



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:32 AM UTC

PDB ID : 3A8J / pdb_00003a8j
Title : Crystal Structure of ET-EHred complex
Authors : Okamura-Ikeda, K.; Hosaka, H.
Deposited on : 2009-10-06
Resolution : 1.98 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

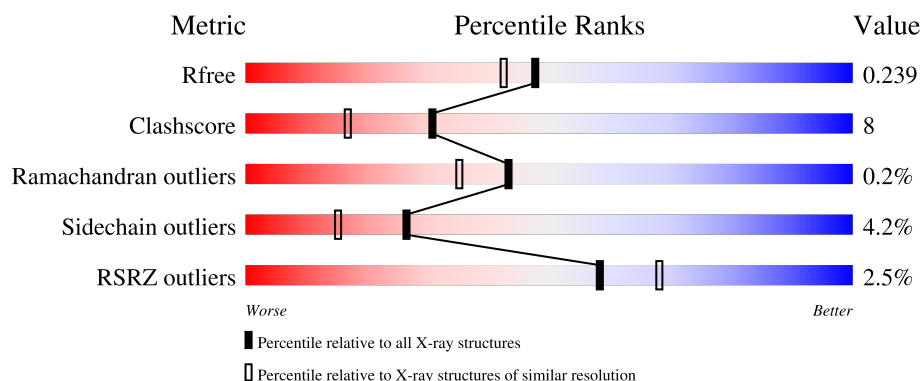
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	364	2% 84% 15% .
1	B	364	84% 13% .
1	C	364	3% 83% 16% .
1	D	364	3% 83% 15% .
2	E	129	5% 84% 12% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	129	4% 75% 21% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14613 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 Aminomethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	2	0
			2823	1782	492	534	15			
1	B	363	Total	C	N	O	S	0	2	0
			2825	1784	492	533	16			
1	C	363	Total	C	N	O	S	0	1	0
			2818	1779	492	532	15			
1	D	363	Total	C	N	O	S	0	2	0
			2839	1794	497	533	15			

- Molecule 2 is a protein called Glycine cleavage system H protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	127	Total	C	N	O	S	0	0	0
			964	606	146	208	4			
2	F	128	Total	C	N	O	S	0	1	0
			982	616	148	213	5			

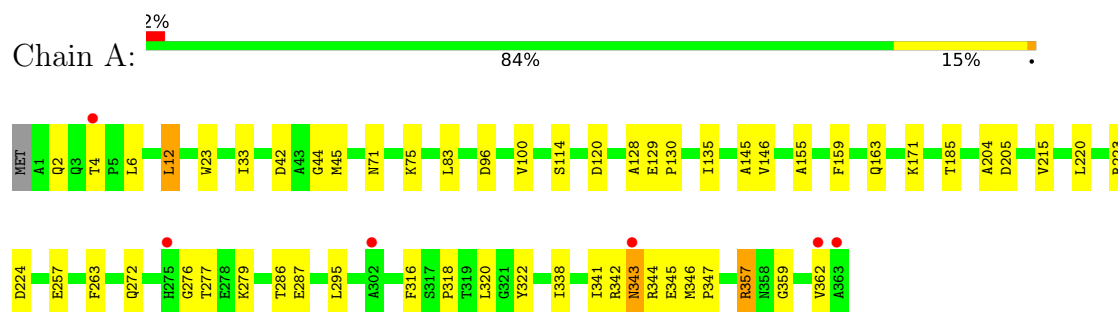
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	332	Total	O	0	0
			332	332		
3	B	326	Total	O	0	0
			326	326		
3	C	280	Total	O	0	0
			280	280		
3	D	273	Total	O	0	0
			273	273		
3	E	77	Total	O	0	0
			77	77		
3	F	74	Total	O	0	0
			74	74		

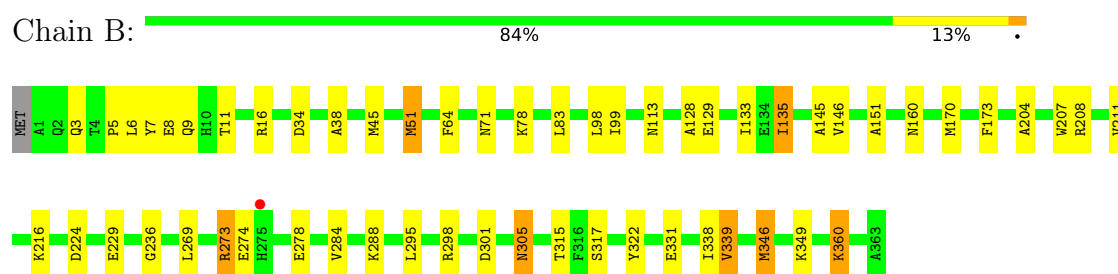
3 Residue-property plots [i](#)

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.

