Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:52 PM GMT

PDB ID	:	4MY3
Title	:	Crystal Structure of GCN5-related N-acetyltransferase from Kribbella flavida
Authors	:	Kim, Y.; Mack, J.; Endres, M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2013-09-27
Resolution	:	2.57 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:

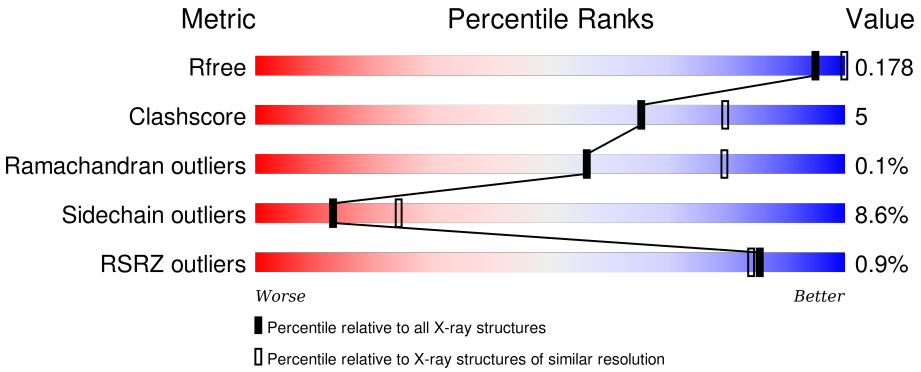
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.57 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	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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	392	84% 14%
1	B	392	83% 15%
1	C	392	76% 20%
1	D	392	85% 11%
1	E	392	85% 12%

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Mol	Chain	Length	Quality of chain
1	F	392	

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
3	EDO	D	402	-	-	X	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18203 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 GCN5-related N-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	Se	0	1	0
			2958	1867	538	548	5			
1	B	392	Total	C	N	O	Se	0	0	0
			2988	1884	541	558	5			
1	C	386	Total	C	N	O	Se	0	0	0
			2947	1861	534	547	5			
1	D	384	Total	C	N	O	Se	0	2	0
			2954	1864	539	546	5			
1	E	386	Total	C	N	O	Se	0	2	0
			2969	1873	542	549	5			
1	F	386	Total	C	N	O	Se	0	3	0
			2976	1879	542	550	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP D2PVF8
A	-1	ASN	-	EXPRESSION TAG	UNP D2PVF8
A	0	ALA	-	EXPRESSION TAG	UNP D2PVF8
A	1	VAL	MET	SEE REMARK 999	UNP D2PVF8
B	-2	SER	-	EXPRESSION TAG	UNP D2PVF8
B	-1	ASN	-	EXPRESSION TAG	UNP D2PVF8
B	0	ALA	-	EXPRESSION TAG	UNP D2PVF8
B	1	VAL	MET	SEE REMARK 999	UNP D2PVF8
C	-2	SER	-	EXPRESSION TAG	UNP D2PVF8
C	-1	ASN	-	EXPRESSION TAG	UNP D2PVF8
C	0	ALA	-	EXPRESSION TAG	UNP D2PVF8
C	1	VAL	MET	SEE REMARK 999	UNP D2PVF8
D	-2	SER	-	EXPRESSION TAG	UNP D2PVF8
D	-1	ASN	-	EXPRESSION TAG	UNP D2PVF8
D	0	ALA	-	EXPRESSION TAG	UNP D2PVF8
D	1	VAL	MET	SEE REMARK 999	UNP D2PVF8
E	-2	SER	-	EXPRESSION TAG	UNP D2PVF8

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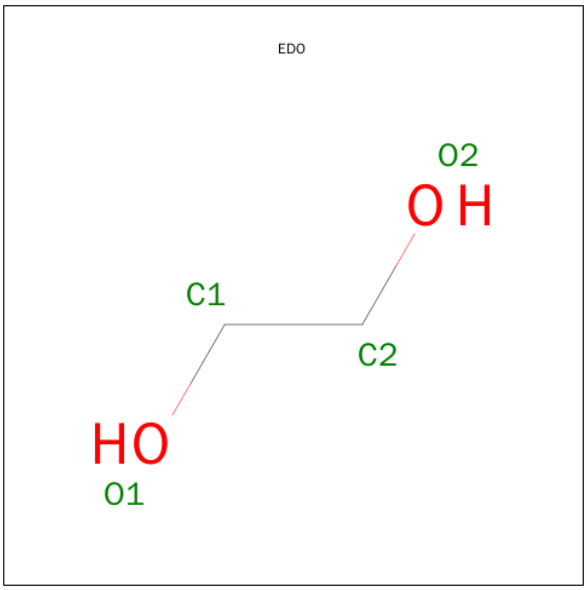
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	EXPRESSION TAG	UNP D2PVF8
E	0	ALA	-	EXPRESSION TAG	UNP D2PVF8
E	1	VAL	MET	SEE REMARK 999	UNP D2PVF8
F	-2	SER	-	EXPRESSION TAG	UNP D2PVF8
F	-1	ASN	-	EXPRESSION TAG	UNP D2PVF8
F	0	ALA	-	EXPRESSION TAG	UNP D2PVF8
F	1	VAL	MET	SEE REMARK 999	UNP D2PVF8

