
1:D:249:ILE:HD12	1:D:379:SER:CB	2.39	0.53
1:A:377:PHE:CE1	1:A:415:GLN:HG3	2.44	0.53
1:D:195:ASP:OD1	1:D:198:LEU:HD22	2.09	0.53
1:A:152:LYS:CD	1:A:193:MET:HB3	2.39	0.52
1:B:150:GLN:HG3	1:B:151:GLU:H	1.74	0.52
1:B:431:ALA:HB1	1:B:440:PRO:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ARG:O	1:B:174:LEU:HD23	2.09	0.52
1:D:194:LEU:HD22	1:D:199:PHE:HA	1.90	0.52
1:A:148:GLU:CD	1:A:157:LYS:HZ1	2.13	0.52
1:A:453:ARG:HD2	1:C:527:HIS:CG	2.45	0.52
1:B:316:ARG:C	1:B:317:PHE:HD1	2.12	0.52
1:C:444:GLU:OE1	3:C:702:HOH:O	2.19	0.52
1:D:211:THR:O	1:D:215:ARG:HB2	2.10	0.52
1:D:266:THR:HA	1:D:495:MET:HA	1.92	0.52
1:B:194:LEU:HD23	1:B:198:LEU:HG	1.92	0.52
1:B:250:PRO:O	1:B:254:LYS:HD3	2.10	0.51
1:C:249:ILE:CD1	1:C:379:SER:CB	2.77	0.51
1:B:527:HIS:CG	1:D:453:ARG:HD2	2.45	0.51
1:D:142:LEU:HA	1:D:215:ARG:HH12	1.75	0.51
1:A:171:ASP:OD1	1:A:173:ARG:HD3	2.10	0.51
1:A:529:TYR:CE1	1:C:478:PRO:HG3	2.46	0.51
1:B:140:ASP:OD2	1:B:140:ASP:N	2.41	0.51
1:D:140:ASP:HA	1:D:143:PHE:H	1.75	0.51
1:B:373:SER:OG	1:B:376:THR:HG23	2.11	0.51
1:D:195:ASP:OD1	1:D:198:LEU:CD2	2.59	0.51
1:C:315:LEU:HD23	1:C:315:LEU:O	2.10	0.50
1:C:249:ILE:HD11	1:C:379:SER:C	2.32	0.50
1:A:152:LYS:HZ1	1:A:193:MET:CB	1.99	0.50
1:B:190:ASP:N	1:B:190:ASP:OD2	2.41	0.50
1:D:198:LEU:HD23	1:D:199:PHE:N	2.26	0.50
1:A:249:ILE:CG1	1:A:379:SER:OG	2.59	0.50
1:A:229:HIS:ND1	1:A:523:LEU:HD21	2.27	0.50
1:D:348:VAL:HG12	1:D:352:GLU:HB2	1.93	0.50
1:A:152:LYS:HD2	1:A:152:LYS:C	2.32	0.50
1:B:453:ARG:HD2	1:D:527:HIS:CG	2.47	0.50
1:B:521:VAL:O	1:B:538:LYS:NZ	2.25	0.50
1:C:294:ILE:HG12	1:C:360:PHE:HD2	1.77	0.50
1:D:144:TYR:HA	1:D:147:ALA:HB3	1.94	0.50
1:D:288:LYS:HE3	1:D:337:ALA:HB2	1.94	0.50
1:D:140:ASP:CG	1:D:143:PHE:HB3	2.32	0.49
1:A:142:LEU:HD23	1:A:146:ILE:HG13	1.95	0.49
1:D:144:TYR:OH	1:D:196:LYS:HD3	2.12	0.49
1:D:277:THR:HA	1:D:423:CYS:HB2	1.93	0.49
1:B:200:LYS:HE2	1:B:204:GLN:HB2	1.93	0.49
1:B:145:THR:O	1:B:148:GLU:HG3	2.13	0.49
1:D:198:LEU:HD23	1:D:199:PHE:H	1.78	0.49
1:A:342:SER:HA	1:A:409:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:LYS:HB3	1:D:353:LYS:HG2	1.95	0.49
1:B:150:GLN:NE2	1:B:152:LYS:NZ	2.60	0.49
1:D:251:GLN:HA	1:D:254:LYS:HE3	1.93	0.49
1:B:142:LEU:HD23	1:B:199:PHE:HZ	1.78	0.48
1:C:287:VAL:O	1:C:291:LYS:HG2	2.13	0.48
1:D:531:ASN:HB3	1:D:534:HIS:O	2.12	0.48
1:C:466:ASP:HB2	1:C:507:MET:HE2	1.96	0.48
