Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:49 AM GMT

PDB ID	:	2UUE
Title	:	REPLACE: A strategy for Iterative Design of Cyclin Binding Groove Inhibitors
Authors	:	Andrews, M.J.; Kontopidis, G.; Mcinnes, C.; Plater, A.; Innes, L.; Cowan, A.; Jewsbury, P.; Fischer, P.M.
Deposited on	:	2007-03-02
Resolution	:	2.06 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:

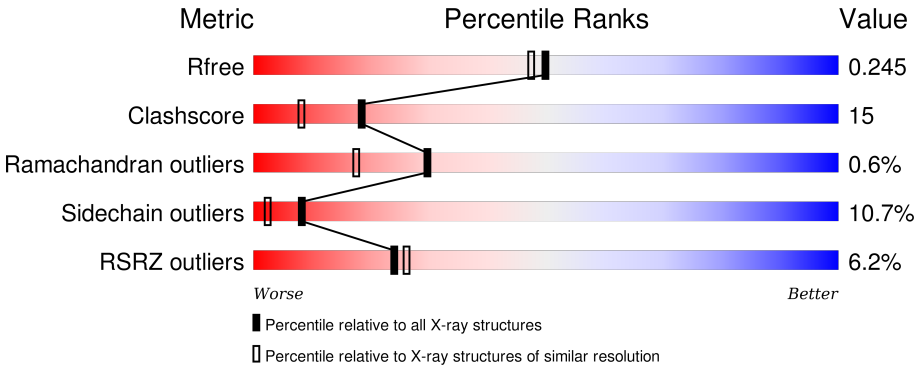
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.06 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	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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	298	8% 69% 25%
1	C	298	7% 69% 23% 6%
2	B	259	4% 75% 20%
2	D	259	5% 75% 20%
3	E	5	60% 20% 20%

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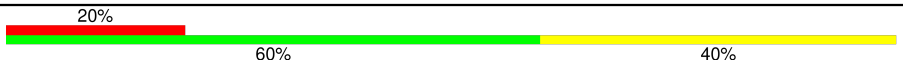
Mol	Chain	Length	Quality of chain
3	F	5	

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
4	MTZ	A	1297	-	-	X	-
5	GVC	F	1433	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9332 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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2378	1547	403	420	8			
1	C	297	Total	C	N	O	S	0	0	1
			2379	1547	404	420	8			

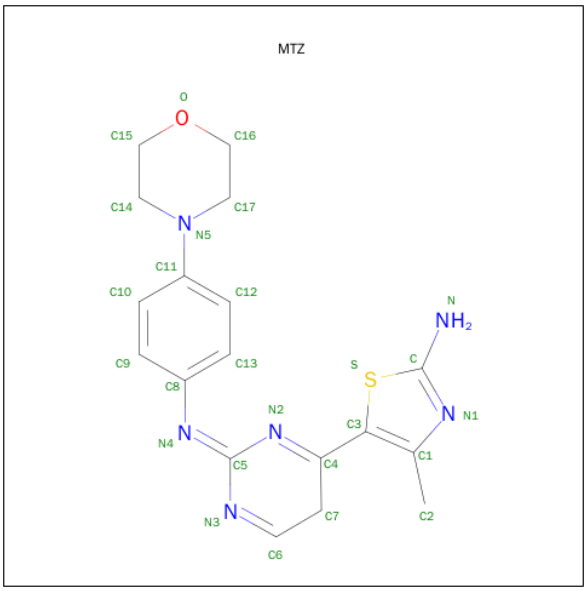
- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2084	1350	339	384	11			

- Molecule 3 is a protein called GVC-TETRAPEPTIDE INHIBITOR.

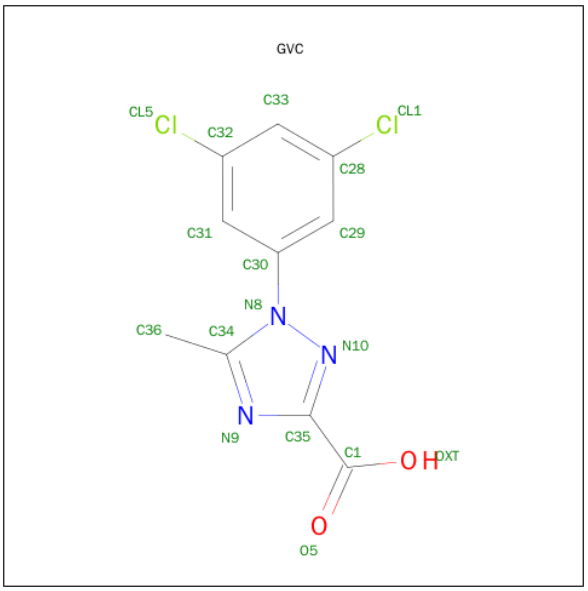
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	5	Total	C	F	N	O	0	0	1
			40	27	1	8	4			
3	F	5	Total	C	F	N	O	0	0	1
			40	27	1	8	4			

- Molecule 4 is 4-METHYL-5-{(2E)-2-[(4-MORPHOLIN-4-YLPHENYL)IMINO]-2,5-DIHYDROPYRIMIDIN-4-YL}-1,3-THIAZOL-2-AMINE (three-letter code: MTZ) (formula: $C_{18}H_{20}N_6OS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	18	6	1	1		
4	C	1	Total	C	N	O	S	0	0
			26	18	6	1	1		

- Molecule 5 is 1-(3,5-DICHLOROPHENYL)-5-METHYL-1H-1,2,4-TRIAZOLE-3-CARBOX YLIC ACID (three-letter code: GVC) (formula: $C_{10}H_7Cl_2N_3O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	Cl	N	O	0	0
			16	10	2	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total	C	Cl	N	O	0	0
			16	10	2	3	1		