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

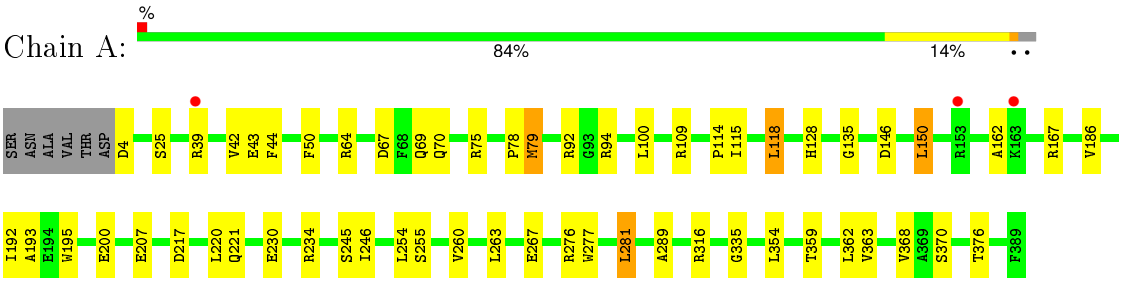
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	72	Total O 72 72	0	0
4	B	66	Total O 66 66	0	0
4	C	45	Total O 45 45	0	0
4	D	82	Total O 82 82	0	0
4	E	77	Total O 77 77	0	0
4	F	59	Total O 59 59	0	0

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 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.

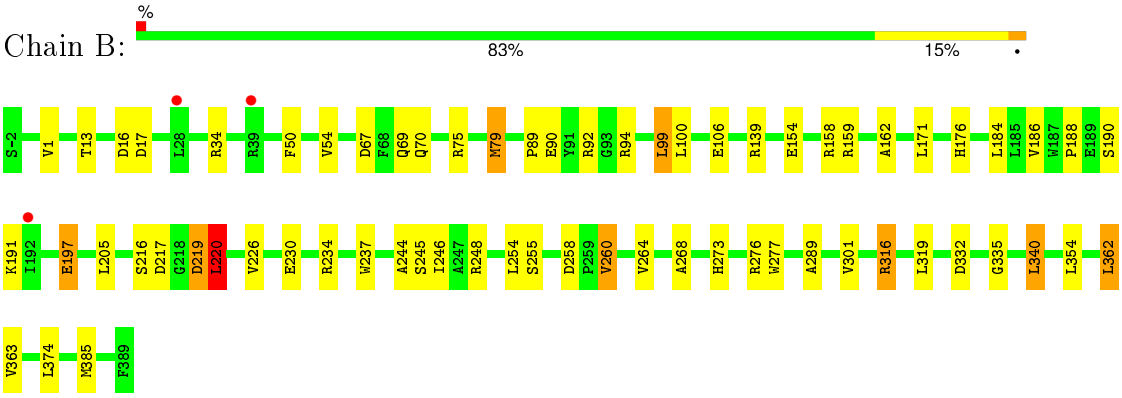
- Molecule 1: GCN5-related N-acetyltransferase

Chain A:



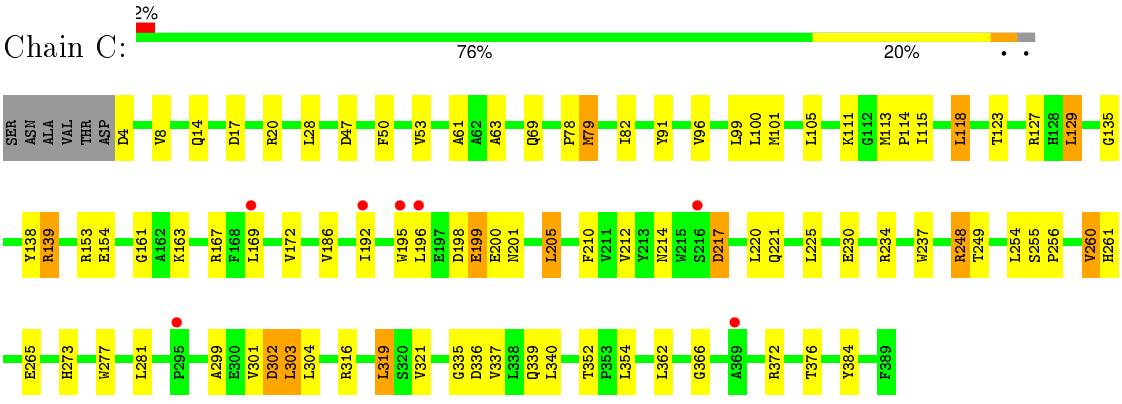
- Molecule 1: GCN5-related N-acetyltransferase