1:A:377:PHE:HZ	1:A:411:ASP:OD1	1.97	0.48
1:A:426:ALA:HB3	1:A:498:MET:HG2	1.96	0.48
1:C:349:ASN:OD1	1:C:352:GLU:HG3	2.14	0.48
1:D:151:GLU:HA	1:D:151:GLU:OE1	2.14	0.48
2:A:601:5XY:O27	1:B:319:LYS:HE3	2.14	0.48
1:D:259:LEU:HD13	1:D:500:TRP:CH2	2.49	0.48
1:B:309:GLY:O	1:B:330:ASN:HA	2.13	0.48
1:A:453:ARG:HD2	1:C:527:HIS:CD2	2.49	0.48
1:D:223:PHE:O	1:D:227:THR:HG23	2.14	0.48
1:B:353:LYS:HB3	1:B:412:PHE:CE2	2.49	0.48
1:B:189:SER:O	1:B:191:GLY:N	2.46	0.47
1:B:478:PRO:HG3	1:D:529:TYR:CE1	2.48	0.47
1:C:277:THR:HA	1:C:423:CYS:HB2	1.96	0.47
1:D:188:THR:CG2	1:D:192:VAL:HG12	2.44	0.47
1:A:316:ARG:HD3	2:C:601:5XY:C24	2.44	0.47
1:B:316:ARG:NH2	1:B:319:LYS:HD3	2.29	0.47
1:B:359:GLN:O	1:B:363:LYS:HG3	2.15	0.47
1:A:143:PHE:HZ	1:A:152:LYS:HA	1.79	0.47
1:A:215:ARG:HB3	1:A:217:LYS:HE3	1.96	0.47
1:C:259:LEU:HD13	1:C:500:TRP:CH2	2.50	0.47
1:B:223:PHE:O	1:B:227:THR:HG23	2.14	0.47
1:B:310:LYS:HD2	1:D:473:PHE:CD2	2.50	0.47
1:A:331:PRO:CD	1:A:458:LEU:HD13	2.45	0.47
1:D:259:LEU:HD13	1:D:500:TRP:HH2	1.80	0.47
1:B:152:LYS:HG2	1:B:193:MET:HG2	1.96	0.46
1:B:317:PHE:N	1:B:317:PHE:CD1	2.83	0.46
1:D:145:THR:OG1	1:D:215:ARG:NH2	2.49	0.46
1:C:292:TYR:OH	1:C:454:ASN:HB3	2.15	0.46
1:D:248:TYR:CE2	1:D:249:ILE:HG12	2.49	0.46
1:B:363:LYS:HD3	1:B:444:GLU:OE2	2.14	0.46
1:A:161:ALA:HB1	1:A:214:PHE:HE1	1.79	0.46
1:C:431:ALA:CB	1:C:440:PRO:HG2	2.45	0.46
1:D:208:VAL:O	1:D:212:GLN:HG3	2.15	0.46
1:D:284:GLN:OE1	1:D:417:CYS:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLY:C	1:A:316:ARG:H	2.19	0.46
1:C:137:SER:O	1:C:141:LEU:HG	2.15	0.46
1:A:152:LYS:NZ	1:A:193:MET:CE	2.79	0.46
1:A:223:PHE:O	1:A:227:THR:HG23	2.16	0.46
1:A:512:LYS:HG3	3:A:744:HOH:O	2.16	0.46
1:B:142:LEU:HD23	1:B:199:PHE:CZ	2.50	0.46
1:D:143:PHE:O	1:D:147:ALA:N	2.49	0.46
1:A:152:LYS:HD3	1:A:193:MET:HB3	1.98	0.46
1:B:284:GLN:HG3	1:B:483:VAL:HG12	1.98	0.46
1:C:194:LEU:HA	1:C:198:LEU:HD23	1.98	0.46
1:C:249:ILE:HD11	1:C:379:SER:HB3	1.90	0.46
1:A:316:ARG:HG3	1:C:324:GLU:CD	2.37	0.45
1:A:277:THR:HA	1:A:423:CYS:HB2	1.97	0.45
1:C:260:TRP:HE3	1:C:500:TRP:O	1.99	0.45
1:C:479:ALA:HB2	1:C:489:LEU:HD12	1.98	0.45
1:D:195:ASP:O	1:D:197:ASP:N	2.49	0.45
1:D:316:ARG:NH1	1:D:319:LYS:HE3	2.30	0.45
1:B:373:SER:HB2	1:B:420:GLU:OE2	2.17	0.45
1:B:342:SER:HA	1:B:409:ILE:HD12	1.99	0.45
1:A:249:ILE:HG13	1:A:379:SER:OG	2.15	0.45