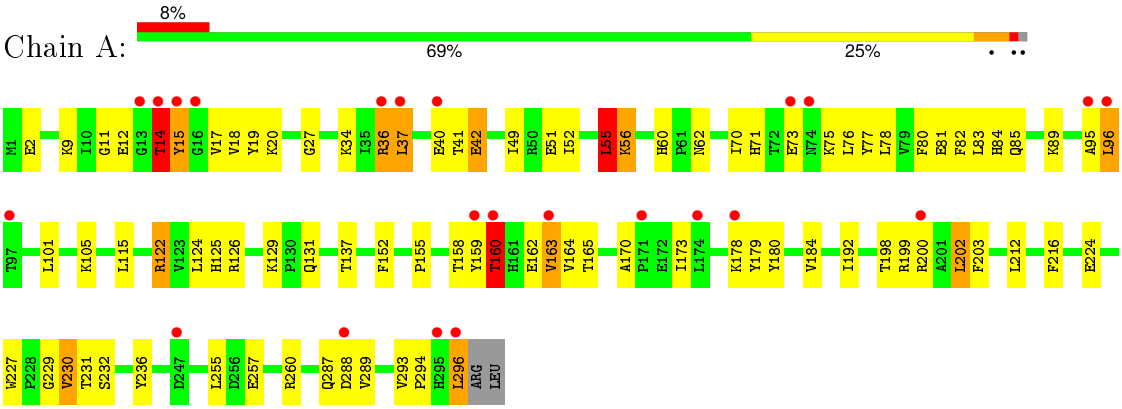
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	49	Total	O	0	0
			49	49		
6	B	64	Total	O	0	0
			64	64		
6	C	65	Total	O	0	0
			65	65		
6	D	63	Total	O	0	0
			63	63		
6	E	2	Total	O	0	0
			2	2		
6	F	1	Total	O	0	0
			1	1		

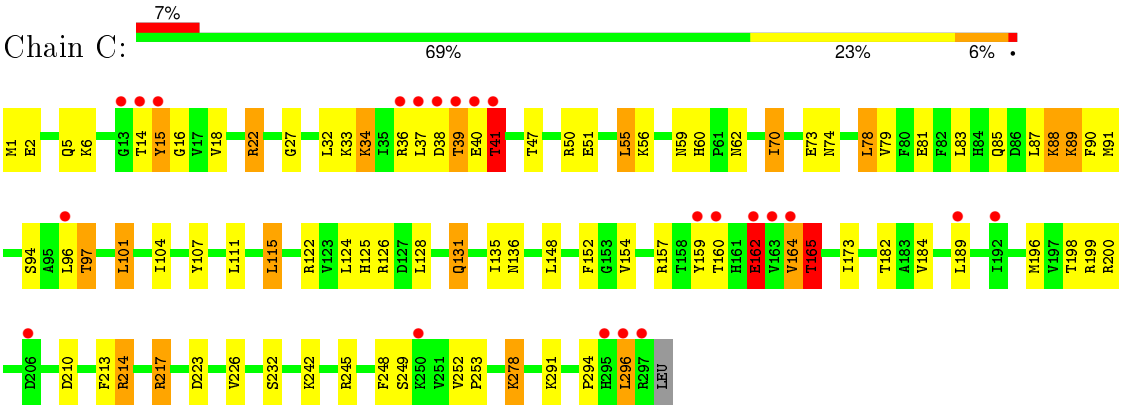
3 Residue-property plots (i)

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.

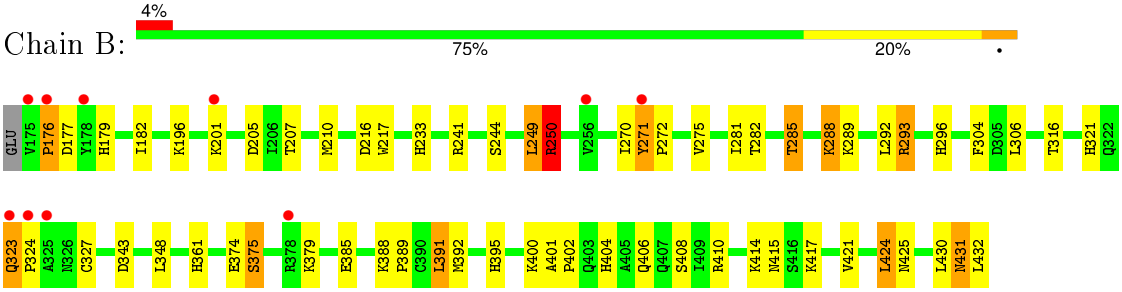
- Molecule 1: CELL DIVISION PROTEIN KINASE 2



- Molecule 1: CELL DIVISION PROTEIN KINASE 2

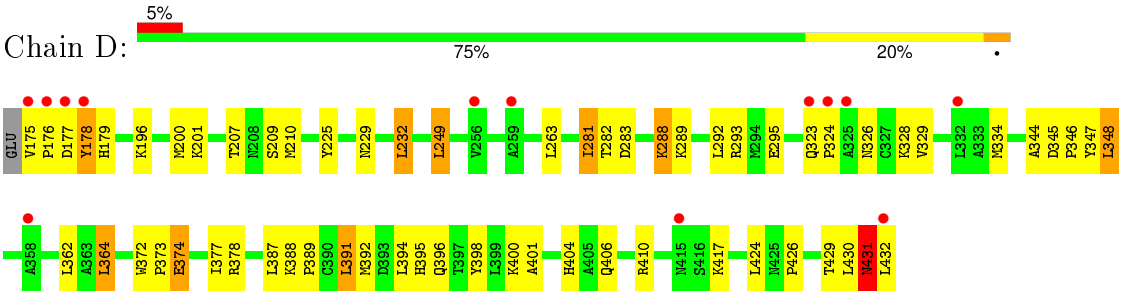


- Molecule 2: CYCLIN A2



- Molecule 2: CYCLIN A2

Chain D:



• Molecule 3: GVC-TETRAPEPTIDE INHIBITOR

Chain E:

• Molecule 3: GVC-TETRAPEPTIDE INHIBITOR

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.56Å 113.80Å 155.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.29 – 2.06 19.90 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (91.29-2.06) 99.0 (19.90-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.244 0.199 , 0.245	Depositor DCC
R_{free} test set	2299 reflections (3.09%)	DCC
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 76777 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9332	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: MTZ, GVC, NH2, PFF

