



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:47 am GMT

PDB ID : 4S13  
Title : Ferulic Acid Decarboxylase (FDC1)  
Authors : Lee, S.G.; Bhuiya, M.W.; Yu, O.; Jez, J.M.  
Deposited on : 2015-01-07  
Resolution : 2.35 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

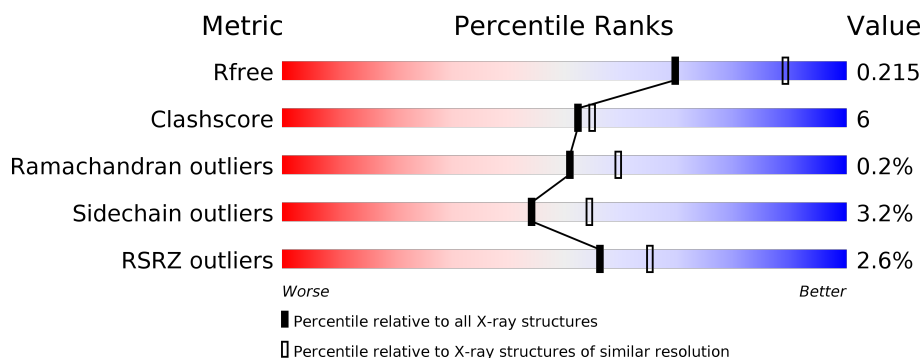
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	100719	1570 (2.36-2.32)
Clashscore	112137	1673 (2.36-2.32)
Ramachandran outliers	110173	1654 (2.36-2.32)
Sidechain outliers	110143	1655 (2.36-2.32)
RSRZ outliers	101464	1576 (2.36-2.32)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	503	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>
1	B	503	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>5%</div> </div> </div>
1	C	503	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>
1	D	503	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>5%</div> </div> </div>
1	E	503	<div> <div></div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>
1	F	503	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>.</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	503	
1	H	503	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	4VP	A	601	-	-	-	X
2	4VP	F	601	-	-	-	X
2	4VP	G	601	-	-	-	X

## 2 Entry composition

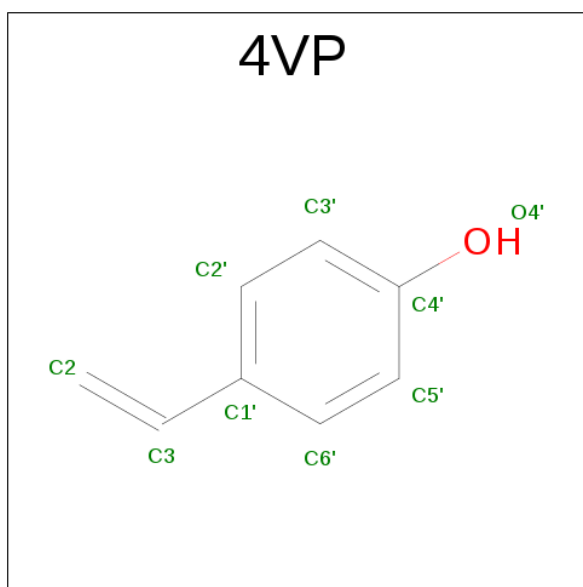
There are 3 unique types of molecules in this entry. The entry contains 31691 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ferulic acid decarboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3705	2387	600	696	22			
1	B	476	Total	C	N	O	S	0	2	0
			3748	2420	604	701	23			
1	C	501	Total	C	N	O	S	0	0	0
			3933	2536	642	733	22			
1	D	480	Total	C	N	O	S	0	1	0
			3775	2436	610	707	22			
1	E	492	Total	C	N	O	S	0	0	0
			3868	2495	630	721	22			
1	F	501	Total	C	N	O	S	0	0	0
			3933	2536	642	733	22			
1	G	472	Total	C	N	O	S	0	1	0
			3718	2399	600	697	22			
1	H	481	Total	C	N	O	S	0	1	0
			3777	2435	611	709	22			

- Molecule 2 is 4-ETHENYLPHENOL (three-letter code: 4VP) (formula: C<sub>8</sub>H<sub>8</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	8	1		
2	C	1	Total	C	O	0	0
			9	8	1		
2	E	1	Total	C	O	0	0
			9	8	1		
2	F	1	Total	C	O	0	0
			9	8	1		
2	G	1	Total	C	O	0	0
			9	8	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total	O	0	0
			152	152		
3	B	190	Total	O	0	0
			190	190		
3	C	131	Total	O	0	0
			131	131		
3	D	185	Total	O	0	0
			185	185		
3	E	165	Total	O	0	0
			165	165		
3	F	137	Total	O	0	0
			137	137		
3	G	100	Total	O	0	0
			100	100		

*Continued on next page...*

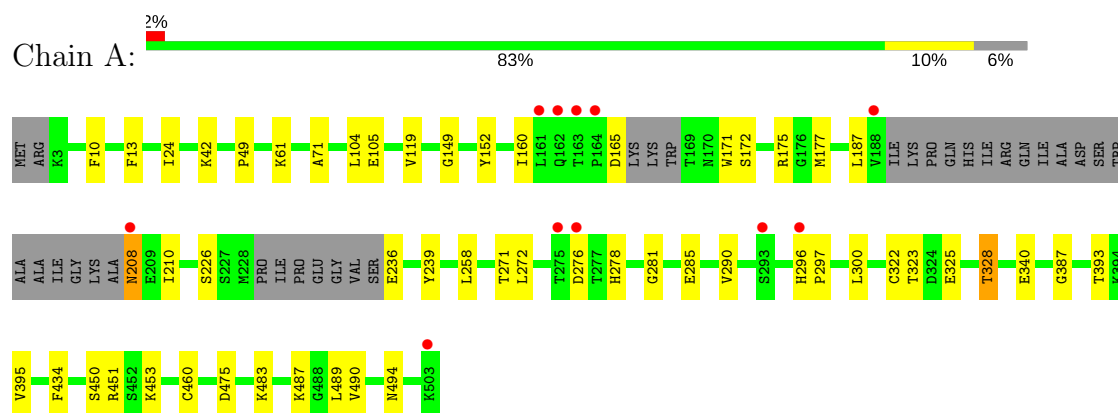
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	129	Total 129	O 129	0	0

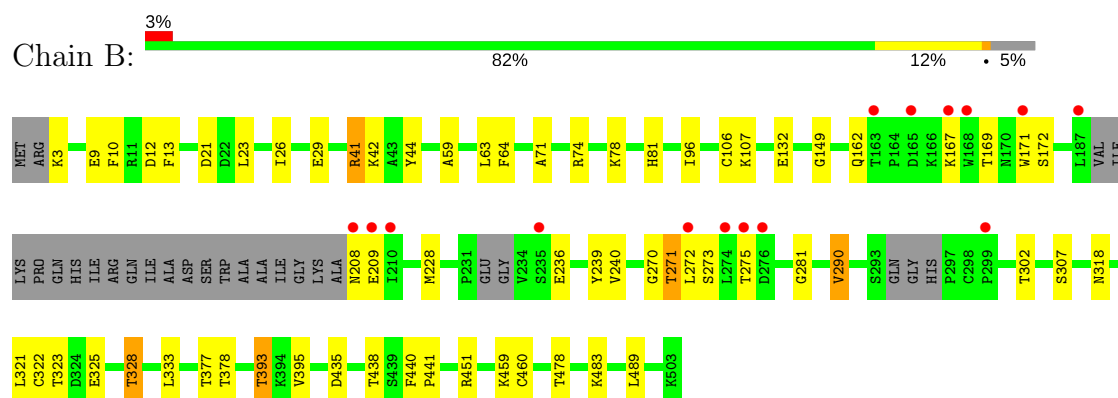
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