1:B:317:PHE:N	1:B:317:PHE:HD1	2.15	0.45
1:A:348:VAL:O	1:A:353:LYS:HE3	2.16	0.45
1:B:212:GLN:H	1:B:212:GLN:HG3	1.55	0.45
1:C:309:GLY:O	1:C:330:ASN:HA	2.17	0.45
1:A:471:PHE:CE1	1:A:475:VAL:HG21	2.52	0.45
1:D:457:SER:O	1:D:460:HIS:HB3	2.16	0.45
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.64	0.45
1:A:208:VAL:O	1:A:212:GLN:HG3	2.17	0.44
1:D:148:GLU:O	1:D:150:GLN:N	2.46	0.44
1:B:285:SER:HB3	1:B:288:LYS:HD2	2.00	0.44
1:A:155:VAL:HG22	1:A:194:LEU:HD11	1.99	0.44
1:D:175:LYS:O	1:D:179:ASP:N	2.46	0.44
1:C:410:LEU:HD23	1:C:410:LEU:HA	1.85	0.44
1:A:140:ASP:HB3	1:A:196:LYS:NZ	2.32	0.44
1:B:249:ILE:HD11	1:B:379:SER:HB3	1.98	0.44
1:A:528:ASN:HD21	1:C:528:ASN:CG	2.20	0.44
1:A:191:GLY:HA3	1:A:192:VAL:HA	1.76	0.44
1:A:180:MET:HG2	1:A:202:CYS:HA	2.00	0.44
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.84	0.44
1:D:524:CYS:HA	1:D:539:LEU:O	2.17	0.44
1:A:152:LYS:NZ	1:A:193:MET:HE3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:VAL:O	1:A:291:LYS:HG2	2.18	0.44
1:B:461:SER:O	1:B:468:SER:HB3	2.18	0.44
1:C:396:GLU:O	1:C:398:LYS:HE2	2.18	0.44
1:B:360:PHE:CE1	1:B:447:LEU:CD2	3.00	0.43
1:A:375:ALA:O	1:A:379:SER:HB3	2.18	0.43
1:B:152:LYS:HG2	1:B:193:MET:CG	2.49	0.43
1:B:316:ARG:HA	1:B:316:ARG:HD2	1.42	0.43
1:C:249:ILE:CG1	1:C:379:SER:HB2	2.48	0.43
1:A:307:TYR:HB3	1:A:339:VAL:HG11	2.00	0.43
1:C:296:VAL:HG11	1:C:454:ASN:HD22	1.84	0.43
1:B:250:PRO:HG2	1:B:251:GLN:NE2	2.33	0.43
1:C:191:GLY:HA3	1:C:192:VAL:HA	1.77	0.43
1:D:288:LYS:HE3	1:D:337:ALA:CB	2.49	0.43
1:A:249:ILE:HG13	1:A:379:SER:HG	1.83	0.43
1:B:505:ASP:HB3	1:B:511:VAL:HG22	2.01	0.43
1:D:152:LYS:NZ	1:D:193:MET:HB2	2.23	0.43
1:D:288:LYS:HA	1:D:291:LYS:HE2	2.01	0.43
1:D:450:GLU:OE1	3:D:603:HOH:O	2.19	0.43
1:B:369:TYR:CZ	1:B:371:GLY:HA3	2.54	0.43
1:B:529:TYR:CE1	1:D:478:PRO:HG3	2.53	0.43
1:A:148:GLU:OE2	1:A:157:LYS:NZ	2.52	0.42
1:D:355:ASP:O	1:D:359:GLN:HG3	2.19	0.42
1:B:292:TYR:HA	1:B:340:VAL:HG11	2.01	0.42
1:B:339:VAL:HG23	1:B:394:LEU:HD13	2.00	0.42
1:B:348:VAL:O	1:B:353:LYS:HE3	2.19	0.42
1:C:228:SER:O	1:C:232:GLU:HG3	2.18	0.42
1:D:334:ASN:ND2	1:D:386:ARG:NH2	2.67	0.42
1:C:369:TYR:CZ	1:C:371:GLY:HA3	2.54	0.42
1:D:250:PRO:O	1:D:254:LYS:HG3	2.20	0.42
1:A:140:ASP:HB3	1:A:196:LYS:HZ2	1.83	0.42
1:A:217:LYS:HD3	1:A:217:LYS:HA	1.91	0.42
1:A:182:ARG:O	1:A:186:GLN:HG2	2.20	0.42
