



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:53 AM UTC

PDB ID : 1Z7L / pdb_00001z7l
Title : Crystal structure of fragment of mouse ubiquitin-activating enzyme
Authors : Szczepanowski, R.H.; Filipek, R.; Bochtler, M.
Deposited on : 2005-03-25
Resolution : 2.80 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

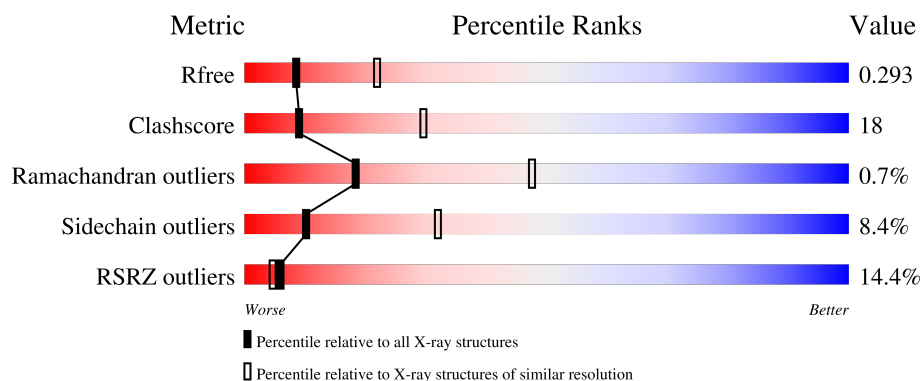
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	276	12% 58% 30% 8%
1	B	276	11% 59% 30% 8%
1	C	276	17% 58% 32% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6144 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 Ubiquitin-activating enzyme E1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2030	1287	353	382	8			
1	B	255	Total	C	N	O	S	0	0	0
			2030	1287	353	382	8			
1	C	255	Total	C	N	O	S	0	0	0
			2030	1287	353	382	8			

There are 30 discrepancies between the modelled and reference sequences:

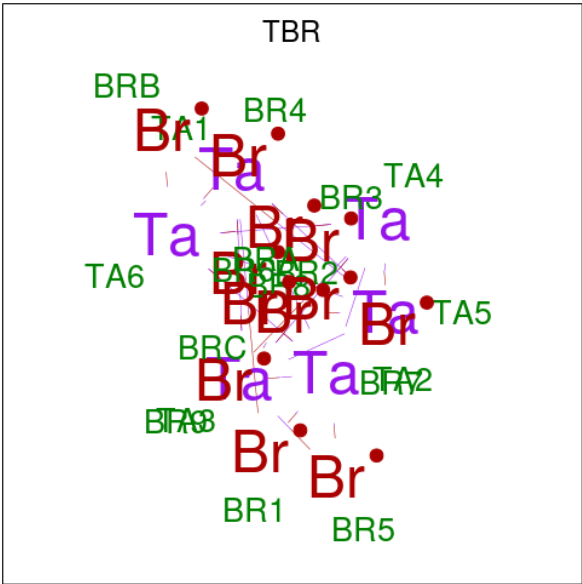
Chain	Residue	Modelled	Actual	Comment	Reference
A	616	MET	-	expression tag	UNP Q02053
A	617	GLY	-	expression tag	UNP Q02053
A	618	HIS	-	expression tag	UNP Q02053
A	619	HIS	-	expression tag	UNP Q02053
A	620	HIS	-	expression tag	UNP Q02053
A	621	HIS	-	expression tag	UNP Q02053
A	622	HIS	-	expression tag	UNP Q02053
A	623	HIS	-	expression tag	UNP Q02053
A	624	GLU	-	expression tag	UNP Q02053
A	625	PHE	-	expression tag	UNP Q02053
B	616	MET	-	expression tag	UNP Q02053
B	617	GLY	-	expression tag	UNP Q02053
B	618	HIS	-	expression tag	UNP Q02053
B	619	HIS	-	expression tag	UNP Q02053
B	620	HIS	-	expression tag	UNP Q02053
B	621	HIS	-	expression tag	UNP Q02053
B	622	HIS	-	expression tag	UNP Q02053
B	623	HIS	-	expression tag	UNP Q02053
B	624	GLU	-	expression tag	UNP Q02053
B	625	PHE	-	expression tag	UNP Q02053
C	616	MET	-	expression tag	UNP Q02053
C	617	GLY	-	expression tag	UNP Q02053
C	618	HIS	-	expression tag	UNP Q02053