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	0/2440	0.74	2/3313 (0.1%)
1	C	0.48	0/2441	0.77	1/3315 (0.0%)
2	B	0.48	0/2133	0.77	2/2896 (0.1%)
2	D	0.49	0/2134	0.76	2/2897 (0.1%)
3	E	1.54	1/26 (3.8%)	1.72	1/33 (3.0%)
3	F	1.50	1/26 (3.8%)	1.66	1/33 (3.0%)
All	All	0.49	2/9200 (0.0%)	0.77	9/12487 (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	3
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	ARG	CB-CG	-6.95	1.33	1.52
3	E	1	ARG	CB-CG	-6.94	1.33	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	250	ARG	NE-CZ-NH1	8.14	124.37	120.30
2	B	250	ARG	NE-CZ-NH2	-6.71	116.94	120.30
2	D	364	LEU	CA-CB-CG	6.27	129.72	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	LEU	CB-CG-CD1	6.14	121.44	111.00
1	C	50	ARG	NE-CZ-NH1	-5.97	117.31	120.30
3	E	1	ARG	CD-NE-CZ	5.96	131.94	123.60
3	F	1	ARG	CD-NE-CZ	5.71	131.60	123.60
1	A	55	LEU	CB-CG-CD2	5.52	120.39	111.00
2	D	232	LEU	CB-CG-CD2	5.39	120.17	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	THR	Peptide
1	C	162	GLU	Peptide
1	C	37	LEU	Peptide
1	C	70	ILE	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	2378	0	2426	86	0
1	C	2379	0	2426	93	0
2	B	2083	0	2107	57	0
2	D	2084	0	2107	46	0
3	E	40	0	41	1	0
3	F	40	0	41	0	0
4	A	26	0	20	13	0
4	C	26	0	20	5	0
5	E	16	0	6	3	0
5	F	16	0	6	3	0
6	A	49	0	0	3	0
6	B	64	0	0	7	0
6	C	65	0	0	15	0
6	D	63	0	0	5	0
6	E	2	0	0	1	0
6	F	1	0	0	0	0
All	All	9332	0	9200	283	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (283) 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:178:LYS:HA	6:A:2035:HOH:O	1.28	1.31
1:C:59:ASN:HB2	6:C:2014:HOH:O	1.49	1.11
5:E:1433:GVC:C29	5:E:1433:GVC:H361	1.73	1.11
1:A:42:GLU:OE2	2:B:275:VAL:HG23	1.50	1.11
5:E:1433:GVC:C36	5:E:1433:GVC:H29	1.80	1.09
1:C:162:GLU:HB2	1:C:164:VAL:HG23	1.37	1.02
2:B:207:THR:HG22	2:B:210:MET:HG3	1.42	1.02
5:F:1433:GVC:H29	5:F:1433:GVC:H361	1.03	1.01
1:C:15:TYR:CE1	1:C:47:THR:OG1	2.09	1.01
1:C:124:LEU:HD22	6:C:2045:HOH:O	1.59	1.00
5:F:1433:GVC:C29	5:F:1433:GVC:H361	1.90	0.99
1:C:124:LEU:HB3	6:C:2045:HOH:O	1.62	0.98
1:A:11:GLY:O	1:A:17:VAL:HG23	1.65	0.97
1:C:15:TYR:HE1	1:C:47:THR:OG1	1.41	0.97
1:C:15:TYR:HD2	1:C:16:GLY:H	1.00	0.97
1:A:95:ALA:O	1:A:96:LEU:HB3	1.65	0.97
2:D:404:HIS:HD2	2:D:406:GLN:H	1.11	0.96
5:F:1433:GVC:H29	5:F:1433:GVC:C36	1.94	0.95
2:B:404:HIS:HD2	2:B:406:GLN:H	1.09	0.93
1:C:6:LYS:NZ	1:C:34:LYS:NZ	2.18	0.91
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.52	0.91
1:A:137:THR:HG22	1:A:296:LEU:HD23	1.53	0.91
1:A:257:GLU:HG3	1:A:260:ARG:HH22	1.34	0.91
1:C:6:LYS:HZ3	1:C:34:LYS:NZ	1.69	0.90
1:C:124:LEU:CB	6:C:2045:HOH:O	2.17	0.90
1:A:56:LYS:HD2	6:B:2037:HOH:O	1.72	0.89
1:C:1:MET:CE	1:C:70:ILE:HD13	2.03	0.89
2:B:288:LYS:NZ	2:B:288:LYS:HB2	1.87	0.88
1:A:56:LYS:CD	6:B:2037:HOH:O	2.22	0.88
1:A:163:VAL:O	1:A:163:VAL:HG13	1.75	0.86
1:A:257:GLU:HG3	1:A:260:ARG:NH2	1.91	0.85
2:B:288:LYS:HZ2	2:B:288:LYS:HB2	1.40	0.85
1:C:214:ARG:HG3	1:C:214:ARG:HH11	1.42	0.84
2:B:282:THR:O	2:B:285:THR:CG2	2.28	0.82
2:B:282:THR:O	2:B:285:THR:HG22	1.79	0.82
4:A:1297:MTZ:H9	4:A:1297:MTZ:N2	1.95	0.81
1:C:173:ILE:HD11	1:C:184:VAL:HG11	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLU:O	4:A:1297:MTZ:H6	1.81	0.80
1:A:17:VAL:HG13	1:A:19:TYR:HE1	1.48	0.78
1:C:88:LYS:O	1:C:88:LYS:HD3	1.84	0.78
1:C:60:HIS:HD2	1:C:62:ASN:H	1.31	0.78
5:E:1433:GVC:H361	5:E:1433:GVC:H29	0.85	0.77
2:D:176:PRO:HD2	2:D:179:HIS:CE1	2.19	0.77
2:B:288:LYS:CB	2:B:288:LYS:NZ	2.47	0.77
1:C:1:MET:HE2	1:C:70:ILE:HD13	1.66	0.77
1:C:124:LEU:CD2	6:C:2045:HOH:O	2.26	0.75
1:C:15:TYR:HD2	1:C:16:GLY:N	1.81	0.74
2:D:175:VAL:HA	2:D:179:HIS:ND1	2.02	0.74
1:C:60:HIS:CD2	1:C:62:ASN:H	2.05	0.74
2:D:225:TYR:HE1	2:D:281:ILE:HD13	1.53	0.74
2:D:207:THR:HG21	6:D:2016:HOH:O	1.88	0.73
1:C:210:ASP:HB2	6:C:2048:HOH:O	1.89	0.73
2:B:217:TRP:CZ2	2:B:281:ILE:HD12	2.24	0.73
1:A:173:ILE:HD11	1:A:184:VAL:HG11	1.72	0.72
1:A:227:TRP:O	1:A:230:VAL:HG22	1.89	0.72
1:A:2:GLU:HG3	6:A:2002:HOH:O	1.88	0.72
1:C:198:THR:O	1:C:199:ARG:HB2	1.90	0.72
2:D:430:LEU:O	2:D:431:ASN:HB2	1.88	0.72
2:B:205:ASP:OD2	2:B:250:ARG:HD2	1.90	0.72
1:A:163:VAL:O	1:A:163:VAL:CG1	2.37	0.72
1:C:73:GLU:OE1	2:D:293:ARG:NH2	2.20	0.72
1:A:14:THR:O	1:A:15:TYR:HB3	1.90	0.71
2:B:176:PRO:HA	2:B:179:HIS:ND1	2.08	0.69
1:C:15:TYR:HE1	1:C:47:THR:HG1	1.03	0.69
1:C:294:PRO:HB2	1:C:296:LEU:HD13	1.73	0.69
1:C:6:LYS:NZ	1:C:34:LYS:HZ1	1.89	0.68
1:C:6:LYS:NZ	1:C:34:LYS:HZ3	1.91	0.68
1:C:51:GLU:O	1:C:55:LEU:HB2	1.93	0.68
2:B:249:LEU:HD22	1:C:27:GLY:HA3	1.76	0.68
1:C:214:ARG:CG	1:C:214:ARG:HH11	2.07	0.68
2:B:404:HIS:CD2	2:B:406:GLN:H	2.01	0.67
4:A:1297:MTZ:C7	4:A:1297:MTZ:C2	2.73	0.67
2:B:430:LEU:O	2:B:431:ASN:HB2	1.93	0.67
1:A:34:LYS:HG3	1:A:77:TYR:CE2	2.30	0.67
1:A:9:LYS:HD2	1:A:17:VAL:HG21	1.76	0.67
1:C:1:MET:HE1	1:C:70:ILE:HD13	1.77	0.67