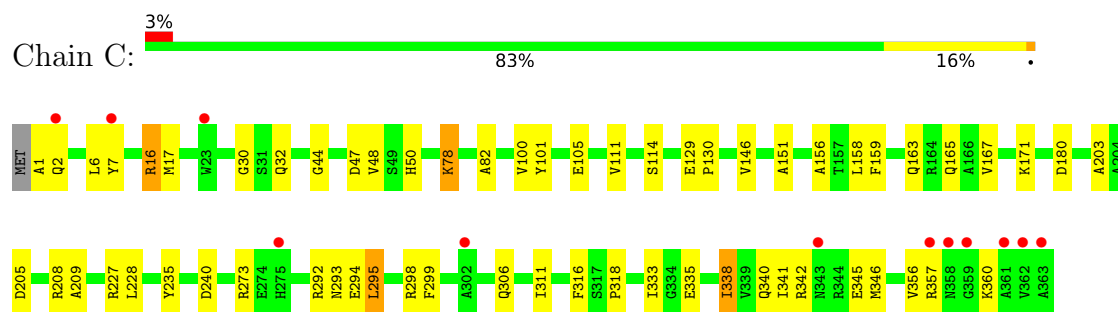
• Molecule 1: Aminomethyltransferase



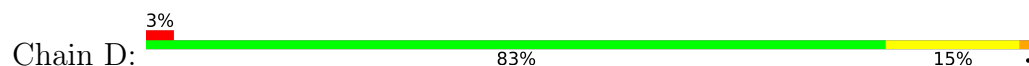
• Molecule 1: Aminomethyltransferase

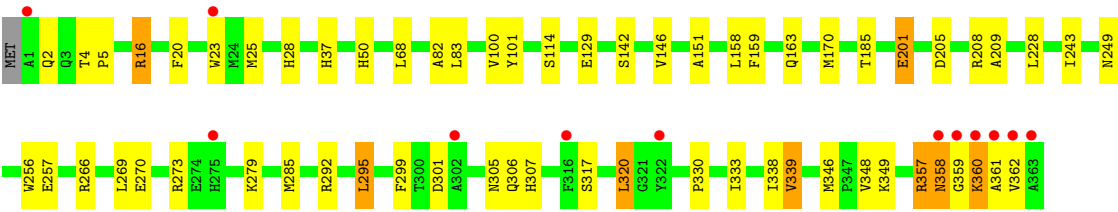


• Molecule 1: Aminomethyltransferase

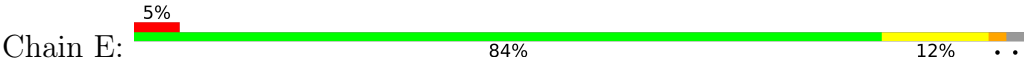


• Molecule 1: Aminomethyltransferase





• Molecule 2: Glycine cleavage system H protein



• Molecule 2: Glycine cleavage system H protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.02Å 88.53Å 97.24Å 91.51° 102.16° 89.66°	Depositor
Resolution (Å)	44.42 – 1.98 44.42 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.2 (44.42-1.98) 97.1 (44.42-1.98)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.172 , 0.238 0.172 , 0.239	Depositor DCC
R_{free} test set	5960 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.066 for -h,k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14613	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LA2