Chain B:



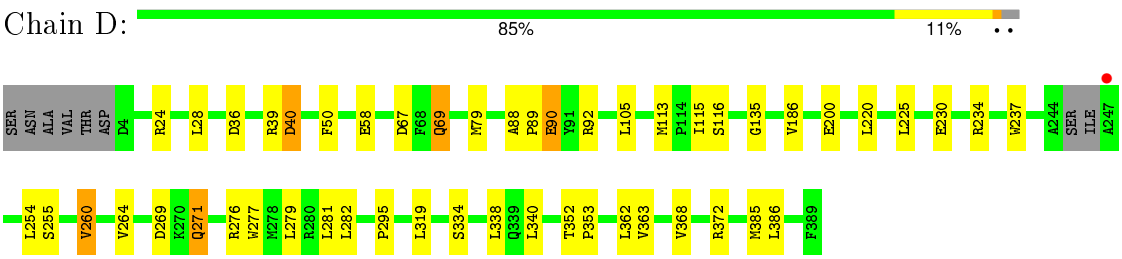
- Molecule 1: GCN5-related N-acetyltransferase

Chain C:



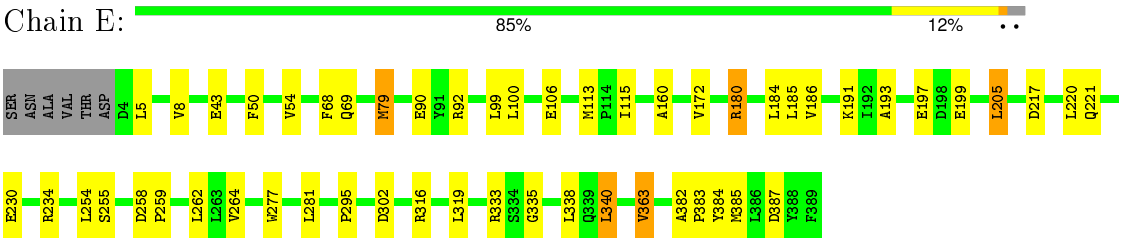
- Molecule 1: GCN5-related N-acetyltransferase

Chain D:



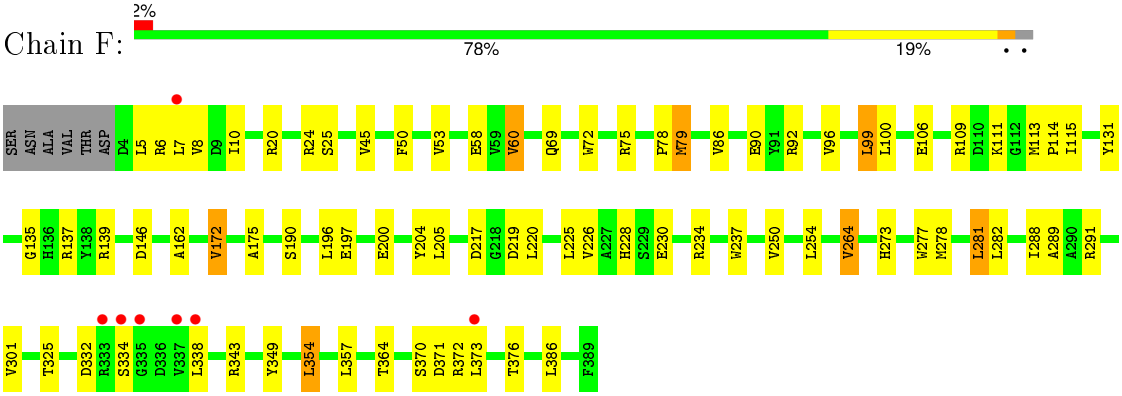
• Molecule 1: GCN5-related N-acetyltransferase

Chain E:



• Molecule 1: GCN5-related N-acetyltransferase

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	89.25Å 167.12Å 183.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.97 – 2.57 47.26 – 2.51	Depositor EDS
% Data completeness (in resolution range)	94.0 (41.97-2.57) 88.9 (47.26-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1161)	Depositor
R, R_{free}	0.176 , 0.235 0.177 , 0.178	Depositor DCC
R_{free} test set	4137 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	40.0	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 35.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 83814 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18203	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: EDO, CL