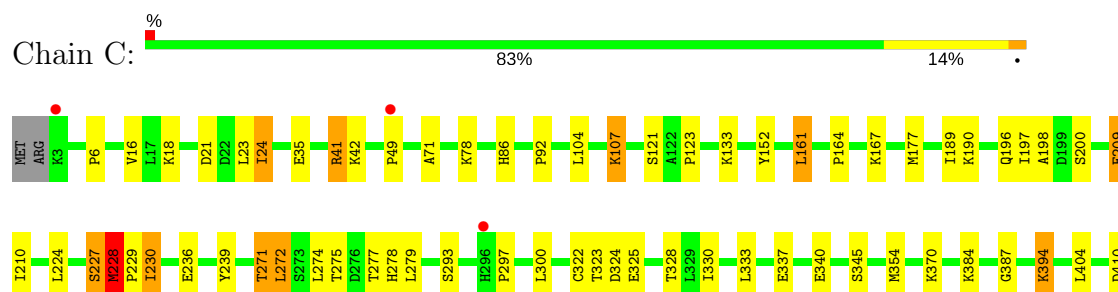
#### • Molecule 1: Ferulic acid decarboxylase 1



#### • Molecule 1: Ferulic acid decarboxylase 1

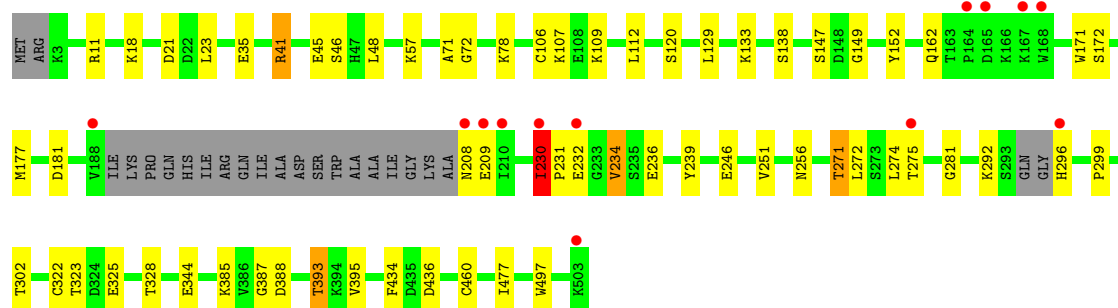
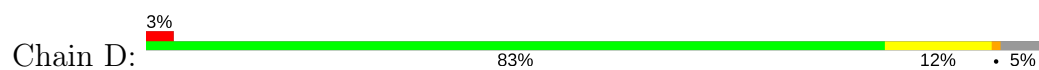


#### • Molecule 1: Ferulic acid decarboxylase 1

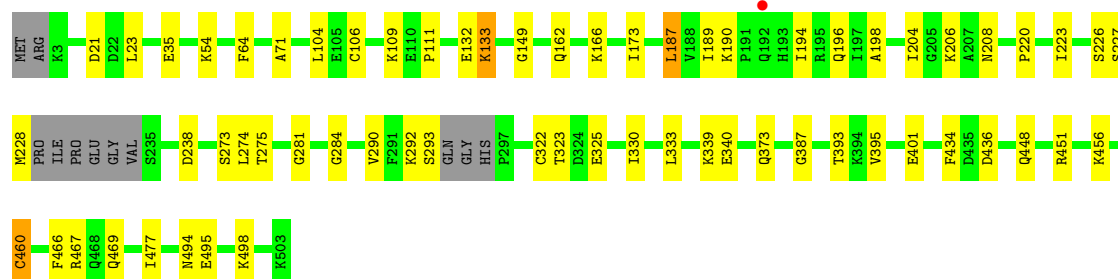
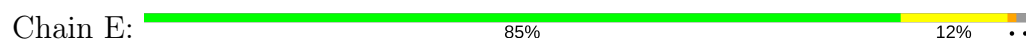




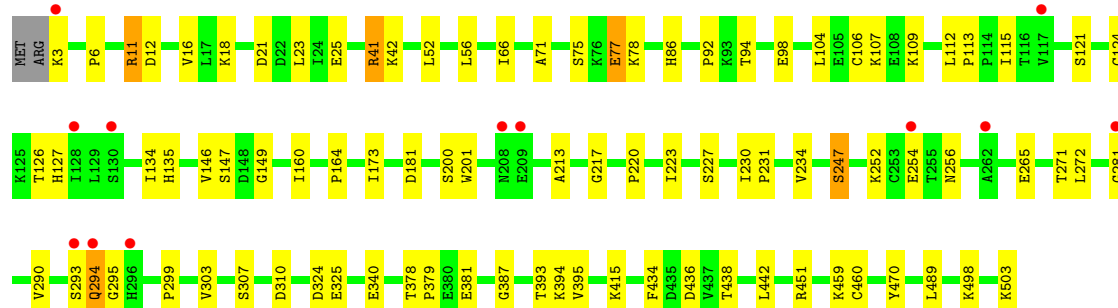
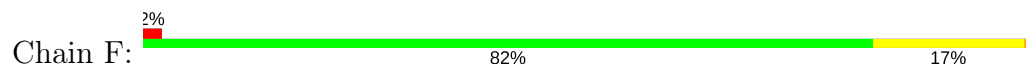
• Molecule 1: Ferulic acid decarboxylase 1



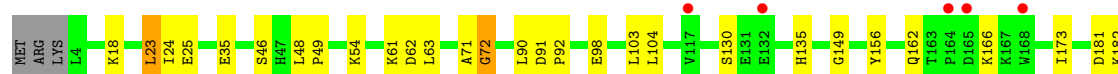
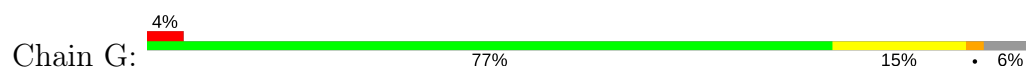
• Molecule 1: Ferulic acid decarboxylase 1



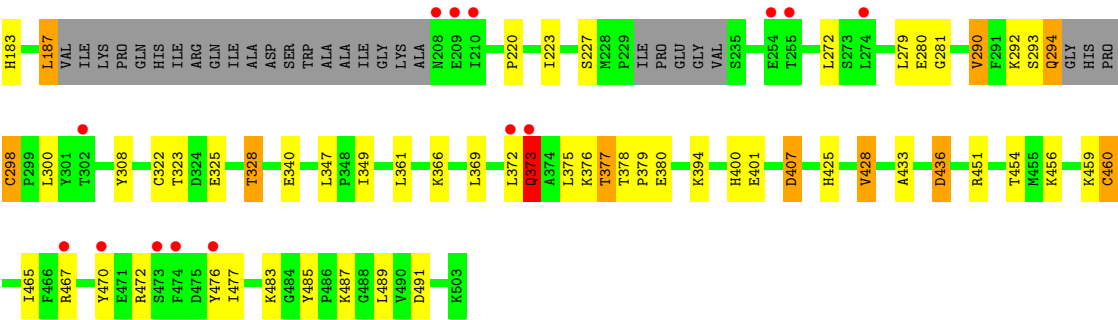
• Molecule 1: Ferulic acid decarboxylase 1



