



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:35 AM UTC

PDB ID : 4MY3 / pdb_00004my3
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

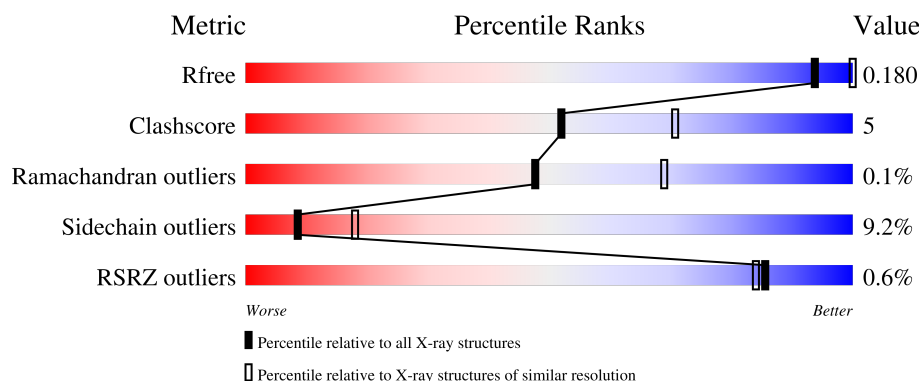
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	392	
1	B	392	
1	C	392	
1	D	392	
1	E	392	

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Mol	Chain	Length	Quality of chain
1	F	392	% 78% 19% ..

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	-

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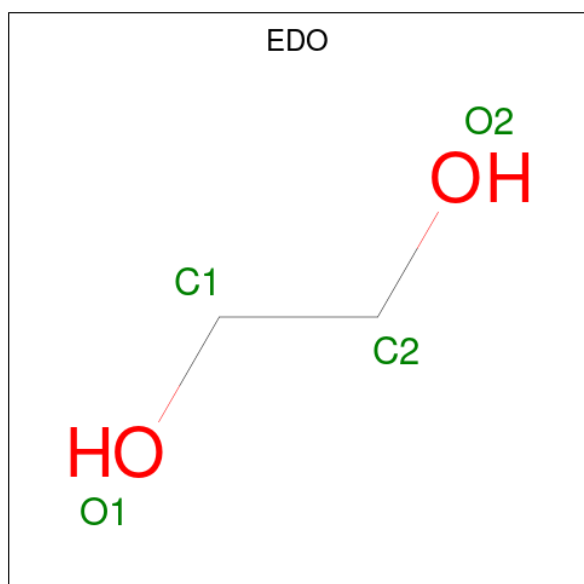
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP D2PVF8
E	0	ALA	-	expression tag	UNP D2PVF8
E	1	VAL	MET	SEE REMARK 999	UNP D2PVF8
F	-2	SER	-	expression tag	UNP D2PVF8
F	-1	ASN	-	expression tag	UNP D2PVF8
F	0	ALA	-	expression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

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

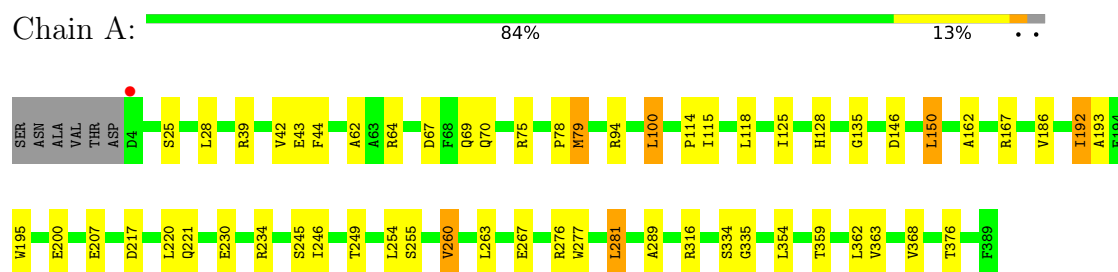
- Molecule 4 is water.