1:C:136:PRO:HB2	1:C:141:LEU:HD21	2.01	0.42
1:B:471:PHE:CZ	1:B:475:VAL:HG11	2.55	0.42
1:D:289:PRO:HD3	1:D:480:LYS:HG2	2.02	0.42
1:D:487:ILE:HD12	1:D:513:GLY:HA3	2.02	0.42
1:A:168:ARG:HD2	3:A:713:HOH:O	2.19	0.42
1:A:195:ASP:OD2	3:A:707:HOH:O	2.21	0.42
1:A:318:ASN:ND2	1:A:466:ASP:OD2	2.52	0.42
1:B:478:PRO:HD2	1:B:490:VAL:O	2.20	0.42
1:D:478:PRO:HD2	1:D:490:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LYS:O	1:A:204:GLN:HB3	2.20	0.42
1:A:259:LEU:HD13	1:A:500:TRP:CH2	2.54	0.41
1:B:150:GLN:HG2	1:B:152:LYS:HD3	2.01	0.41
1:B:150:GLN:HG3	1:B:151:GLU:N	2.35	0.41
1:B:421:VAL:HG21	1:B:426:ALA:HB2	2.00	0.41
1:C:363:LYS:HG2	3:C:728:HOH:O	2.19	0.41
1:C:366:GLY:HA3	1:C:441:ILE:HD11	2.02	0.41
1:B:476:GLY:O	1:B:528:ASN:HB2	2.20	0.41
1:A:152:LYS:HZ3	1:A:193:MET:HA	1.82	0.41
1:D:249:ILE:HG22	1:D:252:LEU:H	1.85	0.41
1:A:142:LEU:HD22	1:A:199:PHE:CZ	2.51	0.41
1:A:316:ARG:O	1:A:317:PHE:HD1	2.03	0.41
1:C:234:TYR:CE1	1:C:260:TRP:CD1	3.08	0.41
1:A:289:PRO:CD	1:A:480:LYS:HG2	2.50	0.41
1:C:249:ILE:HG13	1:C:250:PRO:HD2	2.02	0.41
1:D:215:ARG:HB3	1:D:217:LYS:HE2	2.02	0.41
1:B:141:LEU:HD12	1:B:141:LEU:HA	1.89	0.41
1:C:247:ASP:HA	1:C:253:ALA:HB2	2.03	0.41
1:D:198:LEU:HA	1:D:201:LYS:HB2	2.03	0.41
1:A:217:LYS:N	1:A:217:LYS:HE2	2.36	0.41
1:C:219:VAL:HG21	1:C:494:VAL:HA	2.01	0.41
1:C:273:SER:HB3	1:C:277:THR:HG21	2.03	0.41
1:C:363:LYS:HD3	1:C:444:GLU:OE2	2.19	0.41
1:B:386:ARG:O	1:B:389:ALA:HB3	2.20	0.41
1:C:263:SER:OG	1:C:424:GLU:HG2	2.21	0.41
1:C:438:PHE:CE2	1:C:445:ARG:HB2	2.56	0.41
1:C:199:PHE:O	1:C:203:VAL:HG22	2.21	0.40
1:C:296:VAL:HG11	1:C:454:ASN:ND2	2.36	0.40
1:A:497:MET:CE	1:A:516:PHE:CE1	3.04	0.40
1:C:477:LEU:HD21	1:C:526:PHE:O	2.22	0.40
1:D:315:LEU:HA	1:D:315:LEU:HD12	1.89	0.40
1:C:249:ILE:HG23	1:C:252:LEU:H	1.86	0.40
1:A:139:GLU:H	1:A:139:GLU:HG2	1.12	0.40
1:B:288:LYS:N	1:B:289:PRO:HD2	2.36	0.40
1:B:477:LEU:HA	1:B:477:LEU:HD23	1.89	0.40
1:C:139:GLU:HG3	1:C:200:LYS:CD	2.47	0.40
1:C:466:ASP:CB	1:C:507:MET:HE2	2.52	0.40
1:D:198:LEU:N	1:D:198:LEU:HD23	2.35	0.40
1:D:215:ARG:HB3	1:D:217:LYS:CE	2.51	0.40
1:D:219:VAL:HG13	1:D:220:ILE:HG13	2.02	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%)	390 (96%)	14 (3%)	4 (1%)	19 33
1	B	408/539 (76%)	385 (94%)	22 (5%)	1 (0%)	52 74
1	C	408/539 (76%)	390 (96%)	18 (4%)	0	100 100
1	D	408/539 (76%)	385 (94%)	22 (5%)	1 (0%)	52 74