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	619	HIS	-	expression tag	UNP Q02053
C	620	HIS	-	expression tag	UNP Q02053
C	621	HIS	-	expression tag	UNP Q02053
C	622	HIS	-	expression tag	UNP Q02053
C	623	HIS	-	expression tag	UNP Q02053
C	624	GLU	-	expression tag	UNP Q02053
C	625	PHE	-	expression tag	UNP Q02053

- Molecule 2 is HEXATANTALUM DODECABROMIDE (CCD ID: TBR) (formula: Br₁₂Ta₆).

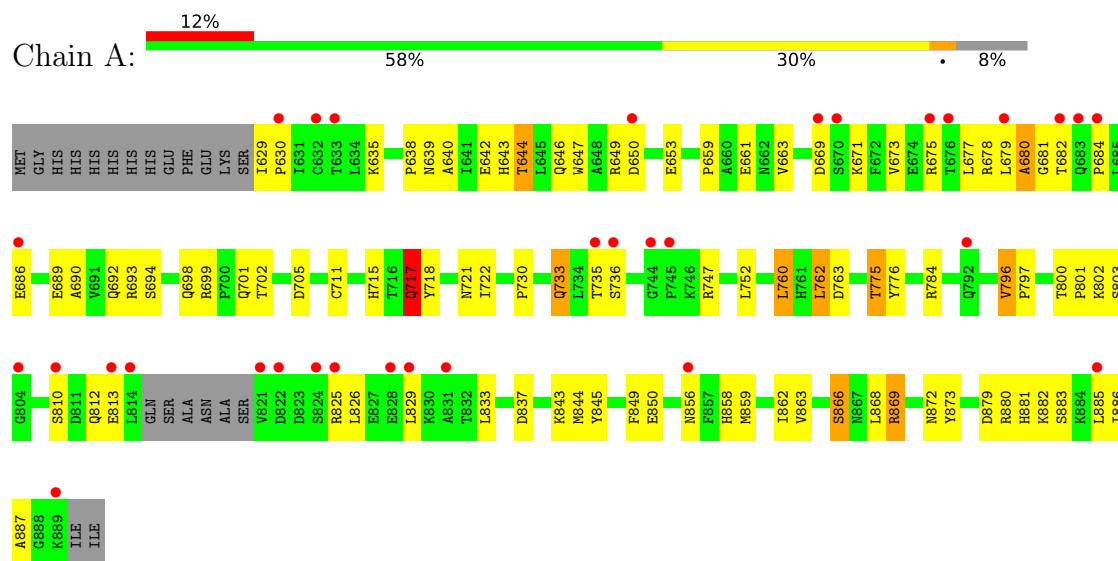


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Br	Ta	0	0
			18	12	6		
2	B	1	Total	Br	Ta	0	0
			18	12	6		
2	C	1	Total	Br	Ta	0	0
			18	12	6		