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	1.31	5/2887 (0.2%)	1.13	4/3910 (0.1%)
1	B	1.26	2/2889 (0.1%)	1.14	10/3912 (0.3%)
1	C	1.20	3/2879 (0.1%)	1.12	5/3899 (0.1%)
1	D	1.21	4/2900 (0.1%)	1.12	5/3929 (0.1%)
2	E	1.07	1/960 (0.1%)	1.04	2/1309 (0.2%)
2	F	1.03	1/978 (0.1%)	1.03	0/1331
All	All	1.22	16/13493 (0.1%)	1.11	26/18290 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	111	VAL	CA-CB	7.21	1.63	1.54
1	A	33	ILE	CA-CB	6.70	1.62	1.54
1	B	339	VAL	CA-CB	6.33	1.62	1.54
1	D	339	VAL	CA-CB	6.10	1.62	1.54
1	D	243	ILE	CA-CB	5.95	1.61	1.54
2	F	77	ILE	CA-CB	5.76	1.59	1.53
2	E	97	ALA	CA-C	5.67	1.55	1.52
1	C	180	ASP	CB-CG	5.58	1.66	1.52
1	C	44	GLY	N-CA	5.57	1.50	1.44
1	A	44	GLY	N-CA	5.50	1.50	1.44
1	A	155	ALA	CA-CB	5.50	1.61	1.53
1	A	263	PHE	CA-C	-5.41	1.46	1.52
1	A	4	THR	N-CA	5.33	1.53	1.45
1	D	37	HIS	CA-C	5.29	1.59	1.52
1	D	317	SER	CA-C	5.17	1.58	1.52
1	B	315	THR	CA-CB	5.09	1.62	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	129	GLU	CA-C-N	-7.90	111.66	119.87
1	D	129	GLU	C-N-CA	-7.90	111.66	119.87
1	D	346	MET	CA-C-N	-7.43	112.68	120.03
1	D	346	MET	C-N-CA	-7.43	112.68	120.03
1	B	331	GLU	N-CA-C	-6.85	101.33	110.24
1	B	211	VAL	N-CA-C	-6.67	103.82	110.62
1	B	51[A]	MET	CA-C-N	-6.07	114.62	123.00
1	B	51[A]	MET	C-N-CA	-6.07	114.62	123.00
1	B	51[B]	MET	CA-C-N	-6.07	114.62	123.00
1	B	51[B]	MET	C-N-CA	-6.07	114.62	123.00
1	B	236	GLY	N-CA-C	-5.90	107.67	114.69
2	E	82	ASP	N-CA-C	5.89	120.00	112.34
1	C	342	ARG	CB-CA-C	-5.87	109.25	117.23
1	A	44	GLY	O-C-N	-5.82	118.54	123.60
1	C	167	VAL	N-CA-C	5.66	117.61	112.29
1	A	276	GLY	N-CA-C	-5.62	105.99	112.29
1	A	263	PHE	N-CA-C	-5.42	101.06	109.24
1	C	360	LYS	N-CA-C	5.40	118.36	109.72
1	B	135	ILE	CA-C-N	-5.19	115.68	123.00
1	B	135	ILE	C-N-CA	-5.19	115.68	123.00
1	C	203	ALA	N-CA-C	5.13	117.27	111.11
1	C	44	GLY	N-CA-C	-5.10	103.33	111.18
1	D	68	LEU	N-CA-C	5.10	116.91	111.36
2	E	111	GLU	N-CA-C	-5.09	105.64	111.14
1	A	71	ASN	N-CA-C	-5.03	104.04	110.53
1	B	71	ASN	N-CA-C	-5.03	104.05	110.53