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

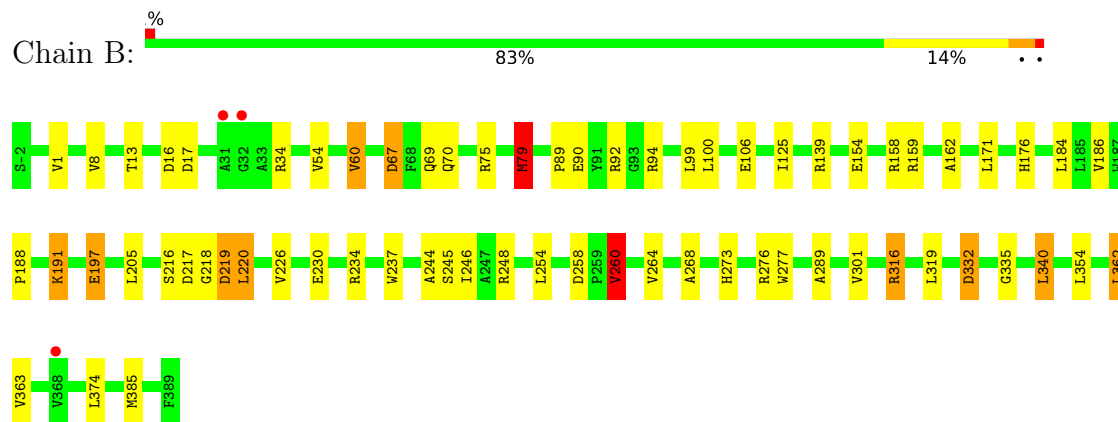
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

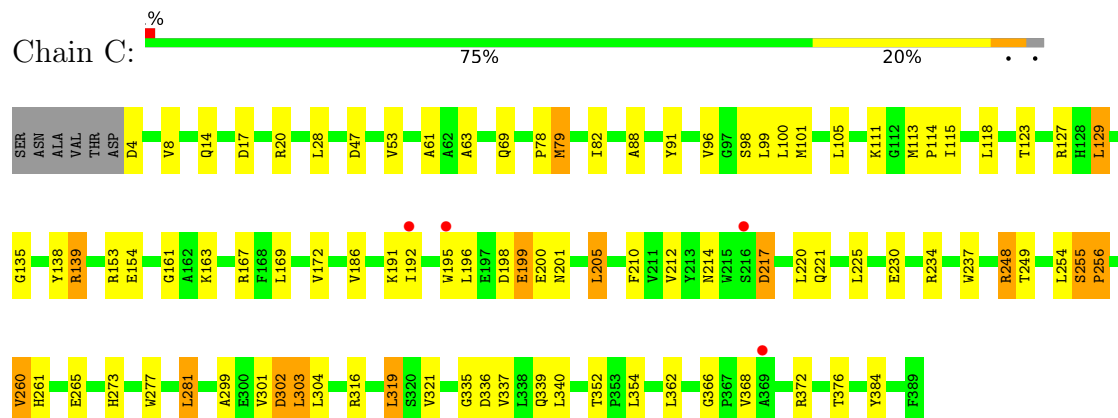
• Molecule 1: GCN5-related N-acetyltransferase



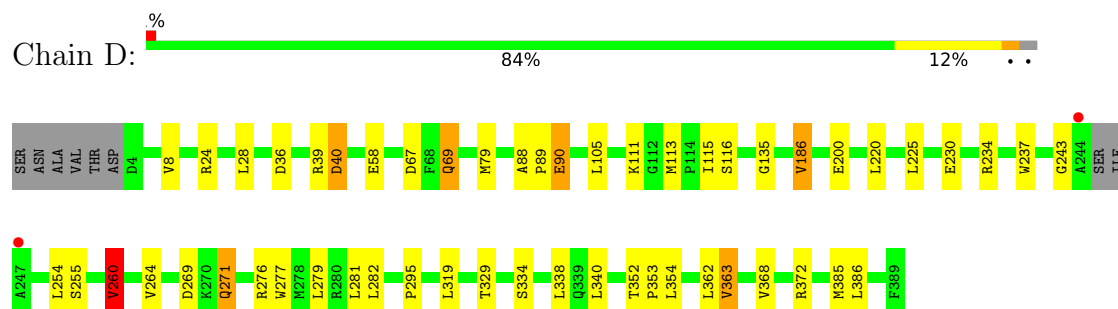
• Molecule 1: GCN5-related N-acetyltransferase