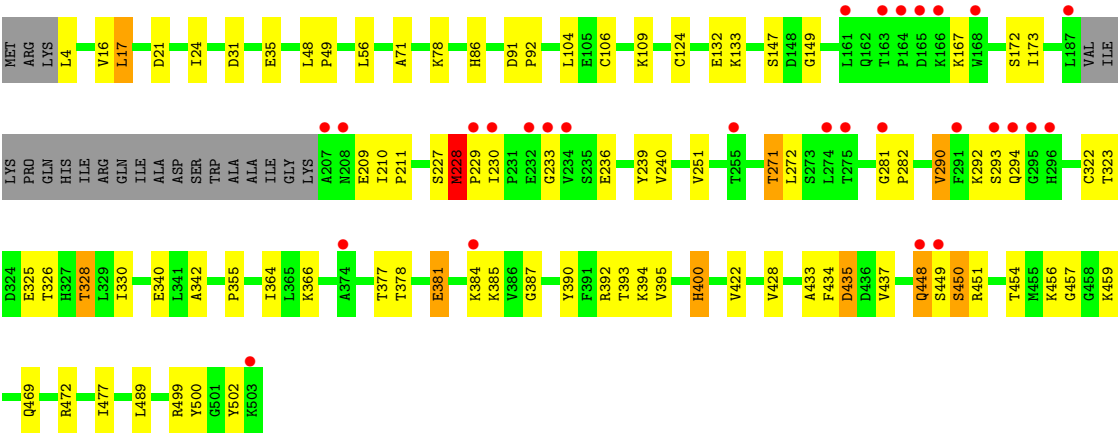
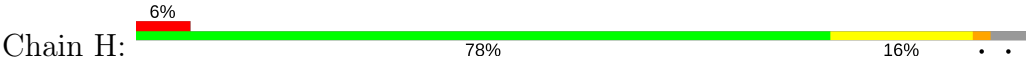
• Molecule 1: Ferulic acid decarboxylase 1







● Molecule 1: Ferulic acid decarboxylase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	251.96Å 121.00Å 159.56Å 90.00° 121.93° 90.00°	Depositor
Resolution (Å)	47.05 – 2.35 49.85 – 2.35	Depositor EDS
% Data completeness (in resolution range)	95.8 (47.05-2.35) 91.5 (49.85-2.35)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.171 , 0.215 0.172 , 0.215	Depositor DCC
$R_{free}$ test set	8147 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	31691	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.95 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.2275e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

Bond lengths and bond angles in the following residue types are not validated in this section: 4VP

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	0.43	0/3794	0.55	0/5147
1	B	0.43	0/3846	0.56	0/5218
1	C	0.41	0/4033	0.54	0/5477
1	D	0.45	0/3872	0.56	0/5256
1	E	0.41	0/3963	0.54	0/5376
1	F	0.41	0/4033	0.55	0/5477
1	G	0.39	0/3811	0.54	0/5170
1	H	0.39	0/3875	0.55	0/5262
All	All	0.42	0/31227	0.55	0/42383

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	C	0	1
1	G	0	3
1	H	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	228	MET	Peptide
1	G	373	GLN	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	G	476	TYR	Peptide
1	G	72	GLY	Peptide
1	H	228	MET	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	3705	0	3702	35	0
1	B	3748	0	3761	45	0
1	C	3933	0	3944	54	1
1	D	3775	0	3781	35	0
1	E	3868	0	3882	40	0
1	F	3933	0	3944	57	0
1	G	3718	0	3722	68	1
1	H	3777	0	3776	69	0
2	A	9	0	8	2	0
2	C	9	0	8	2	0
2	E	9	0	8	1	0
2	F	9	0	8	0	0
2	G	9	0	8	0	0
3	A	152	0	0	8	0
3	B	190	0	0	9	0
3	C	131	0	0	7	0
3	D	185	0	0	11	0
3	E	165	0	0	10	0
3	F	137	0	0	6	0
3	G	100	0	0	7	0
3	H	129	0	0	9	0
All	All	31691	0	30552	382	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (382) 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:D:208:ASN:N	3:D:762:HOH:O	1.93	1.00
1:C:410:ASP:OD2	3:C:736:HOH:O	1.82	0.95
1:G:24[B]:ILE:HD11	1:G:49:PRO:HB2	1.55	0.88
1:C:228:MET:HB3	1:C:229:PRO:HD3	1.55	0.88
1:D:296:HIS:N	3:D:760:HOH:O	2.05	0.88
1:G:90:LEU:O	3:G:726:HOH:O	1.89	0.88
1:D:292:LYS:O	3:D:754:HOH:O	1.90	0.87
1:F:294:GLN:OE1	3:F:825:HOH:O	1.96	0.84
1:B:290:VAL:HG13	1:E:477:ILE:HB	1.59	0.83
1:D:71:ALA:HB3	1:D:325:GLU:HG3	1.57	0.83
1:G:394:LYS:NZ	3:G:778:HOH:O	2.11	0.82
1:B:41:ARG:NH1	1:B:318:ASN:O	2.15	0.79
1:B:41:ARG:NH2	1:B:321:LEU:O	2.16	0.78
1:E:330:ILE:HD13	2:E:601:4VP:H4	1.66	0.78
1:H:133:LYS:NZ	3:H:690:HOH:O	2.16	0.77
1:C:198:ALA:HB1	1:C:274:LEU:HD11	1.66	0.77
1:F:503:LYS:O	3:F:780:HOH:O	2.01	0.77
1:G:71:ALA:HB3	1:G:325:GLU:HG3	1.67	0.77
1:B:59:ALA:O	3:B:701:HOH:O	2.01	0.76
1:B:71:ALA:HB3	1:B:325:GLU:HG3	1.66	0.76
1:G:290:VAL:HG13	1:H:477:ILE:HB	1.65	0.76
1:D:388:ASP:OD2	3:D:731:HOH:O	2.02	0.76
1:B:29:GLU:O	3:B:694:HOH:O	2.02	0.76
1:A:105:GLU:OE1	3:A:744:HOH:O	2.04	0.75
1:F:135:HIS:ND1	1:F:181:ASP:OD2	2.20	0.75
1:C:71:ALA:HB3	1:C:325:GLU:HG3	1.68	0.74
1:F:113:PRO:O	1:F:247:SER:OG	2.04	0.74
1:F:393:THR:HG22	1:F:395:VAL:H	1.53	0.74
1:E:71:ALA:HB3	1:E:325:GLU:HG3	1.69	0.73
1:F:378:THR:OG1	1:F:381:GLU:OE1	2.05	0.73
1:G:477:ILE:HB	1:H:290:VAL:HG13	1.70	0.73
1:H:435:ASP:N	1:H:435:ASP:OD1	2.22	0.73
1:A:475:ASP:OD1	3:A:788:HOH:O	2.06	0.72
1:E:292:LYS:O	3:E:831:HOH:O	2.06	0.72
1:C:487:LYS:NZ	1:C:491:ASP:OD1	2.20	0.72
1:H:381:GLU:N	3:H:726:HOH:O	2.20	0.72
1:F:436:ASP:OD2	3:F:771:HOH:O	2.07	0.71
1:F:11:ARG:NH2	1:F:265:GLU:OE2	2.23	0.71
1:H:71:ALA:HB3	1:H:325:GLU:HG3	1.71	0.71
1:A:393:THR:HG22	1:A:395:VAL:H	1.55	0.70
1:A:171:TRP:HB2	1:A:236:GLU:HG3	1.73	0.70
1:D:230:ILE:HG12	1:D:231:PRO:HD2	1.72	0.70