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	2823	0	2780	43	0
1	B	2825	0	2784	39	0
1	C	2818	0	2776	42	0
1	D	2839	0	2786	58	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	964	0	917	15	0
2	F	982	0	931	30	0
3	A	332	0	0	8	0
3	B	326	0	0	7	0
3	C	280	0	0	6	1
3	D	273	0	0	6	1
3	E	77	0	0	2	0
3	F	74	0	0	3	0
All	All	14613	0	12974	218	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (218) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23[B]:TRP:CE3	1:D:50[B]:HIS:CD2	1.96	1.53
1:D:23[B]:TRP:CZ3	1:D:50[B]:HIS:NE2	1.80	1.46
1:D:23[B]:TRP:CD2	1:D:50[B]:HIS:CD2	2.17	1.30
2:F:36:LEU:HD21	2:F:39[B]:MET:SD	1.72	1.27
1:D:23[B]:TRP:CZ3	1:D:50[B]:HIS:CE1	2.28	1.20
1:D:23[B]:TRP:CH2	1:D:50[B]:HIS:CE1	2.36	1.12
1:D:23[B]:TRP:CE3	1:D:50[B]:HIS:NE2	2.09	1.10
1:D:23[B]:TRP:CZ3	1:D:50[B]:HIS:CD2	2.33	1.08
2:F:39[B]:MET:HA	2:F:39[B]:MET:CE	1.84	1.06
2:F:39[B]:MET:HA	2:F:39[B]:MET:HE2	1.35	1.05
2:E:64:LA2:S6	2:E:64:LA2:S8	2.62	0.98
1:D:23[B]:TRP:CE2	1:D:50[B]:HIS:CG	2.55	0.94
1:B:346:MET:HA	1:B:346:MET:HE2	1.54	0.90
1:A:75:LYS:HD3	3:A:590:HOH:O	1.71	0.89
1:D:23[B]:TRP:CZ2	1:D:50[B]:HIS:CG	2.62	0.88
2:F:36:LEU:CD2	2:F:39[B]:MET:SD	2.60	0.88
1:D:23[B]:TRP:CE3	1:D:50[B]:HIS:HD2	1.93	0.86
1:A:362:VAL:O	1:A:362:VAL:HG23	1.75	0.84
2:F:64:LA2:S6	2:F:64:LA2:S8	2.75	0.84
1:A:223:ARG:HD3	2:E:64:LA2:H8A	1.63	0.81
1:D:23[B]:TRP:CD1	1:D:114:SER:HG	1.99	0.81
1:D:23[B]:TRP:CH2	1:D:50[B]:HIS:ND1	2.48	0.81
1:D:23[B]:TRP:CE2	1:D:50[B]:HIS:HB3	2.17	0.80
1:D:23[B]:TRP:CE2	1:D:50[B]:HIS:CD2	2.69	0.80
1:D:23[B]:TRP:CD2	1:D:50[B]:HIS:HD2	1.92	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:LYS:HD3	3:D:614:HOH:O	1.83	0.78
1:C:146:VAL:HG12	1:C:151:ALA:HB1	1.67	0.76
1:D:23[B]:TRP:CD2	1:D:50[B]:HIS:CG	2.75	0.75
1:D:16:ARG:HD2	1:D:28:HIS:CE1	2.23	0.73
1:A:338:ILE:CG2	1:A:345:GLU:HB3	2.18	0.72
1:B:9:GLN:HE21	1:B:207:TRP:HD1	1.36	0.72
2:F:39[B]:MET:HE2	2:F:39[B]:MET:CA	2.16	0.72
1:D:23[B]:TRP:NE1	1:D:50[B]:HIS:HB3	2.06	0.71
1:D:23[B]:TRP:NE1	1:D:114:SER:OG	2.24	0.70
1:A:362:VAL:O	1:A:362:VAL:CG2	2.40	0.70
1:D:23[B]:TRP:CH2	1:D:50[B]:HIS:CG	2.78	0.70
1:D:23[B]:TRP:CE2	1:D:50[B]:HIS:CB	2.75	0.69
2:F:39[B]:MET:HA	2:F:39[B]:MET:HE3	1.72	0.69
1:A:12:LEU:HD23	1:A:12:LEU:O	1.91	0.69
1:C:16:ARG:HH21	1:C:30:GLY:HA2	1.58	0.68
2:E:119:THR:HG23	3:E:225:HOH:O	1.93	0.68
1:A:12:LEU:HD23	1:A:12:LEU:C	2.19	0.67
1:C:2:GLN:NE2	1:C:2:GLN:HA	2.07	0.67
1:D:146:VAL:HG12	1:D:151:ALA:HB1	1.77	0.67
1:C:16:ARG:NH2	1:C:30:GLY:HA2	2.10	0.66
1:C:16:ARG:HH21	1:C:30:GLY:CA	2.09	0.64
1:D:23[B]:TRP:CH2	1:D:50[B]:HIS:CD2	2.83	0.64
1:C:298:ARG:NH1	1:C:340:GLN:OE1	2.29	0.64
2:E:39:MET:CE	2:E:42:VAL:HB	2.29	0.63
1:C:50:HIS:CD2	1:C:114:SER:HB2	2.34	0.62
1:A:338:ILE:HG21	1:A:345:GLU:HB3	1.80	0.62
1:B:7:TYR:HD1	3:B:463:HOH:O	1.82	0.62
1:A:129:GLU:OE1	3:A:731:HOH:O	2.16	0.61
1:A:359:GLY:HA3	3:A:526:HOH:O	2.00	0.61
1:A:272:GLN:HG3	1:A:277:THR:HG22	1.84	0.60
1:D:257:GLU:OE1	3:D:622:HOH:O	2.17	0.60
1:B:208:ARG:HD3	3:B:723:HOH:O	2.01	0.60
1:B:360:LYS:NZ	1:B:360:LYS:CB	2.64	0.60
1:D:23[B]:TRP:CD1	1:D:114:SER:OG	2.55	0.59
3:A:614:HOH:O	1:C:2:GLN:HG2	2.00	0.59
1:C:2:GLN:HA	1:C:2:GLN:HE21	1.68	0.58
1:A:279:LYS:NZ	3:A:544:HOH:O	2.27	0.58
1:B:301:ASP:OD2	1:B:305:ASN:ND2	2.36	0.58
1:C:316:PHE:O	1:C:318:PRO:HD3	2.04	0.58
1:C:205:ASP:OD1	1:C:208:ARG:NH1	2.38	0.57