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	0.41	0/3021	0.58	1/4100 (0.0%)
1	B	0.43	0/3051	0.62	2/4143 (0.0%)
1	C	0.40	0/3010	0.60	2/4086 (0.0%)
1	D	0.44	0/3017	0.62	0/4093
1	E	0.43	0/3032	0.61	1/4114 (0.0%)
1	F	0.40	0/3040	0.58	0/4126
All	All	0.42	0/18171	0.60	6/24662 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	118	LEU	CA-CB-CG	5.41	127.74	115.30
1	C	260	VAL	CB-CA-C	-5.38	101.19	111.40
1	A	118	LEU	CA-CB-CG	5.34	127.59	115.30
1	B	99	LEU	CA-CB-CG	5.27	127.43	115.30
1	B	220	LEU	CA-CB-CG	5.24	127.36	115.30
1	E	340	LEU	CA-CB-CG	5.20	127.25	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2958	0	2886	27	0
1	B	2988	0	2913	30	0
1	C	2947	0	2874	48	0
1	D	2954	0	2875	24	0
1	E	2969	0	2898	22	0
1	F	2976	0	2902	36	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	D	8	0	12	5	0
4	A	72	0	0	4	0
4	B	66	0	0	0	0
4	C	45	0	0	3	0
4	D	82	0	0	0	0
4	E	77	0	0	0	0
4	F	59	0	0	1	0
All	All	18203	0	17360	176	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 5.