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:SER:OG	3:D:649:HOH:O	1.95	0.69
1:B:393:THR:HG22	1:B:395:VAL:H	1.56	0.69
1:D:11:ARG:NH1	3:D:738:HOH:O	2.08	0.69
1:H:228:MET:HB3	1:H:229:PRO:HD3	1.75	0.69
1:B:162:GLN:O	3:B:689:HOH:O	2.11	0.68
1:D:57:LYS:O	3:D:681:HOH:O	2.11	0.68
1:F:124:CYS:O	1:F:307:SER:OG	2.11	0.68
1:F:498:LYS:O	3:F:736:HOH:O	2.12	0.68
1:A:483:LYS:NZ	3:A:822:HOH:O	2.25	0.68
1:B:162:GLN:NE2	1:B:169:THR:OG1	2.24	0.68
1:G:483:LYS:O	3:G:784:HOH:O	2.12	0.68
1:G:279:LEU:HG	1:G:294:GLN:HG3	1.74	0.67
1:C:354:MET:O	3:C:729:HOH:O	2.12	0.67
1:B:107:LYS:NZ	3:B:759:HOH:O	2.28	0.67
1:B:171:TRP:HB2	1:B:236:GLU:HG2	1.76	0.67
1:F:71:ALA:HB3	1:F:325:GLU:HG3	1.75	0.67
1:F:230:ILE:HG12	1:F:231:PRO:HD2	1.77	0.67
1:H:499:ARG:O	3:H:669:HOH:O	2.11	0.67
1:C:189:ILE:HD13	2:C:601:4VP:H5	1.77	0.66
1:G:104:LEU:HD21	1:G:340:GLU:HB2	1.78	0.66
1:H:400:HIS:HD2	1:H:459:LYS:HG2	1.60	0.66
1:F:217:GLY:HA3	1:F:265:GLU:HG2	1.77	0.66
1:E:393:THR:HG22	1:E:395:VAL:H	1.60	0.66
1:C:71:ALA:O	1:C:328:THR:HG21	1.97	0.65
1:C:394:LYS:O	3:C:788:HOH:O	2.13	0.65
1:G:347:LEU:HB3	1:G:349:ILE:HD13	1.79	0.65
1:E:373:GLN:O	3:E:803:HOH:O	2.14	0.65
1:C:228:MET:HB3	1:C:229:PRO:CD	2.26	0.64
1:A:71:ALA:HB3	1:A:325:GLU:HG3	1.79	0.64
1:G:485:TYR:HB3	1:G:489:LEU:HD23	1.80	0.64
1:F:293:SER:O	1:F:295:GLY:N	2.30	0.64
1:H:149:GLY:HA3	1:H:281:GLY:HA3	1.79	0.64
1:D:208:ASN:OD1	1:D:209:GLU:N	2.30	0.63
1:H:106:CYS:HA	1:H:109:LYS:HD2	1.80	0.63
1:E:228:MET:HG3	1:E:333:LEU:HD13	1.78	0.63
1:E:498:LYS:O	3:E:808:HOH:O	2.15	0.63
1:H:400:HIS:CD2	1:H:459:LYS:HG2	2.32	0.63
1:D:325:GLU:HA	1:D:328:THR:HG22	1.80	0.63
1:A:494:ASN:OD1	1:C:42:LYS:NZ	2.20	0.63
1:B:71:ALA:O	1:B:328:THR:HG21	1.98	0.63
1:B:325:GLU:HA	1:B:328:THR:HG22	1.81	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:LYS:NZ	3:A:842:HOH:O	2.31	0.62
1:F:415:LYS:NZ	3:F:816:HOH:O	2.31	0.62
1:B:171:TRP:HZ3	1:B:240:VAL:HG21	1.65	0.61
1:C:277:THR:HB	1:C:297:PRO:HB2	1.82	0.61
1:G:451:ARG:HA	1:G:454:THR:HB	1.82	0.61
1:H:500:TYR:OH	3:H:644:HOH:O	2.15	0.61
1:G:373:GLN:HE21	1:G:377:THR:HG23	1.66	0.60
1:F:149:GLY:HA3	1:F:281:GLY:HA3	1.82	0.60
1:D:72:GLY:H	1:D:328:THR:HG21	1.66	0.60
1:E:149:GLY:HA3	1:E:281:GLY:HA3	1.81	0.60
1:G:135:HIS:ND1	1:G:181:ASP:OD2	2.28	0.60
1:F:86:HIS:CE1	1:F:92:PRO:HG3	2.35	0.60
1:H:449:SER:OG	1:H:450:SER:N	2.34	0.60
1:G:156:TYR:HA	1:G:173:ILE:HD11	1.83	0.60
1:G:149:GLY:HA3	1:G:281:GLY:HA3	1.84	0.59
1:H:71:ALA:O	1:H:328:THR:HG21	2.02	0.59
1:F:134:ILE:HD13	1:F:303:VAL:HG12	1.84	0.59
1:A:71:ALA:O	1:A:328:THR:HG21	2.01	0.59
1:G:454:THR:HG22	1:G:456:LYS:H	1.68	0.59
1:H:210:ILE:HB	1:H:272:LEU:HB3	1.85	0.59
1:G:61:LYS:NZ	1:G:62:ASP:OD1	2.36	0.58
1:H:228:MET:HB3	1:H:229:PRO:CD	2.31	0.58
1:F:173:ILE:HG22	1:F:227:SER:HA	1.85	0.58
1:A:236:GLU:OE1	1:A:236:GLU:N	2.37	0.58
1:B:162:GLN:OE1	3:B:717:HOH:O	2.16	0.57
1:H:147:SER:OG	1:H:292:LYS:HE3	2.05	0.57
1:H:282:PRO:HG3	1:H:293:SER:H	1.68	0.57
1:B:162:GLN:HE21	1:B:169:THR:HG1	1.53	0.57
1:D:149:GLY:HA3	1:D:281:GLY:HA3	1.87	0.57
1:E:198:ALA:HB1	1:E:274:LEU:HD11	1.87	0.57
1:E:106:CYS:HA	1:E:109:LYS:HD2	1.86	0.57
1:A:451:ARG:HD2	3:A:807:HOH:O	2.06	0.56
1:E:190:LYS:HB3	1:E:194:ILE:HD11	1.88	0.56
1:G:18:LYS:NZ	3:G:749:HOH:O	2.37	0.56
1:H:228:MET:HG3	1:H:330:ILE:HG23	1.86	0.56
1:H:381:GLU:O	1:H:385:LYS:HG2	2.06	0.56
1:D:21:ASP:O	1:D:78:LYS:NZ	2.38	0.56
1:A:208:ASN:HD22	1:A:208:ASN:N	2.03	0.56
1:G:162:GLN:NE2	3:G:746:HOH:O	2.39	0.56
1:D:393:THR:HG22	1:D:395:VAL:H	1.71	0.56
1:D:106:CYS:HA	1:D:109:LYS:HD2	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24[B]:ILE:CD1	1:G:49:PRO:HB2	2.34	0.55
1:G:173:ILE:HG22	1:G:227:SER:HA	1.87	0.55
1:C:86:HIS:CE1	1:C:92:PRO:HG3	2.41	0.55
1:E:104:LEU:HD11	1:E:339:LYS:HD3	1.89	0.55
1:F:173:ILE:CG2	1:F:227:SER:HA	2.37	0.55
1:D:35:GLU:HG2	1:F:489:LEU:HD11	1.87	0.55
1:F:107:LYS:HD3	1:F:340:GLU:OE1	2.05	0.55
1:G:377:THR:OG1	1:G:378:THR:N	2.40	0.55
1:G:491:ASP:OD1	3:G:765:HOH:O	2.18	0.55
1:F:12:ASP:O	1:F:16:VAL:HG23	2.07	0.55
1:G:46:SER:OG	3:G:723:HOH:O	2.18	0.54
1:F:127:HIS:NE2	1:F:310:ASP:OD1	2.39	0.54
1:G:436:ASP:HA	1:G:456:LYS:HD3	1.88	0.54
1:C:24:ILE:HD12	1:C:49:PRO:HB2	1.88	0.54
1:C:325:GLU:HA	1:C:328:THR:HG22	1.90	0.54
1:E:21:ASP:OD2	3:E:853:HOH:O	2.18	0.54
1:G:35:GLU:HG3	1:H:489:LEU:HD11	1.90	0.54
1:C:18:LYS:NZ	3:C:808:HOH:O	2.40	0.54
1:H:209:GLU:HA	1:H:271:THR:HG23	1.89	0.54
1:A:104:LEU:HD21	1:A:340:GLU:HB2	1.89	0.54
1:G:436:ASP:OD1	1:G:456:LYS:HD3	2.07	0.54
1:A:236:GLU:N	3:A:831:HOH:O	2.40	0.54
1:G:428:VAL:HG11	1:H:433:ALA:HB2	1.90	0.54
1:F:21:ASP:O	1:F:78:LYS:NZ	2.40	0.53
1:A:149:GLY:HA3	1:A:281:GLY:HA3	1.90	0.53
1:H:451:ARG:HH21	1:H:457:GLY:HA3	1.74	0.53
1:D:387:GLY:HA3	1:D:434:PHE:CZ	2.44	0.53
1:G:72:GLY:H	1:G:328:THR:HG21	1.74	0.53
1:C:21:ASP:O	1:C:78:LYS:NZ	2.41	0.52
1:A:387:GLY:HA3	1:A:434:PHE:CZ	2.44	0.52
1:B:208:ASN:HB3	1:B:273:SER:HB2	1.91	0.52
1:G:433:ALA:HB2	1:H:428:VAL:HG11	1.91	0.52