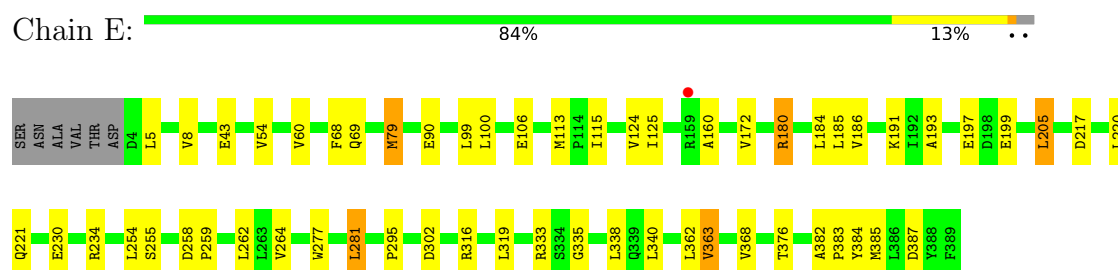
• Molecule 1: GCN5-related N-acetyltransferase



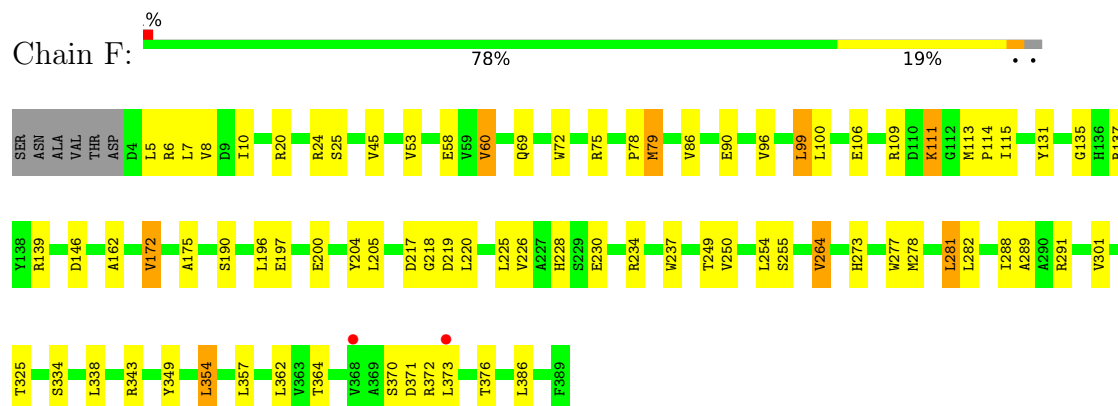
- Molecule 1: GCN5-related N-acetyltransferase



- Molecule 1: GCN5-related N-acetyltransferase



- Molecule 1: GCN5-related N-acetyltransferase



4 Data and refinement statistics

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 41.97 – 2.57	Depositor EDS
% Data completeness (in resolution range)	94.0 (41.97-2.57) 93.9 (41.97-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1161)	Depositor
R, R_{free}	0.176 , 0.235 0.182 , 0.180	Depositor DCC
R_{free} test set	4204 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.52	0/3021	0.85	1/4100 (0.0%)
1	B	0.55	0/3051	0.90	5/4143 (0.1%)
1	C	0.53	0/3010	0.91	6/4086 (0.1%)
1	D	0.55	0/3017	0.89	4/4093 (0.1%)
1	E	0.56	0/3032	0.87	1/4114 (0.0%)
1	F	0.52	0/3040	0.85	4/4126 (0.1%)
All	All	0.54	0/18171	0.88	21/24662 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	260	VAL	CB-CA-C	-8.12	101.19	112.14
1	F	255	SER	CA-C-N	-7.62	112.32	120.47
1	F	255	SER	C-N-CA	-7.62	112.32	120.47
1	C	255	SER	CA-C-N	-7.59	112.20	121.00
1	C	255	SER	C-N-CA	-7.59	112.20	121.00
1	B	79	MSE	N-CA-C	6.78	119.64	108.99
1	B	260	VAL	CB-CA-C	-6.71	103.30	111.88
1	A	260	VAL	CB-CA-C	-6.63	103.19	112.14
1	D	260	VAL	CB-CA-C	-6.57	103.28	112.14
1	F	218	GLY	N-CA-C	-6.52	105.51	114.64
1	D	329	THR	CA-C-N	6.48	126.51	119.90
1	D	329	THR	C-N-CA	6.48	126.51	119.90
1	B	60	VAL	N-CA-C	-6.00	108.00	113.71
1	B	260	VAL	N-CA-CB	5.56	116.69	110.51
1	D	243	GLY	N-CA-C	5.50	118.63	110.60
1	B	218	GLY	N-CA-C	-5.47	107.97	114.48
1	E	124	VAL	N-CA-C	5.38	115.58	110.42
1	C	88	ALA	CA-C-N	5.29	124.93	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	ALA	C-N-CA	5.29	124.93	119.05
1	C	256	PRO	N-CA-C	-5.27	108.65	114.92
1	F	249	THR	N-CA-C	5.05	117.63	109.40