All (176) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ALA:HB2	1:B:197:GLU:HG2	1.54	0.89
1:E:230:GLU:OE1	1:E:234:ARG:NH1	2.21	0.73
1:A:276:ARG:NH1	4:A:550:HOH:O	2.21	0.72
1:F:115:ILE:HG22	1:F:281:LEU:HD22	1.71	0.72
1:C:47:ASP:O	1:C:111:LYS:NZ	2.24	0.71
1:D:67:ASP:HA	1:D:113:MSE:HE1	1.73	0.69
1:C:82:ILE:HG21	1:C:101:MSE:HE1	1.74	0.68
1:A:230:GLU:OE1	1:A:234:ARG:NH1	2.28	0.66
1:C:316:ARG:HH12	1:C:335:GLY:H	1.45	0.64
1:C:352:THR:HG21	4:C:406:HOH:O	1.98	0.62
1:E:43:GLU:OE2	1:E:191:LYS:NZ	2.32	0.62
1:F:162:ALA:HB2	1:F:197:GLU:HB3	1.80	0.61
1:C:225:LEU:HD13	1:C:237:TRP:CE2	2.34	0.61
1:A:316:ARG:NH1	1:A:335:GLY:O	2.33	0.61
1:B:159:ARG:NH1	1:F:58:GLU:OE2	2.34	0.61
1:A:69:GLN:HB2	1:A:186:VAL:HB	1.81	0.61
1:B:16:ASP:OD1	1:B:34:ARG:NH1	2.33	0.61
1:C:198:ASP:HB3	1:C:201:ASN:HB2	1.83	0.61
1:F:175:ALA:HB2	1:F:228[B]:HIS:HE1	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:ARG:NH1	1:C:335:GLY:H	1.98	0.60
1:C:69:GLN:HB2	1:C:186:VAL:HB	1.83	0.60
1:B:332:ASP:OD1	1:B:332:ASP:N	2.35	0.60
1:C:101:MSE:HG2	1:C:129:LEU:HD13	1.84	0.60
1:A:115:ILE:HG22	1:A:281:LEU:HD22	1.83	0.59
1:F:172:VAL:HG23	1:F:226:VAL:HG21	1.83	0.59
1:A:200:GLU:HG3	1:C:28:LEU:HD23	1.85	0.59
1:C:261:HIS:CD2	3:D:402:EDO:H22	2.38	0.59
1:B:230:GLU:O	1:B:234:ARG:HG3	2.02	0.59
1:C:299:ALA:HB3	1:C:321:VAL:HG22	1.85	0.59
1:B:340:LEU:HB3	1:B:363:VAL:HG12	1.86	0.57
1:D:115:ILE:HG22	1:D:281:LEU:HD22	1.86	0.57
1:F:230:GLU:O	1:F:234:ARG:HG3	2.04	0.57
1:C:230:GLU:O	1:C:234:ARG:HG3	2.05	0.56
1:A:75:ARG:NH2	1:A:289:ALA:O	2.37	0.56
1:E:115:ILE:HG22	1:E:281:LEU:HD22	1.87	0.56
1:C:138:TYR:CE2	1:C:256:PRO:HG3	2.40	0.56
1:C:139:ARG:HB3	1:C:273:HIS:HB2	1.88	0.55
1:E:255:SER:HB2	1:E:384:TYR:CZ	2.40	0.55
1:C:17:ASP:OD1	1:C:20:ARG:NH2	2.38	0.55
1:F:225:LEU:HD13	1:F:237:TRP:CE2	2.41	0.55
1:F:217:ASP:HB2	1:F:219:ASP:H	1.72	0.55
1:B:70:GLN:HB2	1:B:79:MSE:HG2	1.90	0.54
1:B:316:ARG:NH1	1:B:335:GLY:O	2.40	0.54
1:C:302:ASP:HB3	1:C:337:VAL:HG23	1.90	0.54
1:A:150:LEU:HD11	1:A:263:LEU:HB3	1.89	0.54
1:A:146:ASP:O	1:A:150:LEU:HD23	2.08	0.54
1:D:269:ASP:OD2	1:D:271:GLN:HG2	2.08	0.54
1:B:176:HIS:CE1	1:B:184:LEU:HD13	2.43	0.53
1:C:214:ASN:HD21	1:C:221:GLN:NE2	2.06	0.53
1:C:195:TRP:CH2	1:C:212:VAL:HG21	2.44	0.52
1:A:67:ASP:N	1:A:67:ASP:OD1	2.39	0.52
1:F:146:ASP:HB3	1:F:264:VAL:HG22	1.90	0.52
1:D:69:GLN:HB3	1:D:186:VAL:HG13	1.92	0.52
1:D:230:GLU:O	1:D:234:ARG:HG3	2.10	0.51
1:C:376:THR:HG21	1:D:295:PRO:O	2.09	0.51
1:A:44:PHE:CE1	1:A:64[B]:ARG:HG3	2.45	0.51
1:F:343:ARG:NH1	4:F:442:HOH:O	2.39	0.51
1:F:370:SER:HA	1:F:373:LEU:HD23	1.93	0.51
1:F:111:LYS:HB3	1:F:113:MSE:HE2	1.93	0.51
1:A:162:ALA:HB1	1:A:193:ALA:HB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ARG:HD2	1:F:204:TYR:OH	2.11	0.50
1:A:276:ARG:NH2	4:A:526:HOH:O	2.45	0.50
1:F:75:ARG:NH2	1:F:289:ALA:O	2.45	0.50
1:A:245:SER:OG	1:A:246:ILE:N	2.42	0.50
1:D:225:LEU:HD13	1:D:237:TRP:CE2	2.47	0.50
1:E:79:MSE:HB2	1:E:115:ILE:HG13	1.94	0.49
1:F:78:PRO:O	1:F:114:PRO:HD2	2.11	0.49
1:A:135:GLY:HA3	1:A:277:TRP:CZ2	2.48	0.49
1:E:302:ASP:OD2	1:E:316:ARG:NH2	2.44	0.48
1:E:220:LEU:HD23	1:E:221:GLN:N	2.28	0.48
1:C:255:SER:HB3	1:C:384:TYR:CZ	2.49	0.48
1:B:260:VAL:O	1:B:264:VAL:HG23	2.14	0.48
1:F:139:ARG:HB3	1:F:273:HIS:HB2	1.95	0.48
1:C:78:PRO:O	1:C:114:PRO:HD2	2.13	0.48
1:D:135:GLY:HA3	1:D:277:TRP:CZ2	2.49	0.48
1:B:154:GLU:H	1:B:154:GLU:CD	2.16	0.47
1:F:20:ARG:HG2	1:F:24:ARG:NH2	2.29	0.47
1:F:291:ARG:HD2	1:F:349:TYR:CE1	2.49	0.47
1:C:115:ILE:HG22	1:C:281:LEU:HD22	1.97	0.47
1:C:214:ASN:HD21	1:C:221:GLN:HE21	1.61	0.47
1:C:256:PRO:O	3:D:402:EDO:H21	2.15	0.47
1:B:245:SER:OG	1:B:246:ILE:N	2.46	0.47
1:A:167:ARG:NH2	1:A:207:GLU:O	2.48	0.46
1:F:135:GLY:HA3	1:F:277:TRP:CZ2	2.51	0.46
1:C:304:LEU:HB3	1:C:339:GLN:HG2	1.97	0.46
1:C:200:GLU:HB2	4:C:423:HOH:O	2.16	0.46
1:C:79:MSE:HB2	1:C:115:ILE:HG13	1.99	0.45
1:B:69:GLN:HB2	1:B:186:VAL:HB	1.97	0.45
1:A:39:ARG:O	1:A:42:VAL:HG22	2.15	0.45
1:E:185:LEU:HD12	1:E:387:ASP:HB2	1.99	0.45
1:C:79:MSE:CB	1:C:115:ILE:HG13	2.46	0.45
1:E:338:LEU:HD11	1:E:363:VAL:HG13	1.98	0.45