1:H:294:GLN:H	1:H:294:GLN:CD	2.12	0.52
1:G:373:GLN:NE2	1:G:470:TYR:HD1	2.06	0.52
1:H:437:VAL:O	1:H:456:LYS:HG3	2.09	0.52
1:B:81:HIS:CD2	1:B:96:ILE:HD13	2.46	0.51
1:F:252:LYS:HE2	1:F:256:ASN:O	2.11	0.51
1:E:162:GLN:HG2	1:E:166:LYS:HA	1.91	0.51
1:F:146:VAL:O	1:F:147:SER:HB2	2.10	0.51
1:A:160:ILE:HG22	1:A:258:LEU:HD22	1.92	0.51
1:G:24[B]:ILE:HD13	1:H:502:TYR:CZ	2.45	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:ILE:HG22	1:F:247:SER:HB3	1.93	0.51
1:G:183:HIS:HD2	1:G:300:LEU:HG	1.76	0.50
1:B:3:LYS:HD3	1:D:234:VAL:HA	1.92	0.50
1:F:126:THR:HG22	1:F:127:HIS:CD2	2.46	0.50
1:G:18:LYS:HE2	1:G:23:LEU:HD22	1.93	0.50
1:C:209:GLU:HG3	1:C:271:THR:HG21	1.92	0.50
1:G:290:VAL:CG1	1:H:477:ILE:HB	2.38	0.50
1:A:285:GLU:OE2	2:A:601:4VP:O4'	2.30	0.50
1:F:104:LEU:HD11	1:F:340:GLU:HB2	1.94	0.50
1:C:41:ARG:NH2	1:C:324:ASP:OD2	2.44	0.49
1:D:209:GLU:HG2	1:D:271:THR:OG1	2.12	0.49
1:H:4:LEU:HD13	1:H:16:VAL:HG12	1.93	0.49
1:C:152:TYR:CZ	1:C:177:MET:HB2	2.47	0.49
1:H:24:ILE:HG12	1:H:49:PRO:HB2	1.93	0.49
1:B:106[B]:CYS:HG	1:B:239:TYR:HE1	1.58	0.49
1:F:25:GLU:HG2	1:F:52:LEU:HD23	1.95	0.49
1:G:292:LYS:O	1:G:293:SER:HB2	2.13	0.49
1:G:375:LEU:HB3	1:G:377:THR:HG22	1.94	0.49
1:A:290:VAL:HB	1:C:477:ILE:HB	1.93	0.49
1:F:112:LEU:O	3:F:770:HOH:O	2.19	0.49
1:H:366:LYS:NZ	3:H:728:HOH:O	2.11	0.49
1:C:133:LYS:NZ	3:C:802:HOH:O	2.46	0.49
1:E:456:LYS:NZ	3:E:761:HOH:O	2.43	0.49
1:H:435:ASP:HA	1:H:457:GLY:CA	2.42	0.49
1:B:478:THR:HG21	1:B:483:LYS:HE3	1.94	0.49
1:E:436:ASP:OD1	1:E:436:ASP:N	2.46	0.49
1:D:152:TYR:CZ	1:D:177:MET:HB2	2.48	0.49
1:F:11:ARG:NH2	1:F:265:GLU:CD	2.66	0.49
1:G:379:PRO:HD3	1:G:470:TYR:CD1	2.48	0.49
1:H:387:GLY:HA3	1:H:434:PHE:CZ	2.48	0.49
1:D:272:LEU:HD11	1:D:299:PRO:HB2	1.94	0.48
1:C:228:MET:SD	2:C:601:4VP:H3	2.52	0.48
1:C:121:SER:O	1:C:123:PRO:HD3	2.14	0.48
1:H:4:LEU:N	3:H:680:HOH:O	2.45	0.48
1:A:278:HIS:HB2	1:A:300:LEU:HD13	1.95	0.48
1:G:280:GLU:N	1:G:294:GLN:OE1	2.47	0.48
1:B:489:LEU:HD11	1:E:35:GLU:HG2	1.94	0.48
1:F:11:ARG:NH2	1:F:265:GLU:OE1	2.47	0.48
1:D:477:ILE:HB	1:F:290:VAL:HB	1.96	0.48
1:F:160:ILE:HB	1:F:213:ALA:HB3	1.95	0.48
1:F:106:CYS:HA	1:F:109:LYS:HD2	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLY:HA3	1:B:281:GLY:HA3	1.95	0.47
1:E:111:PRO:HB2	1:E:238:ASP:HB3	1.95	0.47
1:C:230:ILE:HG22	3:C:811:HOH:O	2.13	0.47
1:B:21:ASP:O	1:B:78:LYS:NZ	2.48	0.47
1:F:379:PRO:HG3	1:F:470:TYR:CE1	2.49	0.47
1:A:210:ILE:HB	1:A:272:LEU:HB3	1.96	0.47
1:A:296:HIS:CG	1:A:297:PRO:HD2	2.50	0.47
1:D:436:ASP:N	1:D:436:ASP:OD1	2.47	0.47
1:F:18:LYS:HG2	1:F:23:LEU:HD22	1.96	0.47
1:G:373:GLN:NE2	1:G:377:THR:HG23	2.28	0.47
1:G:465:ILE:HB	1:G:470:TYR:CE2	2.50	0.47
1:H:173:ILE:HG21	1:H:227:SER:HA	1.97	0.47
1:A:239:TYR:OH	3:A:791:HOH:O	2.20	0.47
1:C:107:LYS:HE3	1:C:340:GLU:OE1	2.14	0.47
1:G:366:LYS:HE3	1:G:407:ASP:HA	1.96	0.47
1:B:9:GLU:HB2	1:B:12:ASP:HB2	1.96	0.46
1:E:54:LYS:NZ	3:E:859:HOH:O	2.47	0.46
1:A:325:GLU:HA	1:A:328:THR:HG22	1.97	0.46
1:G:373:GLN:HG2	1:G:376:LYS:HA	1.97	0.46
1:H:393:THR:HG22	1:H:395:VAL:H	1.79	0.46
1:B:208:ASN:N	3:B:763:HOH:O	2.47	0.46
1:E:448:GLN:OE1	3:E:708:HOH:O	2.21	0.46
1:E:132:GLU:HG2	1:E:133:LYS:HG2	1.97	0.46
1:G:477:ILE:HB	1:H:290:VAL:CG1	2.44	0.46
3:D:619:HOH:O	1:F:451:ARG:HD2	2.15	0.46
1:F:56:LEU:HD11	1:F:66:ILE:HG13	1.97	0.46
1:C:164:PRO:CD	1:C:200:SER:HB3	2.45	0.46
1:B:162:GLN:N	3:B:689:HOH:O	2.34	0.46
1:D:322:CYS:HA	1:D:323:THR:HA	1.76	0.46
1:G:162:GLN:OE1	1:G:166:LYS:HG3	2.16	0.46
1:F:86:HIS:HE1	1:F:92:PRO:HG3	1.81	0.46
1:G:361:LEU:HD12	1:H:422:VAL:HG12	1.98	0.46
1:H:377:THR:OG1	1:H:378:THR:N	2.49	0.46
1:C:190:LYS:NZ	1:C:196:GLN:OE1	2.28	0.45
1:H:355:PRO:CD	1:H:364:ILE:HD13	2.46	0.45
1:C:224:LEU:O	1:C:227:SER:HB2	2.16	0.45
1:G:173:ILE:HD12	1:G:223:ILE:HD11	1.99	0.45
1:H:86:HIS:CE1	1:H:92:PRO:HG3	2.50	0.45
1:B:132:GLU:CD	1:B:132:GLU:H	2.18	0.45
1:B:377:THR:OG1	1:B:378:THR:N	2.48	0.45
1:D:41:ARG:HD3	1:D:45:GLU:OE2	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:378:THR:OG1	3:H:726:HOH:O	2.20	0.45
1:B:209:GLU:HA	1:B:271:THR:HG23	1.99	0.45
1:D:171:TRP:HB2	1:D:236:GLU:CG	2.46	0.45
1:F:387:GLY:HA3	1:F:434:PHE:CZ	2.52	0.45
1:G:380:GLU:N	1:G:380:GLU:OE1	2.45	0.45
1:G:401:GLU:HG3	1:G:460:CYS:SG	2.56	0.45
1:F:41:ARG:NH2	1:F:324:ASP:OD2	2.49	0.45
1:A:24:ILE:HG12	1:A:49:PRO:HB2	1.99	0.45
1:G:372:LEU:O	1:G:375:LEU:HB2	2.17	0.45
1:A:450:SER:O	1:A:453:LYS:HG3	2.16	0.45
1:D:18:LYS:HG3	1:D:23:LEU:HD22	1.98	0.45
1:E:322:CYS:HA	1:E:323:THR:HA	1.82	0.44
1:G:293:SER:OG	1:G:294:GLN:N	2.49	0.44
1:H:21:ASP:O	1:H:78:LYS:NZ	2.49	0.44
1:D:256:ASN:HB2	3:D:785:HOH:O	2.17	0.44
1:E:466:PHE:HB2	1:E:469:GLN:HG3	2.00	0.44
1:F:272:LEU:HD11	1:F:299:PRO:HB3	2.00	0.44
1:G:18:LYS:HG3	1:G:23:LEU:HD22	1.98	0.44
1:A:42:LYS:HD2	1:C:481:PHE:CE2	2.52	0.44
1:B:26:ILE:HA	3:B:661:HOH:O	2.16	0.44
1:B:451:ARG:HD2	3:B:622:HOH:O	2.18	0.44
1:F:6:PRO:O	1:F:220:PRO:HG2	2.17	0.44
1:E:187:LEU:HD21	1:E:189:ILE:HD11	2.00	0.44