1:C:91:MET:CE	1:C:196:MET:HG3	2.26	0.66
2:B:207:THR:CG2	2:B:210:MET:HG3	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLU:O	4:C:1298:MTZ:H6	1.95	0.66
1:C:162:GLU:HB2	1:C:164:VAL:CG2	2.20	0.65
1:C:22:ARG:CD	6:C:2005:HOH:O	2.45	0.65
1:A:14:THR:O	1:A:15:TYR:CB	2.44	0.65
2:D:388:LYS:O	2:D:392:MET:HG2	1.96	0.65
2:D:178:TYR:HA	6:D:2005:HOH:O	1.96	0.65
2:B:327:CYS:HB3	6:B:2043:HOH:O	1.97	0.65
4:A:1297:MTZ:H2C3	4:A:1297:MTZ:H7C2	1.77	0.65
1:C:88:LYS:C	1:C:88:LYS:HD3	2.16	0.65
1:A:60:HIS:HD2	1:A:62:ASN:H	1.44	0.65
2:B:207:THR:HG23	2:B:210:MET:H	1.61	0.64
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.78	0.64
2:D:404:HIS:CD2	2:D:406:GLN:H	2.04	0.64
1:C:278:LYS:HE2	2:D:177:ASP:O	1.97	0.64
1:C:223:ASP:OD1	1:C:226:VAL:HG23	1.98	0.63
4:A:1297:MTZ:C9	4:A:1297:MTZ:N2	2.61	0.63
1:A:17:VAL:HG13	1:A:19:TYR:CE1	2.33	0.63
2:D:207:THR:HG22	2:D:210:MET:HG3	1.81	0.63
1:C:15:TYR:CD2	1:C:16:GLY:N	2.62	0.62
2:D:225:TYR:CE1	2:D:281:ILE:HD13	2.34	0.62
1:A:173:ILE:HD11	1:A:184:VAL:CG1	2.29	0.62
1:C:91:MET:CE	1:C:196:MET:CG	2.77	0.62
2:B:282:THR:HB	2:B:285:THR:HG23	1.82	0.61
1:A:294:PRO:HB2	1:A:296:LEU:HD13	1.83	0.61
2:B:288:LYS:HZ3	2:B:288:LYS:CB	2.13	0.60
1:C:6:LYS:HZ3	1:C:34:LYS:HZ1	1.43	0.59
1:A:36:ARG:O	1:A:36:ARG:HG2	2.02	0.59
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.38	0.59
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.84	0.59
1:A:84:HIS:HE1	1:A:296:LEU:HD21	1.67	0.59
1:A:170:ALA:HB3	1:A:173:ILE:HD12	1.85	0.59
2:B:217:TRP:CH2	2:B:281:ILE:HD12	2.38	0.59
1:C:128:LEU:HD13	1:C:189:LEU:HD13	1.85	0.59
6:A:2010:HOH:O	2:D:249:LEU:HD13	2.03	0.58
1:C:22:ARG:HD2	6:C:2005:HOH:O	2.03	0.58
1:C:6:LYS:HZ1	1:C:34:LYS:NZ	2.00	0.58
1:A:60:HIS:CD2	1:A:62:ASN:H	2.21	0.58
1:C:85:GLN:NE2	1:C:89:LYS:HB3	2.19	0.57
2:D:207:THR:HG23	2:D:209:SER:H	1.68	0.57
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.72	0.57
2:D:430:LEU:O	2:D:431:ASN:CB	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:LYS:NZ	6:B:2052:HOH:O	1.83	0.56
1:A:84:HIS:NE2	1:A:296:LEU:HG	2.20	0.56
2:B:388:LYS:O	2:B:392:MET:HG3	2.05	0.56
1:A:125:HIS:O	1:A:126:ARG:HB2	2.06	0.56
1:C:214:ARG:HG2	6:C:2049:HOH:O	2.05	0.56
1:C:173:ILE:HD11	1:C:184:VAL:CG1	2.32	0.56
2:D:334:MET:HE2	6:D:2022:HOH:O	2.05	0.56
2:D:175:VAL:HA	2:D:179:HIS:CE1	2.40	0.56
1:A:227:TRP:O	1:A:230:VAL:CG2	2.54	0.55
2:B:270:ILE:HG22	2:B:271:TYR:CD1	2.41	0.55
2:D:175:VAL:O	2:D:175:VAL:HG13	2.07	0.55
1:C:83:LEU:O	4:C:1298:MTZ:N4	2.39	0.55
2:D:282:THR:O	2:D:283:ASP:CB	2.51	0.55
1:A:224:GLU:OE2	1:A:231:THR:OG1	2.13	0.55
1:A:80:PHE:CG	4:A:1297:MTZ:H2C2	2.42	0.55
1:A:2:GLU:HG2	1:C:73:GLU:CD	2.27	0.54
1:C:165:THR:HG22	6:C:2036:HOH:O	2.07	0.54
1:A:159:TYR:O	1:A:160:THR:C	2.45	0.54
2:B:321:HIS:ND1	2:B:375:SER:HB2	2.22	0.54
1:A:83:LEU:O	4:A:1297:MTZ:N4	2.41	0.54
2:D:229:ASN:HB3	6:D:2043:HOH:O	2.07	0.54
1:C:162:GLU:CB	1:C:164:VAL:HG23	2.26	0.54
3:E:1:ARG:HD2	6:E:2001:HOH:O	2.08	0.53
2:B:233:HIS:HD2	6:B:2040:HOH:O	1.90	0.53
4:A:1297:MTZ:H2C2	4:A:1297:MTZ:H7C1	1.91	0.53
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.42	0.53
1:C:101:LEU:HD13	1:C:104:ILE:HD12	1.91	0.53
4:A:1297:MTZ:C2	4:A:1297:MTZ:H7C2	2.38	0.52
1:C:91:MET:HE2	1:C:196:MET:CG	2.39	0.52
1:A:49:ILE:CG2	2:B:306:LEU:HD12	2.39	0.52
1:A:84:HIS:CE1	1:A:296:LEU:CD2	2.93	0.51
1:C:214:ARG:CG	6:C:2049:HOH:O	2.57	0.51
1:A:56:LYS:HE3	1:A:56:LYS:O	2.10	0.51
1:C:1:MET:HA	1:C:1:MET:HE2	1.92	0.51
1:A:2:GLU:H	1:A:2:GLU:CD	2.13	0.51
1:C:278:LYS:CE	2:D:177:ASP:O	2.59	0.51
4:A:1297:MTZ:C2	4:A:1297:MTZ:H7C1	2.40	0.51
1:C:125:HIS:O	1:C:126:ARG:HB2	2.11	0.51
1:A:11:GLY:O	1:A:17:VAL:CG2	2.50	0.51
2:B:288:LYS:HZ3	2:B:288:LYS:HB3	1.75	0.51
1:C:32:LEU:CD2	1:C:79:VAL:HG22	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:TYR:CD2	1:C:15:TYR:N	2.79	0.50
1:A:198:THR:O	1:A:199:ARG:HB2	2.10	0.50
1:C:18:VAL:HG22	1:C:33:LYS:HG3	1.93	0.50
1:C:91:MET:HE3	1:C:196:MET:CG	2.40	0.50
1:C:159:TYR:HB2	1:C:162:GLU:HB3	1.93	0.50
1:C:91:MET:CE	1:C:196:MET:HG2	2.42	0.50
1:A:36:ARG:O	1:A:36:ARG:CG	2.60	0.50
1:C:115:LEU:HD12	1:C:189:LEU:HD22	1.92	0.50
1:A:71:HIS:CD2	2:B:296:HIS:CE1	3.00	0.50
1:C:214:ARG:NH1	1:C:214:ARG:CG	2.71	0.49
1:A:84:HIS:CE1	1:A:296:LEU:HD21	2.47	0.49
1:C:1:MET:HE1	1:C:70:ILE:CD1	2.41	0.49
1:A:70:ILE:HB	1:A:77:TYR:HB2	1.94	0.49
1:A:49:ILE:HG23	2:B:306:LEU:CD1	2.41	0.49
1:A:159:TYR:N	1:A:159:TYR:CD1	2.79	0.49
1:A:17:VAL:HG22	1:A:18:VAL:N	2.26	0.49
1:C:78:LEU:N	1:C:78:LEU:HD23	2.28	0.49
2:D:323:GLN:O	2:D:323:GLN:HG2	2.11	0.49
1:A:137:THR:HG22	1:A:296:LEU:CD2	2.34	0.49
2:B:233:HIS:HE1	6:B:2045:HOH:O	1.96	0.49
2:B:343:ASP:OD1	2:B:404:HIS:HE1	1.96	0.49
1:C:148:LEU:HD13	1:C:164:VAL:HG13	1.95	0.49
2:D:326:ASN:HB3	2:D:329:VAL:HB	1.94	0.49
2:D:176:PRO:CD	2:D:179:HIS:CE1	2.92	0.49