1:E:69:GLN:HB2	1:E:186:VAL:HB	1.99	0.45
1:A:276:ARG:NH2	1:B:268:ALA:HB3	2.32	0.45
1:D:40:ASP:OD1	1:D:40:ASP:N	2.49	0.45
1:B:89:PRO:HA	1:B:92:ARG:HD2	1.99	0.45
1:C:199:GLU:H	1:C:199:GLU:HG3	1.38	0.45
1:D:90:GLU:HG3	1:F:204:TYR:CE1	2.52	0.45
1:D:277:TRP:CE2	1:D:385:MSE:HE3	2.53	0.44
1:C:135:GLY:HA3	1:C:277:TRP:CZ2	2.53	0.44
1:E:230:GLU:O	1:E:234:ARG:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HD12	1:A:234:ARG:HG2	2.00	0.44
1:C:91:TYR:HB3	1:C:96:VAL:HG21	2.00	0.44
1:F:131:TYR:HB3	1:F:278:MSE:HB3	1.99	0.44
1:A:234:ARG:NH2	4:A:518:HOH:O	2.51	0.44
1:C:205:LEU:HD23	1:C:210:PHE:HB3	1.99	0.44
1:B:92:ARG:O	1:B:94:ARG:HG3	2.18	0.44
1:D:28:LEU:HD12	1:F:200:GLU:HG2	1.98	0.44
1:D:260:VAL:O	1:D:264:VAL:HG23	2.17	0.44
1:C:248:ARG:HE	1:C:249:THR:HG23	1.83	0.44
1:F:5:LEU:HD13	1:F:96:VAL:HG22	2.00	0.44
1:C:101:MSE:O	1:C:105:LEU:HG	2.18	0.44
1:B:219:ASP:OD2	1:B:219:ASP:N	2.49	0.44
1:A:359:THR:O	1:B:230:GLU:HA	2.18	0.43
1:C:53:VAL:HB	1:C:61:ALA:HB3	1.99	0.43
1:A:78:PRO:O	1:A:114:PRO:HD2	2.17	0.43
1:A:128:HIS:HB2	4:A:556:HOH:O	2.18	0.43
1:F:79:MSE:HB2	1:F:115:ILE:HG13	1.99	0.43
1:E:316:ARG:NH1	1:E:335:GLY:O	2.52	0.43
1:A:70:GLN:HB2	1:A:79:MSE:HG2	2.00	0.43
1:E:277:TRP:CD2	1:E:385:MSE:HE3	2.52	0.43
1:C:372:ARG:O	1:C:376:THR:HG23	2.19	0.43
1:B:139:ARG:HB3	1:B:273:HIS:HB2	2.00	0.43
1:B:75:ARG:NH2	1:B:289:ALA:O	2.50	0.43
1:E:184:LEU:HD21	1:E:384:TYR:CE1	2.54	0.42
1:A:192:ILE:O	1:A:195:TRP:HB3	2.19	0.42
1:F:72:TRP:HB3	1:F:291:ARG:HG3	2.00	0.42
1:F:354:LEU:HD23	1:F:371:ASP:CG	2.39	0.42
1:C:303:LEU:HA	1:C:337:VAL:HG22	2.00	0.42
1:F:53:VAL:O	1:F:60:VAL:HG12	2.19	0.42
1:B:362:LEU:HD12	1:B:362:LEU:HA	1.92	0.42
1:C:319:LEU:HD22	1:C:321:VAL:HG13	2.02	0.42
1:B:258:ASP:OD2	1:B:260:VAL:HG22	2.18	0.42
1:B:277:TRP:CE2	1:B:385:MSE:HE3	2.55	0.42
1:F:220:LEU:HB3	1:F:250:VAL:HG22	2.02	0.42
1:D:352:THR:HA	1:D:353:PRO:HD3	1.95	0.42
1:D:338:LEU:HA	1:D:338:LEU:HD12	1.84	0.42
1:E:193:ALA:O	1:E:197:GLU:HB2	2.20	0.42
1:E:180:ARG:NH2	1:F:372:ARG:HD3	2.35	0.42
1:C:336:ASP:O	1:C:366:GLY:HA2	2.20	0.42
1:D:276:ARG:HE	3:D:402:EDO:H11	1.84	0.41
1:B:176:HIS:NE2	1:B:184:LEU:HD13	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:ALA:HB2	1:E:205:LEU:HB2	2.02	0.41
1:B:237:TRP:NE1	1:B:260:VAL:HG13	2.36	0.41
1:E:68:PHE:HB2	1:E:79:MSE:HG3	2.00	0.41
1:D:338:LEU:HD11	1:D:363:VAL:CG1	2.49	0.41
1:D:36:ASP:OD1	1:D:39:ARG:NH2	2.53	0.41
1:B:158:ARG:NH1	1:B:159:ARG:O	2.53	0.41
1:F:288:ILE:HA	1:F:288:ILE:HD13	1.93	0.41
1:F:10:ILE:O	1:F:45:VAL:HG13	2.20	0.41
1:F:20:ARG:HG2	1:F:24:ARG:HH22	1.84	0.41
1:F:7[A]:LEU:HD21	1:F:99:LEU:O	2.21	0.41
1:D:340:LEU:HG	1:D:363:VAL:HG22	2.03	0.41
1:E:180:ARG:HD3	1:E:295:PRO:HD3	2.02	0.41
1:B:188:PRO:HG2	1:B:191:LYS:HG3	2.02	0.41
1:C:167:ARG:HA	1:C:167:ARG:HD2	1.94	0.41
1:F:109:ARG:HG2	1:F:282:LEU:HB3	2.02	0.41
1:D:116:SER:O	1:D:279:LEU:HD12	2.20	0.41
1:B:301:VAL:HG21	1:B:374:LEU:HD21	2.03	0.41
1:E:382:ALA:HA	1:E:383:PRO:HD3	1.97	0.41
1:C:261:HIS:CG	3:D:402:EDO:H22	2.56	0.40
1:C:161:GLY:O	1:C:196:LEU:HD13	2.20	0.40
1:A:267:GLU:HG3	1:B:276:ARG:HD2	2.03	0.40
1:A:220:LEU:HD23	1:A:221:GLN:N	2.36	0.40
1:C:4:ASP:N	1:C:4:ASP:OD1	2.55	0.40
1:E:258:ASP:HA	1:E:259:PRO:HD3	1.98	0.40
1:D:105:LEU:HD22	1:D:282:LEU:HD21	2.03	0.40
1:D:276:ARG:HD3	3:D:402:EDO:H11	2.03	0.40
1:F:354:LEU:HD12	1:F:357:LEU:HD12	2.04	0.40
1:C:123:THR:O	1:C:127:ARG:HG3	2.22	0.40
1:B:220:LEU:HD23	1:B:244:ALA:HA	2.04	0.40
1:E:295:PRO:O	1:F:376:THR:HG21	2.21	0.40
1:C:217:ASP:OD2	1:C:217:ASP:N	2.52	0.40
1:C:63:ALA:HB2	1:C:100:LEU:HD21	2.03	0.40
1:D:88:ALA:HA	1:D:89:PRO:HD3	1.90	0.40
1:C:154:GLU:HB2	4:C:436:HOH:O	2.21	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	385/392 (98%)	376 (98%)	9 (2%)	0	100 100
1	B	390/392 (100%)	381 (98%)	8 (2%)	1 (0%)	46 70
1	C	384/392 (98%)	372 (97%)	11 (3%)	1 (0%)	46 70
1	D	382/392 (97%)	375 (98%)	7 (2%)	0	100 100
1	E	386/392 (98%)	376 (97%)	10 (3%)	0	100 100
1	F	387/392 (99%)	378 (98%)	9 (2%)	0	100 100
All	All	2314/2352 (98%)	2258 (98%)	54 (2%)	2 (0%)	56 79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	14	GLN
1	B	216	SER