All	All	1632/2156 (76%)	1550 (95%)	76 (5%)	6 (0%)	39 60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	THR
1	A	318	ASN
1	B	190	ASP
1	A	315	LEU
1	D	196	LYS
1	A	216	ARG

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	353/462 (76%)	345 (98%)	8 (2%)	58 83
1	B	353/462 (76%)	346 (98%)	7 (2%)	63 86
1	C	353/462 (76%)	350 (99%)	3 (1%)	86 96
1	D	353/462 (76%)	346 (98%)	7 (2%)	63 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1412/1848 (76%)	1387 (98%)	25 (2%)	66 87

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	GLU
1	A	140	ASP
1	A	152	LYS
1	A	169	THR
1	A	241	SER
1	A	360	PHE
1	A	379	SER
1	A	519	ASP
1	B	140	ASP
1	B	150	GLN
1	B	152	LYS
1	B	169	THR
1	B	216	ARG
1	B	318	ASN
1	B	360	PHE
1	C	169	THR
1	C	318	ASN
1	C	543	ARG
1	D	197	ASP
1	D	198	LEU
1	D	316	ARG
1	D	318	ASN
1	D	360	PHE
1	D	519	ASP
1	D	543	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	GLN
1	A	528	ASN
1	B	150	GLN
1	B	240	GLN
1	D	515	HIS
1	D	528	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	5XY	A	601	-	32,40,40	3.77	10 (31%)	33,54,54	1.42	4 (12%)
2	5XY	C	601	-	32,40,40	3.86	10 (31%)	33,54,54	1.29	4 (12%)

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	5XY	A	601	-	-	0/14/33/33	0/3/5/5
2	5XY	C	601	-	-	0/14/33/33	0/3/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	5XY	C11-N12	-10.29	1.31	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	5XY	C13-C09	-10.21	1.34	1.53
2	C	601	5XY	C11-N12	-10.01	1.32	1.47
2	A	601	5XY	C13-C09	-9.82	1.35	1.53
2	A	601	5XY	C10-C11	2.41	1.57	1.52
2	C	601	5XY	C10-C11	2.45	1.57	1.52
2	C	601	5XY	C19-N18	2.71	1.42	1.35
2	A	601	5XY	C02-N03	2.77	1.42	1.35
2	A	601	5XY	C19-N18	2.91	1.42	1.35
2	C	601	5XY	C02-N03	3.36	1.43	1.35
2	A	601	5XY	C04-N03	3.58	1.42	1.36
2	A	601	5XY	C17-N18	3.62	1.42	1.36
2	C	601	5XY	C17-N18	3.82	1.42	1.36
2	C	601	5XY	C07-N08	4.15	1.42	1.35
2	A	601	5XY	C07-N08	4.38	1.42	1.35
2	C	601	5XY	C04-N03	4.59	1.44	1.36
2	A	601	5XY	C14-N12	6.33	1.42	1.32
2	C	601	5XY	C14-N12	6.42	1.42	1.32
2	A	601	5XY	C13-N12	11.72	1.62	1.46
2	C	601	5XY	C13-N12	12.09	1.62	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	5XY	C11-N12-C13	-4.16	100.82	111.54
2	C	601	5XY	O27-C19-N18	-2.88	118.73	123.77
2	A	601	5XY	C11-C10-C09	-2.15	101.26	104.28
2	C	601	5XY	C20-C19-N18	2.09	120.69	114.69
2	A	601	5XY	C11-N12-C14	2.11	129.33	123.40