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	28	0
1	B	2988	0	2913	31	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	178	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 (178) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:225:LEU:HD13	1:C:237:TRP:CE2	2.34	0.61
1:F:162:ALA:HB2	1:F:197:GLU:HB3	1.80	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
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:B:230:GLU:O	1:B:234:ARG:HG3	2.02	0.59
1:C:261:HIS:CD2	3:D:402:EDO:H22	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:154:GLU:H	1:B:154:GLU:CD	2.16	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:OD1	1:A:67:ASP:N	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:C:376:THR:HG21	1:D:295:PRO:O	2.09	0.51
1:D:230:GLU:O	1:D:234:ARG:HG3	2.10	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
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:C:255:SER:HB3	1:C:384:TYR:CZ	2.49	0.48
1:E:220:LEU:HD23	1:E:221:GLN:N	2.28	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: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:F:354:LEU:HD23	1:F:371:ASP:CG	2.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:39:ARG:O	1:A:42:VAL:HG22	2.15	0.45
1:B:69:GLN:HB2	1:B:186:VAL:HB	1.97	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:69:GLN:HB2	1:E:186:VAL:HB	1.99	0.45
1:E:338:LEU:HD11	1:E:363:VAL:HG13	1.98	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:C:135:GLY:HA3	1:C:277:TRP:CZ2	2.53	0.44
1:D:277:TRP:CE2	1:D:385:MSE:HE3	2.53	0.44
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:E:230:GLU:O	1:E:234:ARG:HG3	2.16	0.44
1:B:245:SER:OG	1:B:246:ILE:N	2.46	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:C:248:ARG:HE	1:C:249:THR:HG23	1.83	0.44
1:D:260:VAL:O	1:D:264:VAL:HG23	2.17	0.44
1:F:5:LEU:HD13	1:F:96:VAL:HG22	2.00	0.44
1:B:219:ASP:OD2	1:B:219:ASP:N	2.49	0.44
1:C:101:MSE:O	1:C:105:LEU:HG	2.18	0.44
1:A:78:PRO:O	1:A:114:PRO:HD2	2.17	0.43
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:128:HIS:HB2	4:A:556:HOH:O	2.18	0.43
1:E:316:ARG:NH1	1:E:335:GLY:O	2.52	0.43
1:F:79:MSE:HB2	1:F:115:ILE:HG13	1.99	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:A:62:ALA:C	1:A:100:LEU:HD11	2.43	0.43
1:C:372:ARG:O	1:C:376:THR:HG23	2.19	0.43