1:F:438:THR:O	1:F:459:LYS:HE3	2.18	0.44
1:B:41:ARG:HD3	1:B:44:TYR:HD2	1.83	0.44
1:E:223:ILE:HA	1:E:223:ILE:HD12	1.92	0.44
1:E:104:LEU:HD22	1:E:340:GLU:OE2	2.17	0.44
1:F:294:GLN:HG2	1:F:294:GLN:H	1.54	0.44
1:F:442:LEU:HA	1:F:442:LEU:HD12	1.88	0.44
1:H:326:THR:O	1:H:330:ILE:HB	2.18	0.44
1:A:208:ASN:N	1:A:208:ASN:ND2	2.66	0.44
1:B:74:ARG:NH2	1:B:78:LYS:O	2.44	0.44
1:G:91:ASP:HA	1:G:92:PRO:HD2	1.86	0.44
1:A:489:LEU:HD11	1:C:35:GLU:HG3	1.99	0.43
1:C:438:THR:O	1:C:459:LYS:HE3	2.17	0.43
1:F:104:LEU:HA	1:F:104:LEU:HD12	1.74	0.43
1:G:373:GLN:HG2	1:G:376:LYS:CA	2.48	0.43
1:C:230:ILE:HD11	1:C:239:TYR:CD2	2.54	0.43
1:E:190:LYS:HD2	1:E:196:GLN:OE1	2.18	0.43
1:F:164:PRO:HG3	1:F:201:TRP:CD2	2.53	0.43
1:C:18:LYS:HE2	1:C:23:LEU:HD22	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:451:ARG:HD2	3:E:732:HOH:O	2.17	0.43
1:H:322:CYS:HA	1:H:323:THR:HA	1.73	0.43
1:H:104:LEU:HD21	1:H:340:GLU:HB2	2.01	0.43
1:B:322:CYS:HA	1:B:323:THR:HA	1.80	0.43
1:H:435:ASP:HA	1:H:457:GLY:HA2	2.00	0.43
1:H:91:ASP:HA	1:H:92:PRO:HD3	1.87	0.43
1:B:228:MET:HB2	1:B:333:LEU:HD12	2.00	0.43
1:E:173:ILE:HG22	1:E:226:SER:O	2.19	0.43
1:H:48:LEU:HB3	1:H:49:PRO:HD2	2.01	0.43
1:A:175:ARG:CZ	1:A:187:LEU:HD22	2.49	0.43
1:C:422:VAL:HG12	1:C:423:THR:HG23	2.00	0.43
1:C:471:GLU:OE1	1:C:472:ARG:NH1	2.51	0.43
1:H:133:LYS:CE	3:H:690:HOH:O	2.65	0.43
1:H:167:LYS:HA	1:H:167:LYS:HD3	1.49	0.43
1:H:384:LYS:HE3	1:H:392:ARG:NH2	2.33	0.43
1:C:415:LYS:HG2	3:C:799:HOH:O	2.19	0.42
1:E:220:PRO:O	1:E:223:ILE:HG22	2.19	0.42
1:E:208:ASN:HA	1:E:273:SER:HA	2.00	0.42
1:G:173:ILE:CG2	1:G:227:SER:HA	2.48	0.42
1:H:31:ASP:O	1:H:35:GLU:HB2	2.19	0.42
3:A:721:HOH:O	1:C:451:ARG:HD2	2.18	0.42
1:C:333:LEU:O	1:C:337:GLU:HG2	2.20	0.42
1:H:228:MET:HG2	1:H:330:ILE:HG12	2.02	0.42
1:E:387:GLY:HA3	1:E:434:PHE:CZ	2.55	0.42
1:G:187:LEU:HA	1:G:298:CYS:SG	2.60	0.42
1:A:10:PHE:O	1:A:13:PHE:HB3	2.20	0.42
1:B:10:PHE:O	1:B:13:PHE:HB3	2.20	0.42
1:B:270:GLY:HA3	1:B:302:THR:O	2.20	0.42
1:F:223:ILE:HA	1:F:223:ILE:HD12	1.94	0.42
1:H:104:LEU:HA	1:H:104:LEU:HD23	1.78	0.42
1:H:384:LYS:HD2	1:H:434:PHE:CZ	2.54	0.42
1:G:325:GLU:HA	1:G:328:THR:HG22	2.02	0.42
1:H:469:GLN:HG2	3:H:606:HOH:O	2.20	0.42
1:G:25:GLU:OE2	1:G:54:LYS:NZ	2.53	0.42
1:B:438:THR:O	1:B:459:LYS:HE3	2.20	0.42
1:D:112:LEU:HD23	1:D:112:LEU:HA	1.83	0.42
1:B:272:LEU:HD12	1:B:273:SER:N	2.34	0.42
1:C:228:MET:HG2	1:C:330:ILE:HD13	2.01	0.42
1:C:387:GLY:HA3	1:C:434:PHE:CZ	2.55	0.42
1:E:284:GLY:CA	1:E:290:VAL:HG22	2.49	0.42
1:E:227:SER:HB2	1:E:333:LEU:CD1	2.49	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:4VP:H4	2:A:601:4VP:H1	1.81	0.41
1:D:46:SER:HB2	1:D:48:LEU:HG	2.02	0.41
1:E:293:SER:HB2	3:E:831:HOH:O	2.20	0.41
1:H:17:LEU:HA	1:H:17:LEU:HD12	1.86	0.41
1:H:132:GLU:OE2	1:H:133:LYS:HE2	2.20	0.41
1:C:322:CYS:HA	1:C:323:THR:HA	1.70	0.41
1:C:418:ILE:HD12	1:C:418:ILE:HA	1.90	0.41
1:F:231:PRO:O	1:F:234:VAL:HG12	2.20	0.41
1:H:86:HIS:HE1	1:H:92:PRO:HG3	1.85	0.41
1:C:277:THR:CB	1:C:297:PRO:HB2	2.48	0.41
1:D:302:THR:OG1	3:D:676:HOH:O	2.21	0.41
1:E:204:ILE:HG13	1:E:206:LYS:HG2	2.02	0.41
1:G:322:CYS:HA	1:G:323:THR:HA	1.73	0.41
1:B:63:LEU:HA	1:B:64:PHE:HB3	2.02	0.41
1:C:161:LEU:HB3	1:C:197:ILE:HG21	2.02	0.41
1:B:42:LYS:HE3	1:E:494:ASN:OD1	2.21	0.41
1:C:104:LEU:HD21	1:C:340:GLU:HB2	2.02	0.41
1:C:278:HIS:HB2	1:C:300:LEU:HD13	2.02	0.41
1:D:497:TRP:CZ3	1:F:42:LYS:HD3	2.56	0.41
1:A:322:CYS:HA	1:A:323:THR:HA	1.79	0.41
1:G:63:LEU:HD21	1:G:308:TYR:CG	2.55	0.41
1:E:293:SER:C	3:E:855:HOH:O	2.58	0.41
1:H:230:ILE:HG21	1:H:236:GLU:OE2	2.21	0.41
1:C:210:ILE:HB	1:C:272:LEU:HG	2.03	0.41
1:C:442:LEU:HD23	1:C:442:LEU:HA	1.66	0.41
1:G:400:HIS:ND1	1:G:459:LYS:HG2	2.36	0.41
1:G:467:ARG:H	1:H:448:GLN:HE22	1.69	0.41
1:B:440:PHE:HA	1:B:441:PRO:HD3	1.94	0.41
1:D:129:LEU:HD22	1:D:133:LYS:HB3	2.02	0.41
1:G:369:LEU:HD23	1:G:369:LEU:HA	1.87	0.41
1:A:42:LYS:HE3	1:C:494:ASN:OD1	2.21	0.40
1:C:6:PRO:HG3	1:C:16:VAL:HG11	2.02	0.40
1:D:162:GLN:N	3:D:677:HOH:O	2.34	0.40
1:G:103:LEU:HD23	1:G:103:LEU:HA	1.91	0.40
1:H:342:ALA:HB2	1:H:390:TYR:OH	2.21	0.40
1:C:164:PRO:HD2	1:C:200:SER:HB3	2.03	0.40
1:C:404:LEU:O	1:C:464:CYS:HB2	2.22	0.40
1:F:94:THR:HG22	1:F:98:GLU:HB2	2.03	0.40
1:G:46:SER:HB2	1:G:48:LEU:HG	2.02	0.40
1:A:487:LYS:HA	1:A:490:VAL:HB	2.02	0.40
1:C:279:LEU:HD23	1:C:279:LEU:HA	1.80	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:434:PHE:O	1:H:457:GLY:HA2	2.21	0.40
1:A:152:TYR:CZ	1:A:177:MET:HB2	2.56	0.40
1:E:401:GLU:HG3	1:E:460:CYS:SG	2.62	0.40
1:H:236:GLU:O	1:H:240:VAL:HG23	2.21	0.40
1:H:472:ARG:HB2	1:H:472:ARG:CZ	2.52	0.40
1:B:208:ASN:OD1	1:B:275:THR:HG23	2.21	0.40
1:B:393:THR:CG2	1:B:395:VAL:H	2.31	0.40
1:F:126:THR:HG22	1:F:127:HIS:HD2	1.87	0.40
1:F:75:SER:HB2	1:F:77:GLU:OE2	2.21	0.40
1:G:373:GLN:CG	1:G:377:THR:H	2.34	0.40
1:H:210:ILE:HA	1:H:211:PRO:HD3	1.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:LYS:NZ	1:G:98:GLU:OE2[2_756]	2.15	0.05