1:B:269:LEU:HD12	3:B:608:HOH:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:VAL:HG12	1:B:151:ALA:HB1	1.87	0.57
1:D:292:ARG:H	1:D:295:LEU:HD22	1.69	0.56
1:A:359:GLY:CA	3:A:526:HOH:O	2.52	0.56
1:C:341:ILE:HD12	1:C:346:MET:HG3	1.86	0.56
2:F:74:SER:OG	2:F:111:GLU:OE2	2.23	0.56
1:A:220:LEU:HD22	2:E:64:LA2:H8	1.87	0.56
1:D:170:MET:HE3	1:D:185:THR:HG23	1.88	0.56
2:F:39[B]:MET:HE1	2:F:61:GLU:C	2.31	0.56
1:B:298:ARG:HB2	1:B:338:ILE:HD11	1.88	0.55
1:B:64:PHE:CB	1:B:133:ILE:HD11	2.37	0.55
2:E:13:HIS:ND1	2:E:121:TYR:OH	2.32	0.54
1:C:293:ASN:O	1:C:294:GLU:HB2	2.08	0.54
2:F:39[B]:MET:HE2	2:F:61:GLU:O	2.09	0.53
1:B:9:GLN:HE21	1:B:207:TRP:CD1	2.21	0.53
1:B:349:LYS:HE2	3:B:626:HOH:O	2.08	0.53
1:A:287:GLU:HG3	1:A:346:MET:CE	2.40	0.52
1:A:114:SER:HA	3:A:685:HOH:O	2.09	0.52
1:B:7:TYR:O	1:B:11:THR:HG23	2.10	0.52
1:C:1:ALA:N	3:C:657:HOH:O	2.37	0.52
1:D:299:PHE:CE2	1:D:333:ILE:HA	2.44	0.52
1:D:201:GLU:H	1:D:201:GLU:CD	2.18	0.52
1:D:359:GLY:H	1:D:360:LYS:HD2	1.75	0.52
2:F:39[B]:MET:CE	2:F:39[B]:MET:CA	2.67	0.52
1:A:344:ARG:HD3	1:A:346:MET:SD	2.50	0.51
1:A:341:ILE:O	1:A:344:ARG:HG3	2.11	0.51
2:F:123:ALA:HA	2:F:126:GLU:HB2	1.93	0.51
1:C:16:ARG:HH21	1:C:30:GLY:N	2.09	0.51
1:A:128:ALA:HB3	1:A:135:ILE:HD11	1.92	0.51
2:E:116:LEU:HB3	2:E:120:ALA:HB3	1.92	0.51
1:B:34[C]:ASP:OD2	1:B:216:LYS:HE2	2.11	0.50
2:E:27:GLY:HA2	2:E:101:ILE:HG12	1.93	0.50
1:B:51[B]:MET:SD	1:B:113:ASN:HA	2.52	0.49
1:A:45:MET:HA	1:A:145:ALA:O	2.12	0.49
1:D:285:MET:HG3	1:D:348:VAL:HG12	1.95	0.49
2:F:52:SER:O	2:F:53:ALA:C	2.54	0.49
1:D:20:PHE:O	1:D:23[B]:TRP:HB2	2.12	0.49
1:D:279:LYS:HE2	3:D:577:HOH:O	2.13	0.48
1:A:272:GLN:HG3	1:A:277:THR:CG2	2.43	0.48
2:E:114:SER:HB2	3:E:236:HOH:O	2.13	0.48
1:D:205:ASP:OD1	1:D:208:ARG:NH1	2.46	0.48
1:D:23[B]:TRP:CZ2	1:D:50[B]:HIS:ND1	2.75	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:LYS:NZ	1:B:360:LYS:HB3	2.28	0.48
1:C:299:PHE:CE2	1:C:333:ILE:HA	2.49	0.48
1:C:105:GLU:OE1	3:C:667:HOH:O	2.20	0.48
1:C:293:ASN:ND2	3:C:491:HOH:O	2.47	0.48
1:D:307:HIS:HB3	1:D:330:PRO:CG	2.44	0.48
2:F:123:ALA:HB2	3:F:245:HOH:O	2.13	0.48
1:A:96:ASP:OD2	1:A:120:ASP:OD2	2.32	0.48
1:D:5:PRO:HG2	1:D:142:SER:OG	2.14	0.48
2:F:39[B]:MET:CE	2:F:61:GLU:O	2.62	0.48
1:C:158:LEU:HD22	1:C:209:ALA:HB1	1.96	0.48
1:D:159:PHE:HB3	1:D:163:GLN:HB2	1.95	0.48
1:B:38:ALA:HB2	1:B:216:LYS:HD3	1.96	0.47
1:C:357:ARG:NH2	3:C:583:HOH:O	2.46	0.47
2:E:39:MET:HE1	2:E:42:VAL:HB	1.94	0.47
1:A:224:ASP:HB2	2:E:64:LA2:H5	1.95	0.47
1:C:292:ARG:H	1:C:295:LEU:HD22	1.78	0.47
1:B:224:ASP:HB2	2:F:64:LA2:H5	1.97	0.47
2:F:25:THR:OG1	2:F:103:LYS:HD3	2.14	0.47
2:F:46:GLU:HA	2:F:46:GLU:OE1	2.15	0.47
1:B:360:LYS:HE3	3:B:674:HOH:O	2.14	0.47
1:A:286:THR:HA	1:A:322:TYR:CD1	2.50	0.47
1:A:6:LEU:CD2	1:A:204:ALA:HA	2.45	0.46
1:D:357:ARG:O	1:D:358:ASN:HB2	2.15	0.46
2:F:64:LA2:H4A	2:F:64:LA2:H7	1.49	0.46
1:D:360:LYS:HE3	1:D:360:LYS:HB3	1.60	0.46
2:F:45:PRO:O	2:F:80:VAL:HG11	2.15	0.46
1:C:78:LYS:HB2	1:C:78:LYS:HE2	1.75	0.46
1:D:16:ARG:HD2	1:D:28:HIS:HE1	1.78	0.46
1:A:287:GLU:HG3	1:A:346:MET:HE3	1.97	0.46
1:C:227:ARG:HD2	1:C:227:ARG:C	2.41	0.46
1:B:129:GLU:OE2	1:D:23[A]:TRP:CH2	2.69	0.46
1:B:273:ARG:HG2	1:B:274:GLU:N	2.31	0.46
1:C:50:HIS:CD2	1:C:114:SER:CB	2.99	0.46
1:C:338:ILE:HG12	1:C:345:GLU:HB3	1.97	0.45
1:B:6:LEU:HD21	1:B:204:ALA:HA	1.97	0.45