1:B:75:ARG:NH2	1:B:289:ALA:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ARG:HB3	1:B:273:HIS:HB2	2.00	0.43
1:A:192:ILE:O	1:A:195:TRP:HB3	2.19	0.42
1:B:67:ASP:O	1:B:67:ASP:CG	2.62	0.42
1:E:184:LEU:HD21	1:E:384:TYR:CE1	2.54	0.42
1:F:72:TRP:HB3	1:F:291:ARG:HG3	2.00	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: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:C:319:LEU:HD22	1:C:321:VAL:HG13	2.02	0.42
1:F:220:LEU:HB3	1:F:250:VAL:HG22	2.02	0.42
1:D:338:LEU:HD12	1:D:338:LEU:HA	1.84	0.42
1:D:352:THR:HA	1:D:353:PRO:HD3	1.95	0.42
1:E:193:ALA:O	1:E:197:GLU:HB2	2.20	0.42
1:C:336:ASP:O	1:C:366:GLY:HA2	2.20	0.42
1:E:180:ARG:NH2	1:F:372:ARG:HD3	2.35	0.42
1:B:176:HIS:NE2	1:B:184:LEU:HD13	2.35	0.41
1:D:276:ARG:HE	3:D:402:EDO:H11	1.84	0.41
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:D:36:ASP:OD1	1:D:39:ARG:NH2	2.53	0.41
1:D:338:LEU:HD11	1:D:363:VAL:CG1	2.49	0.41
1:E:68:PHE:HB2	1:E:79:MSE:HG3	2.00	0.41
1:B:158:ARG:NH1	1:B:159:ARG:O	2.53	0.41
1:F:10:ILE:O	1:F:45:VAL:HG13	2.20	0.41
1:F:288:ILE:HD13	1:F:288:ILE:HA	1.93	0.41
1:F:7[A]:LEU:HD21	1:F:99:LEU:O	2.21	0.41
1:F:20:ARG:HG2	1:F:24:ARG:HH22	1.84	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:D:116:SER:O	1:D:279:LEU:HD12	2.20	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:F:109:ARG:HG2	1:F:282:LEU:HB3	2.02	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:A:267:GLU:HG3	1:B:276:ARG:HD2	2.03	0.40
1:C:161:GLY:O	1:C:196:LEU:HD13	2.20	0.40
1:C:261:HIS:CG	3:D:402:EDO:H22	2.56	0.40
1:A:220:LEU:HD23	1:A:221:GLN:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:ASP:OD1	1:C:4:ASP:N	2.55	0.40
1:D:105:LEU:HD22	1:D:282:LEU:HD21	2.03	0.40
1:E:258:ASP:HA	1:E:259:PRO:HD3	1.98	0.40
1:B:220:LEU:HD23	1:B:244:ALA:HA	2.04	0.40
1:C:123:THR:O	1:C:127:ARG:HG3	2.22	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:63:ALA:HB2	1:C:100:LEU:HD21	2.03	0.40
1:C:154:GLU:HB2	4:C:436:HOH:O	2.21	0.40
1:C:217:ASP:OD2	1:C:217:ASP:N	2.52	0.40
1:D:88:ALA:HA	1:D:89:PRO:HD3	1.90	0.40
1:E:295:PRO:O	1:F:376:THR:HG21	2.21	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	385/392 (98%)	376 (98%)	9 (2%)	0	100	100
1	B	390/392 (100%)	381 (98%)	8 (2%)	1 (0%)	36	56
1	C	384/392 (98%)	372 (97%)	11 (3%)	1 (0%)	36	56
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%)	48	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	14	GLN