1:A:71:HIS:CE1	2:B:296:HIS:CE1	3.00	0.49
2:B:293:ARG:HG3	2:B:293:ARG:HH11	1.78	0.48
2:B:241:ARG:O	2:B:244:SER:HB2	2.13	0.48
4:C:1298:MTZ:C2	4:C:1298:MTZ:C7	2.91	0.48
2:B:385:GLU:O	2:B:388:LYS:HB2	2.14	0.48
1:A:159:TYR:HD1	1:A:159:TYR:N	2.10	0.48
2:B:430:LEU:O	2:B:431:ASN:CB	2.61	0.48
2:D:334:MET:HE3	6:D:2043:HOH:O	2.13	0.48
1:C:91:MET:HE3	1:C:196:MET:HG2	1.96	0.48
2:B:404:HIS:HD2	2:B:406:GLN:N	1.93	0.47
1:C:1:MET:HA	1:C:1:MET:CE	2.44	0.47
1:A:164:VAL:HG12	1:A:164:VAL:O	2.14	0.47
4:A:1297:MTZ:H141	4:A:1297:MTZ:H12	1.73	0.47
2:D:396:GLN:O	2:D:400:LYS:HD2	2.14	0.47
1:C:159:TYR:O	1:C:160:THR:C	2.52	0.47
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.96	0.47
4:C:1298:MTZ:H2C3	4:C:1298:MTZ:H7C2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ASP:OD2	2:B:250:ARG:CD	2.62	0.47
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.97	0.47
2:D:362:LEU:HD13	2:D:430:LEU:HD21	1.95	0.47
2:D:225:TYR:HE1	2:D:281:ILE:CD1	2.24	0.47
1:C:51:GLU:HG3	1:C:55:LEU:HD22	1.96	0.47
1:A:231:THR:HA	1:A:236:TYR:CD1	2.50	0.47
1:C:1:MET:CA	1:C:1:MET:CE	2.93	0.46
1:C:213:PHE:O	1:C:217:ARG:HG2	2.16	0.46
1:A:229:GLY:O	1:A:230:VAL:C	2.53	0.46
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.51	0.46
2:D:395:HIS:HB2	2:D:430:LEU:HD11	1.96	0.46
2:B:293:ARG:HG3	2:B:293:ARG:NH1	2.30	0.46
1:A:159:TYR:CE1	2:B:270:ILE:HG12	2.51	0.46
1:A:51:GLU:O	1:A:55:LEU:HB2	2.16	0.46
1:C:2:GLU:H	1:C:2:GLU:CD	2.19	0.46
1:C:39:THR:O	1:C:39:THR:OG1	2.32	0.45
1:A:20:LYS:HE3	1:A:82:PHE:CZ	2.51	0.45
2:D:374:GLU:HA	2:D:377:ILE:HD12	1.98	0.45
2:B:401:ALA:N	2:B:402:PRO:CD	2.79	0.45
1:C:41:THR:O	2:D:288:LYS:HE3	2.15	0.45
1:A:122:ARG:HB3	2:B:182:ILE:HG12	1.98	0.45
2:D:323:GLN:HA	2:D:324:PRO:HA	1.59	0.45
1:A:17:VAL:CG1	1:A:19:TYR:HE1	2.25	0.45
2:B:271:TYR:HA	2:B:272:PRO:HD2	1.66	0.45
2:D:347:TYR:OH	2:D:394:LEU:HA	2.16	0.45
1:A:162:GLU:OE1	1:A:180:TYR:OH	2.34	0.45
1:A:27:GLY:HA3	2:D:249:LEU:HD22	1.99	0.45
1:C:94:SER:O	1:C:97:THR:HG23	2.16	0.45
1:C:1:MET:HE3	1:C:1:MET:HB2	1.61	0.44
1:C:83:LEU:HD23	1:C:136:ASN:HB3	1.99	0.44
1:C:36:ARG:HD2	6:C:2009:HOH:O	2.17	0.44
1:A:289:VAL:O	1:A:289:VAL:HG13	2.17	0.44
1:A:84:HIS:O	1:A:85:GLN:HB3	2.18	0.44
1:A:51:GLU:HG3	1:A:55:LEU:HD22	2.00	0.44
2:B:421:VAL:O	2:B:424:LEU:HB2	2.17	0.44
4:A:1297:MTZ:H10	4:A:1297:MTZ:H172	1.87	0.44
1:A:105:LYS:HE2	1:A:105:LYS:HB2	1.77	0.44
1:C:164:VAL:O	1:C:165:THR:HB	2.17	0.44
2:B:207:THR:CG2	2:B:210:MET:H	2.30	0.43
1:C:115:LEU:HA	1:C:115:LEU:HD23	1.76	0.43
1:C:245:ARG:NH2	6:C:2053:HOH:O	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:THR:HG21	6:C:2030:HOH:O	2.19	0.43
2:D:387:LEU:O	2:D:391:LEU:HB2	2.19	0.43
2:B:282:THR:O	2:B:285:THR:HG23	2.12	0.43
2:B:415:ASN:OD1	2:B:417:LYS:HB2	2.18	0.43
2:D:175:VAL:N	2:D:176:PRO:HD3	2.33	0.43
2:D:398:TYR:CD2	2:D:426:PRO:HB3	2.53	0.43
2:B:395:HIS:HB2	2:B:430:LEU:HD11	2.01	0.42
2:B:304:PHE:HD1	6:B:2038:HOH:O	2.02	0.42
2:B:410:ARG:O	2:B:414:LYS:HG3	2.18	0.42
1:A:17:VAL:CG2	1:A:18:VAL:N	2.82	0.42
2:D:263:LEU:HD21	2:D:295:GLU:HG3	2.00	0.42
1:A:288:ASP:OD1	1:A:288:ASP:N	2.52	0.42
1:A:20:LYS:CE	1:A:82:PHE:CZ	3.03	0.42
1:A:255:LEU:HD12	1:A:255:LEU:HA	1.94	0.42
2:B:216:ASP:OD1	2:B:408:SER:HB2	2.19	0.42
2:D:207:THR:HG23	2:D:209:SER:N	2.34	0.42
1:C:107:TYR:O	1:C:111:LEU:HG	2.20	0.42
2:B:323:GLN:HA	2:B:324:PRO:HA	1.89	0.42
1:A:212:LEU:HD22	1:A:216:PHE:CZ	2.54	0.42
1:A:155:PRO:HD3	2:B:316:THR:HG21	2.01	0.41
1:C:6:LYS:HZ1	1:C:34:LYS:HZ3	1.63	0.41
2:D:401:ALA:HB1	2:D:410:ARG:HD2	2.02	0.41
1:A:158:THR:HA	1:A:180:TYR:CE1	2.56	0.41
1:C:124:LEU:CG	6:C:2045:HOH:O	2.48	0.41
1:A:17:VAL:CG1	1:A:19:TYR:CE1	3.02	0.41
1:A:129:LYS:HA	1:A:192:ILE:HD11	2.02	0.41
4:C:1298:MTZ:C2	4:C:1298:MTZ:H7C2	2.50	0.41
1:C:252:VAL:N	1:C:253:PRO:HD3	2.36	0.41
2:D:372:TRP:HA	2:D:373:PRO:HD3	1.88	0.41
1:C:85:GLN:HE22	1:C:89:LYS:HB3	1.86	0.41
1:C:131:GLN:H	1:C:131:GLN:NE2	2.19	0.41
1:A:37:LEU:HD12	1:A:37:LEU:HA	1.80	0.41
1:A:178:LYS:HD3	1:A:179:TYR:CE2	2.56	0.41
1:A:41:THR:HG23	1:A:42:GLU:HB2	2.03	0.41
1:A:85:GLN:HB2	1:A:85:GLN:HE21	1.62	0.41
1:C:182:THR:OG1	2:D:178:TYR:OH	2.39	0.41
2:D:345:ASP:HA	2:D:346:PRO:HA	1.93	0.41
1:C:90:PHE:HB2	1:C:135:ILE:HD11	2.03	0.40
1:A:85:GLN:HA	4:A:1297:MTZ:C12	2.51	0.40
1:A:12:GLU:HA	1:A:18:VAL:HG23	2.03	0.40
1:C:124:LEU:HG	1:C:152:PHE:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	294/298 (99%)	280 (95%)	12 (4%)	2 (1%)	26 14
1	C	295/298 (99%)	282 (96%)	10 (3%)	3 (1%)	19 8
2	B	256/259 (99%)	247 (96%)	8 (3%)	1 (0%)	39 28
2	D	256/259 (99%)	247 (96%)	8 (3%)	1 (0%)	39 28
3	E	2/5 (40%)	2 (100%)	0	0	100 100
3	F	2/5 (40%)	2 (100%)	0	0	100 100
All	All	1105/1124 (98%)	1060 (96%)	38 (3%)	7 (1%)	30 17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	TYR
2	B	176	PRO
1	C	41	THR
2	D	431	ASN
1	A	160	THR
1	C	40	GLU
1	C	165	THR