1:B:346:MET:HE2	1:B:346:MET:CA	2.34	0.45
1:B:128:ALA:HB3	1:B:135:ILE:HD11	1.97	0.45
1:A:338:ILE:HD13	1:A:347:PRO:HA	1.97	0.45
1:A:12:LEU:C	1:A:12:LEU:CD2	2.88	0.45
1:B:269:LEU:CD1	3:B:608:HOH:O	2.63	0.45
1:D:2:GLN:CD	1:D:23[B]:TRP:CH2	2.95	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:56:ASP:HB3	2:E:70:TYR:CE1	2.52	0.45
1:C:7:TYR:CD1	1:C:17:MET:HE3	2.52	0.45
1:D:4:THR:HG22	1:D:50[B]:HIS:CE1	2.51	0.45
1:A:257:GLU:OE2	3:A:709:HOH:O	2.21	0.45
2:F:64:LA2:HDA	2:F:64:LA2:HA	1.69	0.44
1:A:287:GLU:OE2	1:A:347:PRO:HD2	2.18	0.44
1:A:357:ARG:HG3	1:A:362:VAL:CG1	2.48	0.44
1:B:360:LYS:HZ2	1:B:360:LYS:HB2	1.83	0.44
1:D:266:ARG:O	1:D:270:GLU:HG2	2.16	0.44
1:D:2:GLN:OE1	1:D:23[B]:TRP:CH2	2.70	0.44
1:A:2:GLN:HB2	1:A:23:TRP:CE3	2.52	0.44
1:D:320:LEU:O	3:D:582:HOH:O	2.21	0.44
2:E:39:MET:HE3	2:E:42:VAL:HB	1.99	0.43
1:C:50:HIS:HD2	1:C:114:SER:CB	2.32	0.43
1:D:158:LEU:HD13	1:D:209:ALA:CB	2.48	0.43
1:B:83:LEU:C	1:B:83:LEU:HD12	2.44	0.43
1:C:1:ALA:C	1:C:2:GLN:HE21	2.26	0.43
1:C:32:GLN:HG3	3:C:406:HOH:O	2.17	0.43
1:C:356:VAL:HG12	1:C:357:ARG:N	2.33	0.43
1:C:6:LEU:HD12	1:C:47:ASP:CG	2.44	0.43
1:B:6:LEU:CD2	1:B:204:ALA:HA	2.49	0.42
1:C:293:ASN:HA	1:C:311:ILE:HG22	2.00	0.42
1:C:129:GLU:HB3	1:C:130:PRO:HD3	2.00	0.42
1:B:64:PHE:CD2	1:B:133:ILE:CD1	3.02	0.42
1:B:99:ILE:HD12	1:B:173:PHE:HE2	1.84	0.42
1:A:83:LEU:C	1:A:83:LEU:HD12	2.44	0.42
1:A:220:LEU:HD22	2:E:64:LA2:C8	2.50	0.42
1:A:6:LEU:HD23	1:A:204:ALA:HA	2.00	0.42
1:D:23[B]:TRP:HD1	1:D:114:SER:HG	1.59	0.42
1:A:159:PHE:HB3	1:A:163:GLN:HB2	2.01	0.42
1:D:301:ASP:OD2	1:D:305:ASN:HB2	2.20	0.42
1:D:307:HIS:HB3	1:D:330:PRO:HG2	2.01	0.41
1:B:16:ARG:NH2	2:F:34:GLU:OE2	2.30	0.41
1:C:82:ALA:HB2	1:C:101:TYR:CD2	2.55	0.41
2:F:17:ARG:NH2	3:F:221:HOH:O	2.54	0.41
2:F:126:GLU:HB3	3:F:263:HOH:O	2.20	0.41
1:B:360:LYS:NZ	1:B:360:LYS:HB2	2.34	0.41
1:C:48:VAL:HA	1:C:50:HIS:CE1	2.55	0.41
1:C:235:TYR:CZ	1:C:240:ASP:HA	2.56	0.41
1:D:82:ALA:HB2	1:D:101:TYR:CD2	2.55	0.41
1:A:146:VAL:HG13	1:A:215:VAL:HG11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:ASN:HA	3:D:453:HOH:O	2.19	0.41
2:F:58:ALA:HB3	2:F:69:ILE:HB	2.01	0.41
1:A:128:ALA:CB	1:A:135:ILE:HD11	2.50	0.41
1:B:45:MET:HA	1:B:145:ALA:O	2.21	0.41
1:C:156:ALA:HA	1:C:159:PHE:CD2	2.56	0.41
1:C:165:GLN:HE21	1:C:165:GLN:HB2	1.67	0.41
1:D:256:TRP:CZ2	1:D:273:ARG:HD3	2.56	0.41
2:F:39[B]:MET:CE	2:F:61:GLU:C	2.93	0.41
1:C:159:PHE:HB3	1:C:163:GLN:HB2	2.03	0.41
2:F:79:ALA:HB3	2:F:103:LYS:HG3	2.02	0.41
1:B:129:GLU:OE2	1:D:23[A]:TRP:HH2	2.04	0.40
1:B:284:VAL:HG13	1:B:322:TYR:CE1	2.55	0.40
1:D:23[B]:TRP:HB3	1:D:25:MET:HG2	2.03	0.40
1:D:279:LYS:CE	3:D:577:HOH:O	2.68	0.40
2:E:64:LA2:H4A	2:E:64:LA2:H7	1.86	0.40
1:A:129:GLU:HB3	1:A:130:PRO:HD3	2.02	0.40
1:A:357:ARG:HG3	1:A:362:VAL:HG12	2.04	0.40
1:B:160:ASN:HB2	3:B:504:HOH:O	2.21	0.40
1:A:130:PRO:HG3	1:C:2:GLN:HG3	2.02	0.40
2:F:4:PRO:HD2	2:F:9:TYR:OH	2.21	0.40
1:B:98:LEU:HD12	1:B:98:LEU:C	2.46	0.40
1:C:16:ARG:HB3	3:C:662:HOH:O	2.20	0.40
2:F:105:LYS:HA	2:F:105:LYS:HD2	1.89	0.40
1:A:316:PHE:O	1:A:318:PRO:HD3	2.22	0.40
1:A:342:ARG:HB2	1:A:343:ASN:H	1.49	0.40
1:B:229:GLU:OE2	1:B:317:SER:OG	2.36	0.40
1:B:360:LYS:CB	1:B:360:LYS:HZ2	2.35	0.40
1:C:293:ASN:O	1:C:294:GLU:CB	2.68	0.40
2:F:124:LEU:O	2:F:127:ASP:HB3	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:678:HOH:O	3:D:674:HOH:O[1_656]	2.05	0.15