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	289/288 (100%)	267 (92%)	22 (8%)	16 31
1	B	293/288 (102%)	265 (90%)	28 (10%)	10 19
1	C	288/288 (100%)	260 (90%)	28 (10%)	10 18
1	D	288/288 (100%)	268 (93%)	20 (7%)	19 37
1	E	290/288 (101%)	267 (92%)	23 (8%)	15 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	291/288 (101%)	262 (90%)	29 (10%)	9 17
All	All	1739/1728 (101%)	1589 (91%)	150 (9%)	13 24

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	25	SER
1	A	43	GLU
1	A	50	PHE
1	A	79	MSE
1	A	92	ARG
1	A	94	ARG
1	A	100	LEU
1	A	109	ARG
1	A	118	LEU
1	A	150	LEU
1	A	217	ASP
1	A	254	LEU
1	A	255	SER
1	A	260	VAL
1	A	281	LEU
1	A	354	LEU
1	A	362	LEU
1	A	363	VAL
1	A	368	VAL
1	A	370	SER
1	A	376	THR
1	B	1	VAL
1	B	13	THR
1	B	17	ASP
1	B	50	PHE
1	B	54	VAL
1	B	67	ASP
1	B	79	MSE
1	B	90	GLU
1	B	99	LEU
1	B	100	LEU
1	B	106	GLU
1	B	171	LEU
1	B	190	SER
1	B	197	GLU