2	C	601	5XY	C01-C02-N03	2.12	120.76	114.69
2	C	601	5XY	C09-C13-N12	3.32	108.25	103.19
2	A	601	5XY	C09-C13-N12	3.70	108.83	103.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	5XY	2	0
2	C	601	5XY	2	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%)	0.92	52 (12%)	5 5	30, 44, 79, 114	0
1	B	410/539 (76%)	0.81	46 (11%)	7 7	33, 48, 80, 98	0
1	C	410/539 (76%)	0.87	54 (13%)	4 4	31, 44, 80, 95	0
1	D	410/539 (76%)	0.99	66 (16%)	3 2	34, 47, 87, 111	0
All	All	1640/2156 (76%)	0.90	218 (13%)	4 4	30, 46, 81, 114	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	317	PHE	12.7
1	A	188	THR	12.3
1	A	190	ASP	9.3
1	D	188	THR	8.9
1	D	194	LEU	8.4
1	B	143	PHE	8.0
1	D	251	GLN	7.9
1	B	316	ARG	7.6
1	D	148	GLU	7.6
1	C	317	PHE	7.5
1	A	147	ALA	7.3
1	D	140	ASP	7.1
1	D	190	ASP	7.1
1	C	191	GLY	6.8
1	D	149	GLY	6.6
1	C	143	PHE	6.6
1	D	155	VAL	6.5
1	A	153	ILE	6.4
1	D	145	THR	6.4
1	D	144	TYR	6.2
1	D	151	GLU	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	148	GLU	6.1
1	A	149	GLY	6.1
1	C	149	GLY	6.1
1	A	317	PHE	6.0
1	A	199	PHE	6.0
1	A	143	PHE	5.8
1	A	194	LEU	5.8
1	D	199	PHE	5.7
1	D	143	PHE	5.6
1	A	144	TYR	5.5
1	D	250	PRO	5.5
1	B	137	SER	5.4
1	B	317	PHE	5.3
1	B	190	ASP	5.3
1	C	251	GLN	5.3
1	D	196	LYS	5.3
1	B	199	PHE	5.2
1	B	149	GLY	5.1
1	D	249	ILE	5.1
1	A	155	VAL	5.1
1	A	145	THR	5.0
1	A	151	GLU	5.0
1	B	136	PRO	5.0
1	B	192	VAL	4.8
1	C	190	ASP	4.8
1	D	152	LYS	4.8
1	C	136	PRO	4.7
1	A	191	GLY	4.7
1	B	138	LEU	4.7
1	A	250	PRO	4.7
1	B	189	SER	4.7
1	C	249	ILE	4.7
1	A	150	GLN	4.7
1	A	136	PRO	4.7
1	D	195	ASP	4.6
1	C	161	ALA	4.4
1	C	155	VAL	4.4
1	C	199	PHE	4.4
1	D	248	TYR	4.4
1	A	152	LYS	4.4
1	D	255	PHE	4.4
1	A	187	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	136	PRO	4.3
1	D	187	THR	4.3
1	B	194	LEU	4.3
1	D	141	LEU	4.3
1	D	315	LEU	4.3
1	A	248	TYR	4.3
1	D	192	VAL	4.3
1	B	144	TYR	4.2
1	B	147	ALA	4.2
1	C	147	ALA	4.2
1	B	205	SER	4.2
1	A	545	GLY	4.2
1	D	142	LEU	4.1
1	C	250	PRO	4.1
1	A	251	GLN	4.1
1	C	194	LEU	4.0
1	B	148	GLU	4.0
1	B	140	ASP	4.0
1	C	137	SER	4.0
1	A	159	ILE	3.9
1	A	146	ILE	3.9
1	C	142	LEU	3.9
1	A	249	ILE	3.8
1	D	147	ALA	3.8
1	D	257	PRO	3.8
1	A	316	ARG	3.8
1	C	192	VAL	3.8
1	B	193	MET	3.8
1	D	211	THR	3.8
1	D	191	GLY	3.7
1	D	212	GLN	3.7
1	A	140	ASP	3.7
1	C	150	GLN	3.7
1	A	185	LEU	3.7
1	D	253	ALA	3.7
1	A	195	ASP	3.7
1	C	196	LYS	3.6