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	363/364 (100%)	353 (97%)	9 (2%)	1 (0%)	36	27
1	B	363/364 (100%)	354 (98%)	8 (2%)	1 (0%)	36	27
1	C	362/364 (100%)	348 (96%)	14 (4%)	0	100	100
1	D	363/364 (100%)	347 (96%)	14 (4%)	2 (1%)	21	12
2	E	124/129 (96%)	122 (98%)	2 (2%)	0	100	100
2	F	126/129 (98%)	121 (96%)	5 (4%)	0	100	100
All	All	1701/1714 (99%)	1645 (97%)	52 (3%)	4 (0%)	43	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	358	ASN
1	B	278	GLU
1	A	42	ASP
1	D	361	ALA

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	293/292 (100%)	284 (97%)	9 (3%)	35	26
1	B	293/292 (100%)	281 (96%)	12 (4%)	27	16
1	C	292/292 (100%)	282 (97%)	10 (3%)	32	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	293/292 (100%)	279 (95%)	14 (5%)	23	11
2	E	101/103 (98%)	96 (95%)	5 (5%)	22	10
2	F	103/103 (100%)	95 (92%)	8 (8%)	11	3
All	All	1375/1374 (100%)	1317 (96%)	58 (4%)	26	15

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	100	VAL
1	A	171	LYS
1	A	185	THR
1	A	205	ASP
1	A	295	LEU
1	A	320	LEU
1	A	343	ASN
1	A	357	ARG
1	B	3	GLN
1	B	5	PRO
1	B	8	GLU
1	B	78	LYS
1	B	170	MET
1	B	273	ARG
1	B	288	LYS
1	B	295	LEU
1	B	305	ASN
1	B	339	VAL
1	B	346	MET
1	B	360	LYS
1	C	16	ARG
1	C	78	LYS
1	C	100	VAL
1	C	171	LYS
1	C	228	LEU
1	C	273	ARG
1	C	295	LEU
1	C	306	GLN
1	C	335	GLU
1	C	338	ILE
1	D	16	ARG
1	D	83	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	100	VAL
1	D	201	GLU
1	D	228	LEU
1	D	269	LEU
1	D	295	LEU
1	D	306	GLN
1	D	320	LEU
1	D	338	ILE
1	D	339	VAL
1	D	357	ARG
1	D	360	LYS
1	D	362	VAL
2	E	11	LYS
2	E	12	GLU
2	E	105	LYS
2	E	116	LEU
2	E	119	THR
2	F	11	LYS
2	F	16	LEU
2	F	34	GLU
2	F	74	SER
2	F	86	ASP
2	F	109	GLU
2	F	122	GLU
2	F	124	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	B	9	GLN
1	B	177	GLN
1	B	303	GLN
1	B	305	ASN
1	B	340	GLN
1	B	343	ASN
1	C	2	GLN
1	C	9	GLN
1	C	37	HIS
1	C	165	GLN
1	C	293	ASN
1	D	9	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	37	HIS
1	D	152	GLN
1	D	303	GLN
1	D	306	GLN
2	E	2	ASN