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	261/263 (99%)	235 (90%)	26 (10%)	9 3
1	C	261/263 (99%)	225 (86%)	36 (14%)	4 1
2	B	232/233 (100%)	211 (91%)	21 (9%)	12 5
2	D	232/233 (100%)	211 (91%)	21 (9%)	12 5
3	E	3/3 (100%)	2 (67%)	1 (33%)	0 0
3	F	3/3 (100%)	2 (67%)	1 (33%)	0 0
All	All	992/998 (99%)	886 (89%)	106 (11%)	8 2

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	36	ARG
1	A	37	LEU
1	A	40	GLU
1	A	42	GLU
1	A	55	LEU
1	A	56	LYS
1	A	73	GLU
1	A	75	LYS
1	A	76	LEU
1	A	89	LYS
1	A	96	LEU
1	A	101	LEU
1	A	115	LEU
1	A	122	ARG
1	A	131	GLN
1	A	160	THR
1	A	163	VAL
1	A	165	THR
1	A	200	ARG
1	A	202	LEU
1	A	230	VAL
1	A	232	SER
1	A	287	GLN
1	A	293	VAL
1	A	296	LEU
2	B	177	ASP
2	B	196	LYS
2	B	201	LYS
2	B	249	LEU

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Mol	Chain	Res	Type
2	B	250	ARG
2	B	271	TYR
2	B	285	THR
2	B	288	LYS
2	B	289	LYS
2	B	292	LEU
2	B	293	ARG
2	B	323	GLN
2	B	348	LEU
2	B	374	GLU
2	B	375	SER
2	B	391	LEU
2	B	400	LYS
2	B	424	LEU
2	B	425	ASN
2	B	431	ASN
2	B	432	LEU
1	C	5	GLN
1	C	14	THR
1	C	15	TYR
1	C	22	ARG
1	C	34	LYS
1	C	38	ASP
1	C	39	THR
1	C	41	THR
1	C	55	LEU
1	C	56	LYS
1	C	74	ASN
1	C	78	LEU
1	C	87	LEU
1	C	88	LYS
1	C	89	LYS
1	C	96	LEU
1	C	97	THR
1	C	101	LEU
1	C	115	LEU
1	C	122	ARG
1	C	131	GLN
1	C	154	VAL
1	C	157	ARG
1	C	162	GLU
1	C	164	VAL