1	A	141	LEU	3.6
1	D	254	LYS	3.6
1	A	154	PRO	3.6
1	D	157	LYS	3.6
1	C	148	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	142	LEU	3.6
1	A	383	SER	3.5
1	C	545	GLY	3.5
1	B	150	GLN	3.5
1	B	195	ASP	3.5
1	A	196	LYS	3.4
1	C	195	ASP	3.4
1	D	153	ILE	3.3
1	D	256	SER	3.3
1	A	224	MET	3.3
1	B	141	LEU	3.2
1	D	347	GLY	3.2
1	B	153	ILE	3.2
1	C	156	HIS	3.2
1	D	185	LEU	3.2
1	D	159	ILE	3.1
1	D	150	GLN	3.1
1	A	193	MET	3.1
1	D	156	HIS	3.1
1	B	155	VAL	3.1
1	C	157	LYS	3.1
1	C	478	PRO	3.1
1	B	318	ASN	3.1
1	C	188	THR	3.0
1	B	156	HIS	2.9
1	A	189	SER	2.9
1	A	253	ALA	2.9
1	C	315	LEU	2.9
1	A	137	SER	2.9
1	B	360	PHE	2.9
1	C	475	VAL	2.9
1	D	184	THR	2.9
1	D	193	MET	2.8
1	B	478	PRO	2.8
1	A	255	PHE	2.8
1	B	251	GLN	2.8
1	D	383	SER	2.7
1	C	140	ASP	2.7
1	D	198	LEU	2.7
1	D	545	GLY	2.7
1	C	138	LEU	2.7
1	A	156	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	162	LEU	2.6
1	D	137	SER	2.6
1	A	192	VAL	2.6
1	B	475	VAL	2.6
1	C	144	TYR	2.6
1	A	204	GLN	2.6
1	A	254	LYS	2.6
1	B	252	LEU	2.6
1	C	476	GLY	2.6
1	C	189	SER	2.5
1	D	197	ASP	2.5
1	D	160	THR	2.5
1	D	169	THR	2.5
1	C	164	SER	2.5
1	B	250	PRO	2.5
1	C	252	LEU	2.5
1	D	189	SER	2.5
1	B	151	GLU	2.5
1	A	160	THR	2.5
1	A	212	GLN	2.4
1	B	348	VAL	2.4
1	C	494	VAL	2.4
1	B	315	LEU	2.4
1	D	409	ILE	2.4
1	C	458	LEU	2.4
1	C	207	ILE	2.3
1	B	145	THR	2.3
1	C	193	MET	2.3
1	D	207	ILE	2.3
1	C	360	PHE	2.3
1	A	211	THR	2.3
1	C	257	PRO	2.3
1	C	491	VAL	2.3
1	B	545	GLY	2.3
1	C	151	GLU	2.3
1	A	157	LYS	2.3
1	B	249	ILE	2.3
1	C	141	LEU	2.3
1	D	182	ARG	2.3
1	A	184	THR	2.2
1	B	160	THR	2.2
1	D	204	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	205	SER	2.2
1	D	164	SER	2.2
1	C	455	THR	2.2
1	B	142	LEU	2.2
1	D	258	ASP	2.2
1	B	196	LYS	2.2
1	C	316	ARG	2.2
1	C	490	VAL	2.2
1	C	185	LEU	2.2
1	A	529	TYR	2.1
1	B	491	VAL	2.1
1	D	318	ASN	2.1
1	D	183	LEU	2.1
1	D	252	LEU	2.1
1	B	204	GLN	2.1
1	C	472	ALA	2.1
1	B	183	LEU	2.1
1	C	145	THR	2.1
1	C	153	ILE	2.1
1	C	203	VAL	2.0
1	B	191	GLY	2.0
1	A	216	ARG	2.0
1	D	180	MET	2.0
1	D	224	MET	2.0
1	B	154	PRO	2.0
1	D	375	ALA	2.0
1	B	152	LYS	2.0
1	D	206	ASN	2.0
1	C	347	GLY	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

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	5XY	A	601	36/36	0.87	0.26	0.17	48,65,82,85	0
2	5XY	C	601	36/36	0.89	0.23	-0.22	52,67,83,84	0

6.5 Other polymers

There are no such residues in this entry.