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Mol	Chain	Res	Type
1	B	216	SER

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	289/288 (100%)	267 (92%)	22 (8%)	12	26
1	B	293/288 (102%)	263 (90%)	30 (10%)	7	14
1	C	288/288 (100%)	257 (89%)	31 (11%)	6	12
1	D	288/288 (100%)	266 (92%)	22 (8%)	12	26
1	E	290/288 (101%)	263 (91%)	27 (9%)	8	18
1	F	291/288 (101%)	263 (90%)	28 (10%)	8	16
All	All	1739/1728 (101%)	1579 (91%)	160 (9%)	8	18

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	28	LEU
1	A	43	GLU
1	A	79	MSE
1	A	94	ARG
1	A	100	LEU
1	A	118	LEU
1	A	125	ILE
1	A	150	LEU
1	A	192	ILE
1	A	217	ASP
1	A	249	THR
1	A	254	LEU
1	A	255	SER
1	A	260	VAL
1	A	281	LEU
1	A	334	SER

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Mol	Chain	Res	Type
1	A	354	LEU
1	A	362	LEU
1	A	363	VAL
1	A	368	VAL
1	A	376	THR
1	B	1	VAL
1	B	8	VAL
1	B	13	THR
1	B	17	ASP
1	B	54	VAL
1	B	60	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	125	ILE
1	B	171	LEU
1	B	191	LYS
1	B	197	GLU
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	260	VAL
1	B	316	ARG
1	B	319	LEU
1	B	332	ASP
1	B	340	LEU
1	B	354	LEU
1	B	362	LEU
1	C	8	VAL
1	C	79	MSE
1	C	98	SER
1	C	99	LEU
1	C	113	MSE
1	C	118	LEU
1	C	129	LEU

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Mol	Chain	Res	Type
1	C	139	ARG
1	C	153	ARG
1	C	163	LYS
1	C	169	LEU
1	C	172	VAL
1	C	191	LYS
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	281	LEU
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
1	C	368	VAL
1	D	8	VAL
1	D	40	ASP
1	D	58	GLU
1	D	69	GLN
1	D	79	MSE
1	D	90	GLU
1	D	111	LYS
1	D	186	VAL
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	354	LEU
1	D	362	LEU

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Mol	Chain	Res	Type
1	D	363	VAL
1	D	368	VAL
1	D	372	ARG
1	D	386	LEU
1	E	5	LEU
1	E	8	VAL
1	E	54	VAL
1	E	60	VAL
1	E	79	MSE
1	E	90	GLU
1	E	99	LEU
1	E	100	LEU
1	E	106	GLU
1	E	113	MSE
1	E	125	ILE
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	281	LEU
1	E	319	LEU
1	E	333	ARG
1	E	340	LEU
1	E	362	LEU
1	E	363	VAL
1	E	368	VAL
1	E	376	THR
1	F	6	ARG
1	F	8	VAL
1	F	25	SER
1	F	60	VAL
1	F	69	GLN
1	F	79	MSE
1	F	86	VAL
1	F	90	GLU
1	F	99	LEU
1	F	100	LEU
1	F	106	GLU

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Mol	Chain	Res	Type
1	F	111	LYS
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	334	SER
1	F	338	LEU
1	F	354	LEU
1	F	362	LEU
1	F	364	THR
1	F	386	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	176	HIS
1	C	14	GLN
1	C	69	GLN
1	C	136	HIS
1	C	221	GLN
1	D	128	HIS
1	E	261	HIS
1	F	69	GLN

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 oligosaccharides 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	402	-	3,3,3	0.52	0	2,2,2	0.09	0
3	EDO	D	401	-	3,3,3	0.48	0	2,2,2	0.24	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	402	-	-	0/1/1/1	-
3	EDO	D	401	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	401	EDO	O1-C1-C2-O2

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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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%)	-0.41	1 (0%)	90 89	16, 34, 62, 86	1 (0%)
1	B	387/392 (98%)	-0.32	3 (0%)	82 81	17, 33, 61, 77	0
1	C	381/392 (97%)	-0.08	4 (1%)	79 77	19, 41, 70, 87	0
1	D	379/392 (96%)	-0.53	2 (0%)	87 86	12, 29, 54, 75	2 (0%)
1	E	381/392 (97%)	-0.45	1 (0%)	90 89	15, 31, 57, 74	2 (0%)
1	F	381/392 (97%)	-0.32	2 (0%)	87 86	13, 36, 66, 91	3 (0%)
All	All	2290/2352 (97%)	-0.35	13 (0%)	85 84	12, 34, 64, 91	8 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	247	ALA	3.3
1	E	159[A]	ARG	3.0
1	C	216	SER	2.6
1	B	31	ALA	2.6
1	C	195	TRP	2.4
1	C	192	ILE	2.4
1	B	368	VAL	2.4
1	F	368	VAL	2.3
1	D	244	ALA	2.2
1	B	32	GLY	2.2
1	F	373	LEU	2.2
1	C	369	ALA	2.2
1	A	4	ASP	2.1

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	D	402	4/4	0.82	0.23	45,47,49,50	0
3	EDO	D	401	4/4	0.89	0.20	45,45,46,47	0
2	CL	A	401	1/1	0.95	0.12	52,52,52,52	0
2	CL	B	401	1/1	0.98	0.05	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.