## 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	464/503 (92%)	448 (97%)	15 (3%)	1 (0%)	51	59
1	B	470/503 (93%)	453 (96%)	17 (4%)	0	100	100
1	C	499/503 (99%)	476 (95%)	21 (4%)	2 (0%)	38	42
1	D	475/503 (94%)	455 (96%)	19 (4%)	1 (0%)	51	59
1	E	486/503 (97%)	472 (97%)	14 (3%)	0	100	100
1	F	499/503 (99%)	482 (97%)	16 (3%)	1 (0%)	51	59
1	G	465/503 (92%)	445 (96%)	18 (4%)	2 (0%)	38	42

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	478/503 (95%)	453 (95%)	23 (5%)	2 (0%)	38	42
All	All	3836/4024 (95%)	3684 (96%)	143 (4%)	9 (0%)	51	59

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	228	MET
1	F	294	GLN
1	G	436	ASP
1	H	228	MET
1	C	293	SER
1	D	230	ILE
1	G	428	VAL
1	H	233	GLY
1	A	119	VAL

### 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	413/438 (94%)	404 (98%)	9 (2%)	57	70
1	B	420/438 (96%)	409 (97%)	11 (3%)	51	63
1	C	436/438 (100%)	419 (96%)	17 (4%)	37	48
1	D	422/438 (96%)	402 (95%)	20 (5%)	30	38
1	E	429/438 (98%)	421 (98%)	8 (2%)	62	74
1	F	436/438 (100%)	425 (98%)	11 (2%)	53	64
1	G	415/438 (95%)	398 (96%)	17 (4%)	35	45
1	H	421/438 (96%)	405 (96%)	16 (4%)	38	48
All	All	3392/3504 (97%)	3283 (97%)	109 (3%)	44	54

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	A	165	ASP
1	A	172	SER
1	A	208	ASN
1	A	226	SER
1	A	271	THR
1	A	276	ASP
1	A	328	THR
1	A	460	CYS
1	B	23	LEU
1	B	41	ARG
1	B	167	LYS
1	B	172	SER
1	B	271	THR
1	B	290	VAL
1	B	307	SER
1	B	328	THR
1	B	393	THR
1	B	435	ASP
1	B	460	CYS
1	C	24	ILE
1	C	41	ARG
1	C	107	LYS
1	C	161	LEU
1	C	209	GLU
1	C	227	SER
1	C	230	ILE
1	C	236	GLU
1	C	271	THR
1	C	272	LEU
1	C	275	THR
1	C	345	SER
1	C	370	LYS
1	C	384	LYS
1	C	394	LYS
1	C	422	VAL
1	C	460	CYS
1	D	41	ARG
1	D	107	LYS
1	D	138[A]	SER
1	D	138[B]	SER
1	D	147	SER
1	D	172	SER