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	$\# Z > 2$
2	LA2	F	64	2	17,19,20	0.64	0	12,21,23	2.70	4 (33%)
2	LA2	E	64	2	17,19,20	0.61	0	12,21,23	2.97	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
2	LA2	F	64	2	-	11/18/20/22	-
2	LA2	E	64	2	-	8/18/20/22	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	64	LA2	C7-C8-S8	-8.23	105.17	113.74
2	F	64	LA2	C7-C8-S8	-6.84	106.61	113.74
2	E	64	LA2	CE-NZ-C1	5.58	133.21	122.82
2	F	64	LA2	CE-NZ-C1	3.74	129.78	122.82
2	F	64	LA2	CD-CE-NZ	-3.55	102.23	112.20
2	F	64	LA2	C3-C2-C1	-2.56	106.08	113.19

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	64	LA2	C5-C6-C7-C8
2	E	64	LA2	C6-C7-C8-S8
2	F	64	LA2	C4-C5-C6-C7
2	F	64	LA2	C5-C6-C7-C8
2	F	64	LA2	C6-C7-C8-S8
2	E	64	LA2	CG-CD-CE-NZ
2	E	64	LA2	C3-C4-C5-C6
2	F	64	LA2	C3-C4-C5-C6
2	E	64	LA2	CA-CB-CG-CD
2	E	64	LA2	C1-C2-C3-C4
2	F	64	LA2	C2-C3-C4-C5
2	F	64	LA2	CD-CE-NZ-C1
2	F	64	LA2	C1-C2-C3-C4
2	F	64	LA2	CE-CD-CG-CB
2	F	64	LA2	CA-CB-CG-CD
2	E	64	LA2	C2-C3-C4-C5
2	E	64	LA2	CE-CD-CG-CB
2	F	64	LA2	C-CA-CB-CG
2	F	64	LA2	C4-C5-C6-S6

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	64	LA2	4	0
2	E	64	LA2	6	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 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	363/364 (99%)	-0.30	6 (1%) 69 78	10, 19, 41, 59	2 (0%)
1	B	363/364 (99%)	-0.34	1 (0%) 90 93	12, 20, 40, 56	2 (0%)
1	C	363/364 (99%)	-0.07	12 (3%) 49 59	10, 23, 46, 66	1 (0%)
1	D	363/364 (99%)	0.09	12 (3%) 49 59	14, 26, 46, 71	2 (0%)
2	E	126/129 (97%)	0.49	7 (5%) 30 38	20, 33, 58, 69	0
2	F	127/129 (98%)	0.58	5 (3%) 43 53	13, 36, 51, 66	1 (0%)
All	All	1705/1714 (99%)	-0.05	43 (2%) 58 68	10, 24, 48, 71	8 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	363	ALA	4.9
1	A	363	ALA	4.8
1	D	361	ALA	3.5
2	E	124	LEU	3.3
1	C	361	ALA	3.2
1	A	362	VAL	3.2
2	E	1	SER	3.1
1	B	275	HIS	3.0
1	C	359	GLY	3.0
1	D	23[A]	TRP	3.0
2	E	119	THR	3.0
1	D	316	PHE	3.0
2	E	125	LEU	2.9
1	D	362	VAL	2.9
1	D	322	TYR	2.9
1	C	23	TRP	2.9
2	E	118	ALA	2.8
1	C	363	ALA	2.7
1	C	362	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	275	HIS	2.6
1	D	359	GLY	2.6
2	E	20	ALA	2.5
1	D	302	ALA	2.5
1	A	4	THR	2.5
2	F	124	LEU	2.4
2	E	3	VAL	2.4
1	D	275	HIS	2.4
1	D	360	LYS	2.4
1	C	357	ARG	2.4
1	A	302	ALA	2.3
1	A	343	ASN	2.3
1	C	358	ASN	2.3
1	C	7	TYR	2.2
1	C	343	ASN	2.2
1	C	2	GLN	2.2
2	F	22	GLY	2.2
1	D	358	ASN	2.1
2	F	20	ALA	2.1
2	F	123	ALA	2.1
1	C	275	HIS	2.1
1	C	302	ALA	2.1
1	D	1	ALA	2.1
2	F	3	VAL	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. 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(Å ²)	Q<0.9
2	LA2	F	64	20/21	0.92	0.12	23,47,55,61	0
2	LA2	E	64	20/21	0.95	0.08	24,30,45,51	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.