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Mol	Chain	Res	Type
1	C	165	THR
1	C	200	ARG
1	C	214	ARG
1	C	217	ARG
1	C	232	SER
1	C	242	LYS
1	C	248	PHE
1	C	249	SER
1	C	278	LYS
1	C	291	LYS
1	C	296	LEU
2	D	178	TYR
2	D	196	LYS
2	D	200	MET
2	D	201	LYS
2	D	232	LEU
2	D	249	LEU
2	D	281	ILE
2	D	288	LYS
2	D	289	LYS
2	D	292	LEU
2	D	328	LYS
2	D	348	LEU
2	D	364	LEU
2	D	374	GLU
2	D	378	ARG
2	D	391	LEU
2	D	417	LYS
2	D	424	LEU
2	D	429	THR
2	D	431	ASN
2	D	432	LEU
3	E	3	ILE
3	F	3	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	62	ASN
1	A	85	GLN
1	A	131	GLN

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Mol	Chain	Res	Type
2	B	208	ASN
2	B	323	GLN
2	B	404	HIS
2	B	431	ASN
1	C	60	HIS
1	C	85	GLN
1	C	131	GLN
1	C	287	GLN
2	D	208	ASN
2	D	322	GLN
2	D	404	HIS
2	D	419	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
3	PFF	E	4	3	11,12,13	0.83	0	12,15,17	1.44	2 (16%)
3	PFF	F	4	3	11,12,13	0.72	0	12,15,17	1.52	2 (16%)

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
3	PFF	E	4	3	-	0/4/6/8	0/1/1/1
3	PFF	F	4	3	-	0/4/6/8	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	4	PFF	CE2-CZ-CE1	-2.77	118.89	122.87
3	E	4	PFF	O-C-CA	-2.52	118.93	125.49
3	E	4	PFF	CG-CB-CA	2.30	119.40	114.21
3	F	4	PFF	CD1-CE1-CZ	3.08	121.67	118.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
4	MTZ	A	1297	-	22,29,29	2.00	3 (13%)	22,40,40	1.28	3 (13%)
4	MTZ	C	1298	-	22,29,29	2.22	3 (13%)	22,40,40	1.72	6 (27%)
5	GVC	E	1433	3	14,17,18	1.90	3 (21%)	14,24,26	2.72	7 (50%)
5	GVC	F	1433	3	14,17,18	1.69	2 (14%)	14,24,26	2.76	5 (35%)