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Mol	Chain	Res	Type
1	B	205	LEU
1	B	217	ASP
1	B	219	ASP
1	B	220	LEU
1	B	226	VAL
1	B	248	ARG
1	B	254	LEU
1	B	255	SER
1	B	260	VAL
1	B	316	ARG
1	B	319	LEU
1	B	340	LEU
1	B	354	LEU
1	B	362	LEU
1	C	8	VAL
1	C	50	PHE
1	C	79	MSE
1	C	99	LEU
1	C	113	MSE
1	C	118	LEU
1	C	129	LEU
1	C	139	ARG
1	C	153	ARG
1	C	163	LYS
1	C	169	LEU
1	C	172	VAL
1	C	192	ILE
1	C	199	GLU
1	C	205	LEU
1	C	217	ASP
1	C	220	LEU
1	C	248	ARG
1	C	254	LEU
1	C	260	VAL
1	C	265	GLU
1	C	301	VAL
1	C	302	ASP
1	C	303	LEU
1	C	319	LEU
1	C	340	LEU
1	C	354	LEU
1	C	362	LEU

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Mol	Chain	Res	Type
1	D	40	ASP
1	D	50	PHE
1	D	58	GLU
1	D	69	GLN
1	D	79	MSE
1	D	90	GLU
1	D	92[A]	ARG
1	D	92[B]	ARG
1	D	200	GLU
1	D	220	LEU
1	D	254	LEU
1	D	255	SER
1	D	260	VAL
1	D	271	GLN
1	D	319	LEU
1	D	334	SER
1	D	362	LEU
1	D	368	VAL
1	D	372	ARG
1	D	386	LEU
1	E	5	LEU
1	E	8	VAL
1	E	50	PHE
1	E	54	VAL
1	E	79	MSE
1	E	90	GLU
1	E	92	ARG
1	E	99	LEU
1	E	100	LEU
1	E	106	GLU
1	E	113	MSE
1	E	172	VAL
1	E	180	ARG
1	E	199	GLU
1	E	205	LEU
1	E	217	ASP
1	E	254	LEU
1	E	262	LEU
1	E	264	VAL
1	E	319	LEU
1	E	333	ARG
1	E	340	LEU

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Mol	Chain	Res	Type
1	E	363	VAL
1	F	6	ARG
1	F	8	VAL
1	F	25	SER
1	F	50	PHE
1	F	60	VAL
1	F	69	GLN
1	F	79	MSE
1	F	86	VAL
1	F	90	GLU
1	F	92	ARG
1	F	99	LEU
1	F	100	LEU
1	F	106	GLU
1	F	137	ARG
1	F	172	VAL
1	F	190	SER
1	F	196	LEU
1	F	205	LEU
1	F	254	LEU
1	F	264	VAL
1	F	281	LEU
1	F	301	VAL
1	F	325	THR
1	F	332	ASP
1	F	334	SER
1	F	338	LEU
1	F	354	LEU
1	F	364	THR
1	F	386	LEU

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

Mol	Chain	Res	Type
1	C	14	GLN
1	C	69	GLN
1	C	221	GLN
1	D	201	ASN
1	D	214	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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	EDO	D	401	-	3,3,3	0.52	0	2,2,2	0.28	0
3	EDO	D	402	-	3,3,3	0.56	0	2,2,2	0.12	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
3	EDO	D	401	-	-	0/1/1/1	0/0/0/0
3	EDO	D	402	-	-	0/1/1/1	0/0/0/0

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.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	EDO	5	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	381/392 (97%)	-0.39	3 (0%) 87 86	19, 34, 62, 86	0
1	B	387/392 (98%)	-0.40	3 (0%) 87 86	17, 33, 61, 77	0
1	C	381/392 (97%)	-0.22	7 (1%) 71 68	19, 41, 70, 87	0
1	D	379/392 (96%)	-0.37	1 (0%) 94 94	17, 29, 54, 75	0
1	E	381/392 (97%)	-0.44	0 100 100	15, 31, 57, 74	0
1	F	381/392 (97%)	-0.24	7 (1%) 71 68	16, 36, 66, 91	0
All	All	2290/2352 (97%)	-0.34	21 (0%) 85 84	15, 34, 64, 91	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	192	ILE	4.0
1	F	334	SER	3.4
1	C	369	ALA	3.4
1	B	28	LEU	3.3
1	C	196	LEU	3.3
1	C	216	SER	3.2
1	F	337	VAL	3.1
1	F	338	LEU	2.7
1	C	195	TRP	2.7
1	F	373	LEU	2.5
1	C	169	LEU	2.5
1	B	39	ARG	2.4
1	C	295	PRO	2.3
1	D	247	ALA	2.3
1	F	7[A]	LEU	2.2
1	A	153	ARG	2.2
1	B	192	ILE	2.1
1	F	335	GLY	2.1
1	A	39	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	163	LYS	2.0
1	F	333	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^{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	EDO	D	402	4/4	0.77	0.36	11.44	45,47,49,50	0
2	CL	A	401	1/1	0.95	0.26	1.32	52,52,52,52	0
2	CL	B	401	1/1	0.99	0.08	-2.54	34,34,34,34	0
3	EDO	D	401	4/4	0.92	0.11	-	45,45,46,47	0

6.5 Other polymers (i)

There are no such residues in this entry.