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	181	ASP
1	D	230	ILE
1	D	232	GLU
1	D	234	VAL
1	D	239	TYR
1	D	246	GLU
1	D	251	VAL
1	D	271	THR
1	D	274	LEU
1	D	275	THR
1	D	344	GLU
1	D	385	LYS
1	D	393	THR
1	D	460	CYS
1	E	23	LEU
1	E	64	PHE
1	E	133	LYS
1	E	187	LEU
1	E	275	THR
1	E	460	CYS
1	E	467	ARG
1	E	495	GLU
1	F	3	LYS
1	F	11	ARG
1	F	41	ARG
1	F	77	GLU
1	F	121	SER
1	F	200	SER
1	F	247	SER
1	F	254	GLU
1	F	271	THR
1	F	394	LYS
1	F	460	CYS
1	G	23	LEU
1	G	130	SER
1	G	182	LYS
1	G	187	LEU
1	G	220	PRO
1	G	272	LEU
1	G	290	VAL
1	G	294	GLN
1	G	298	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	328	THR
1	G	373	GLN
1	G	377	THR
1	G	407	ASP
1	G	425	HIS
1	G	460	CYS
1	G	472	ARG
1	G	487	LYS
1	H	17	LEU
1	H	56	LEU
1	H	124	CYS
1	H	172	SER
1	H	239	TYR
1	H	251	VAL
1	H	271	THR
1	H	290	VAL
1	H	328	THR
1	H	381	GLU
1	H	394	LYS
1	H	400	HIS
1	H	435	ASP
1	H	448	GLN
1	H	450	SER
1	H	454	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	162	GLN
1	F	468	GLN
1	G	183	HIS
1	G	373	GLN
1	H	400	HIS

### 5.3.3 RNA ⓘ

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](#)

5 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	4VP	A	601	-	9,9,9	0.63	0	11,11,11	0.92	0
2	4VP	C	601	-	9,9,9	0.64	0	11,11,11	0.86	0
2	4VP	E	601	-	9,9,9	0.77	0	11,11,11	0.76	0
2	4VP	F	601	-	9,9,9	0.77	0	11,11,11	0.67	0
2	4VP	G	601	-	9,9,9	0.72	0	11,11,11	0.77	0

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	4VP	A	601	-	-	0/2/2/2	0/1/1/1
2	4VP	C	601	-	-	0/2/2/2	0/1/1/1
2	4VP	E	601	-	-	0/2/2/2	0/1/1/1
2	4VP	F	601	-	-	0/2/2/2	0/1/1/1
2	4VP	G	601	-	-	0/2/2/2	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	4VP	2	0
2	C	601	4VP	2	0
2	E	601	4VP	1	0

## 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	472/503 (93%)	-0.24	11 (2%) 61 70	22, 37, 66, 87	0
1	B	476/503 (94%)	-0.18	15 (3%) 48 59	23, 36, 66, 110	0
1	C	501/503 (99%)	-0.36	3 (0%) 89 93	25, 40, 64, 87	0
1	D	480/503 (95%)	-0.24	13 (2%) 55 64	19, 35, 66, 95	0
1	E	492/503 (97%)	-0.36	1 (0%) 94 97	24, 37, 62, 82	0
1	F	501/503 (99%)	-0.15	12 (2%) 59 68	22, 46, 75, 94	0
1	G	472/503 (93%)	0.05	19 (4%) 39 50	26, 53, 85, 110	0
1	H	481/503 (95%)	0.05	28 (5%) 24 34	26, 46, 84, 107	0
All	All	3875/4024 (96%)	-0.18	102 (2%) 56 65	19, 40, 74, 110	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	168	TRP	9.3
1	H	168	TRP	7.3
1	D	296	HIS	5.6
1	A	293	SER	5.1
1	B	167	LYS	5.0
1	H	296	HIS	5.0
1	D	168	TRP	4.9
1	B	210	ILE	4.4
1	D	230	ILE	4.2
1	H	233	GLY	4.1
1	H	232	GLU	4.0
1	B	208	ASN	3.9
1	A	188	VAL	3.8
1	G	168	TRP	3.8
1	G	254	GLU	3.8
1	G	476	TYR	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	296	HIS	3.7
1	G	209	GLU	3.7
1	H	275	THR	3.6
1	H	293	SER	3.6
1	F	293	SER	3.5
1	B	165	ASP	3.5
1	D	188	VAL	3.4
1	G	255	THR	3.4
1	H	291	PHE	3.4
1	F	130	SER	3.3
1	D	208	ASN	3.3
1	H	187	LEU	3.2
1	G	210	ILE	3.2
1	B	163	THR	3.2
1	D	209	GLU	3.2
1	H	207	ALA	3.2
1	H	230	ILE	3.1
1	G	372	LEU	3.1
1	B	274	LEU	3.1
1	D	210	ILE	3.1
1	B	275	THR	3.1
1	H	448	GLN	3.0
1	D	167	LYS	3.0
1	G	474	PHE	3.0
1	H	164	PRO	3.0
1	H	274	LEU	3.0
1	D	503	LYS	3.0
1	A	296	HIS	3.0
1	G	208	ASN	3.0
1	F	281	GLY	2.9
1	F	294	GLN	2.9
1	F	254	GLU	2.9
1	B	299	PRO	2.9
1	G	470	TYR	2.9
1	G	373	GLN	2.8
1	F	117	VAL	2.7
1	H	449	SER	2.7
1	F	209	GLU	2.7
1	H	294	GLN	2.7
1	H	165	ASP	2.7
1	A	275	THR	2.7
1	A	503	LYS	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	165	ASP	2.6
1	H	281	GLY	2.6
1	C	3	LYS	2.5
1	H	503	LYS	2.5
1	F	208	ASN	2.5
1	A	162	GLN	2.5
1	G	132	GLU	2.5
1	B	272	LEU	2.5
1	A	161	LEU	2.5
1	B	209	GLU	2.5
1	D	165	ASP	2.5
1	H	295	GLY	2.5
1	F	296	HIS	2.4
1	C	49	PRO	2.4
1	H	166	LYS	2.3
1	G	164	PRO	2.3
1	F	128	ILE	2.3
1	H	161	LEU	2.3
1	F	262	ALA	2.3
1	A	163	THR	2.2
1	A	164	PRO	2.2
1	H	374	ALA	2.2
1	D	232	GLU	2.2
1	E	192	GLN	2.2
1	A	276	ASP	2.2
1	G	117	VAL	2.1
1	H	234	VAL	2.1
1	B	187	LEU	2.1
1	B	276	ASP	2.1
1	B	171	TRP	2.1
1	A	208	ASN	2.1
1	H	255	THR	2.1
1	H	208	ASN	2.1
1	F	3	LYS	2.1
1	G	302	THR	2.1
1	H	163	THR	2.1
1	H	229	PRO	2.1
1	G	274	LEU	2.1
1	D	275	THR	2.1
1	G	473	SER	2.1
1	B	235	SER	2.0
1	H	384	LYS	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	164	PRO	2.0
1	G	467	ARG	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	4VP	F	601	9/9	0.90	0.19	3.49	42,45,53,57	0
2	4VP	G	601	9/9	0.87	0.18	3.49	49,51,61,66	0
2	4VP	A	601	9/9	0.83	0.20	3.38	55,58,64,66	0
2	4VP	E	601	9/9	0.90	0.19	1.90	40,41,62,68	0
2	4VP	C	601	9/9	0.91	0.17	0.86	48,50,54,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.