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
4	MTZ	A	1297	-	-	0/8/30/30	0/3/4/4
4	MTZ	C	1298	-	-	0/8/30/30	0/3/4/4
5	GVC	E	1433	3	-	0/4/6/8	0/2/2/2
5	GVC	F	1433	3	-	0/4/6/8	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1298	MTZ	C3-C4	-6.18	1.38	1.47
4	C	1298	MTZ	C8-N4	-5.10	1.34	1.42
5	E	1433	GVC	C30-N8	-5.08	1.33	1.44
4	A	1297	MTZ	C3-C4	-5.05	1.40	1.47
4	A	1297	MTZ	C8-N4	-5.01	1.34	1.42
5	F	1433	GVC	C30-N8	-4.72	1.34	1.44
5	E	1433	GVC	C29-C30	2.21	1.41	1.38
5	F	1433	GVC	C28-CL1	2.67	1.80	1.74
5	E	1433	GVC	C28-CL1	3.50	1.82	1.74
4	A	1297	MTZ	C6-N3	4.79	1.33	1.27
4	C	1298	MTZ	C6-N3	5.11	1.33	1.27

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1433	GVC	C29-C30-C31	-5.93	114.64	121.69
5	F	1433	GVC	N10-C35-N9	-5.16	110.74	114.88
5	E	1433	GVC	N10-C35-N9	-4.31	111.43	114.88
5	E	1433	GVC	C29-C30-C31	-4.05	116.88	121.69
5	E	1433	GVC	C29-C28-C33	-3.50	117.00	121.69
4	C	1298	MTZ	C12-C11-N5	-2.96	117.40	121.38
4	C	1298	MTZ	O-C15-C14	-2.96	105.05	111.84
4	A	1297	MTZ	N-C-N1	2.03	125.57	122.92
4	C	1298	MTZ	O-C16-C17	2.13	116.73	111.84
4	C	1298	MTZ	C6-C7-C4	2.23	116.25	111.77
5	E	1433	GVC	C36-C34-N9	2.50	128.84	124.15
4	C	1298	MTZ	C8-N4-C5	2.57	127.03	120.73
5	F	1433	GVC	C30-C31-C32	2.75	122.77	118.98
4	A	1297	MTZ	C6-C7-C4	3.24	118.28	111.77
4	A	1297	MTZ	C17-N5-C14	3.28	118.48	111.59
5	F	1433	GVC	C30-C29-C28	3.30	123.53	118.98
5	E	1433	GVC	C30-C29-C28	3.62	123.97	118.98
5	E	1433	GVC	C29-C30-N8	3.67	123.61	119.13
5	F	1433	GVC	C29-C30-N8	3.93	123.92	119.13
4	C	1298	MTZ	C17-N5-C14	4.06	120.12	111.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1433	GVC	C29-C28-CL1	4.25	124.42	119.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1297	MTZ	13	0
4	C	1298	MTZ	5	0
5	E	1433	GVC	3	0
5	F	1433	GVC	3	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	296/298 (99%)	0.44	23 (7%) 16 18	36, 52, 90, 132	0
1	C	297/298 (99%)	0.33	22 (7%) 17 19	33, 48, 91, 129	0
2	B	258/259 (99%)	0.09	10 (3%) 43 47	35, 48, 71, 108	0
2	D	258/259 (99%)	0.14	13 (5%) 32 35	34, 50, 72, 104	0
3	E	3/5 (60%)	0.41	0 100 100	49, 49, 65, 66	0
3	F	3/5 (60%)	0.67	1 (33%) 0 0	46, 46, 62, 75	0
All	All	1115/1124 (99%)	0.26	69 (6%) 24 26	33, 50, 83, 132	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	TYR	13.5
1	C	39	THR	11.3
1	C	14	THR	10.9
1	A	13	GLY	10.6
2	B	175	VAL	8.7
1	C	13	GLY	8.2
1	C	15	TYR	7.7
1	A	16	GLY	7.3
1	A	296	LEU	7.2
1	A	163	VAL	7.1
1	A	14	THR	6.8
2	D	175	VAL	6.6
1	C	164	VAL	5.7
1	A	96	LEU	5.4
1	C	295	HIS	5.2
1	C	96	LEU	4.9
1	A	159	TYR	4.8
1	C	40	GLU	4.8
1	C	297	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	271	TYR	4.6
1	A	95	ALA	4.4
2	B	176	PRO	4.4
1	C	38	ASP	4.2
1	A	160	THR	4.1
1	A	36	ARG	3.9
2	B	324	PRO	3.9
2	D	178	TYR	3.8
1	C	163	VAL	3.8
1	C	159	TYR	3.8
2	B	323	GLN	3.7
1	A	73	GLU	3.4
1	C	160	THR	3.3
3	F	3	ILE	3.2
1	A	74	ASN	3.2
1	A	40	GLU	3.1
1	C	36	ARG	3.0
1	C	37	LEU	2.9
2	D	177	ASP	2.9
1	C	41	THR	2.9
2	D	176	PRO	2.9
2	D	432	LEU	2.8
1	A	37	LEU	2.8
2	D	256	VAL	2.7
2	D	325	ALA	2.7
1	A	171	PRO	2.6
1	C	296	LEU	2.6
1	C	162	GLU	2.6
2	D	415	ASN	2.6
2	B	325	ALA	2.5
1	A	200	ARG	2.5
1	A	174	LEU	2.4
2	D	324	PRO	2.4
1	C	206	ASP	2.3
2	D	358	ALA	2.3
1	A	247	ASP	2.2
1	A	97	THR	2.2
2	B	378	ARG	2.2
1	C	250	LYS	2.2
2	B	201	LYS	2.2
2	D	259	ALA	2.2
1	A	288	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	178	TYR	2.2
1	A	295	HIS	2.1
2	D	332	LEU	2.1
2	D	323	GLN	2.1
2	B	256	VAL	2.1
1	C	192	ILE	2.0
1	A	178	LYS	2.0
1	C	189	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
3	PFF	F	4	12/13	0.87	0.12	-	38,46,58,59	0
3	PFF	E	4	12/13	0.93	0.12	-	43,49,65,80	0

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
5	GVC	F	1433	16/17	0.75	0.26	4.23	65,70,78,80	0
4	MTZ	A	1297	26/26	0.66	0.31	1.07	88,110,127,129	0
5	GVC	E	1433	16/17	0.75	0.20	0.02	52,59,69,79	0
4	MTZ	C	1298	26/26	0.85	0.17	-0.03	44,68,92,95	0

6.5 Other polymers (i)

There are no such residues in this entry.