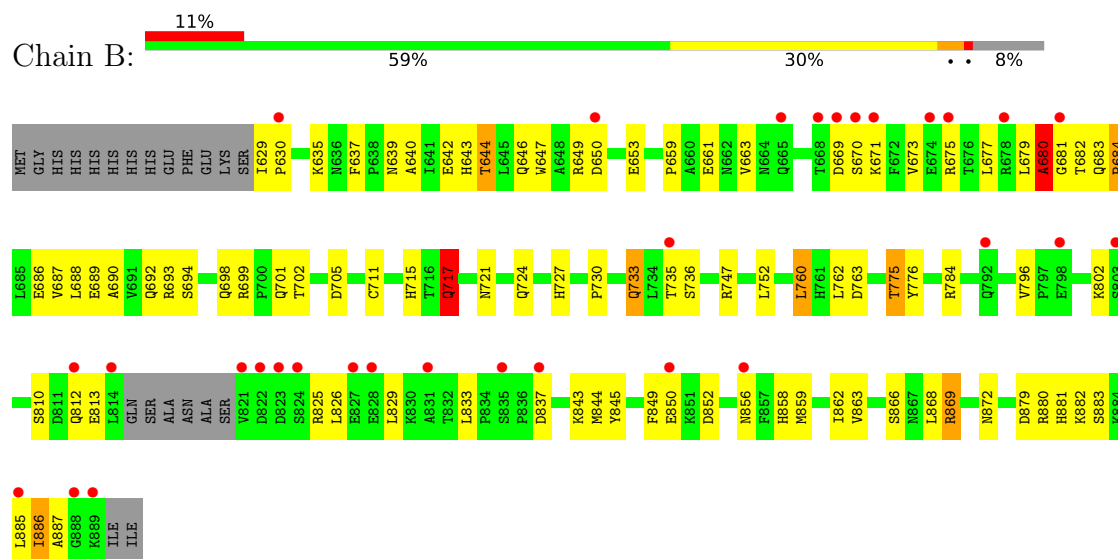
3 Residue-property plots [i](#)

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.

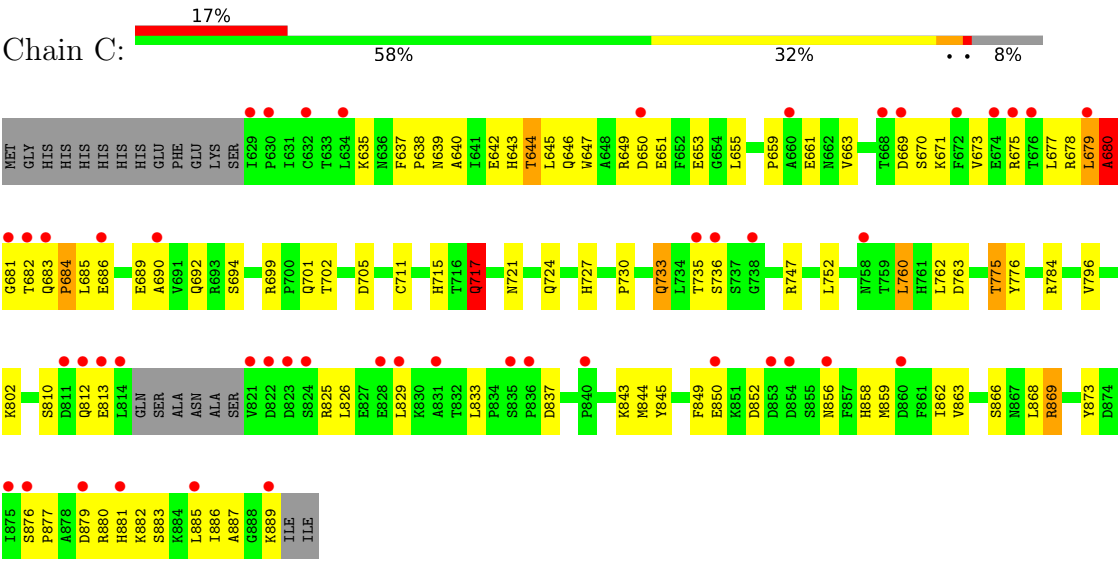
• Molecule 1: Ubiquitin-activating enzyme E1 1



• Molecule 1: Ubiquitin-activating enzyme E1 1



• Molecule 1: Ubiquitin-activating enzyme E1 1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	216.12Å 216.12Å 196.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (10.00-2.80) 96.7 (10.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.06 (at 2.79Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.277 , 0.308 0.266 , 0.293	Depositor DCC
R_{free} test set	2109 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6144	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: TBR

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	0.51	0/2085	1.01	10/2841 (0.4%)
1	B	0.53	0/2085	1.02	10/2841 (0.4%)
1	C	0.51	1/2085 (0.0%)	1.02	11/2841 (0.4%)
All	All	0.52	1/6255 (0.0%)	1.02	31/8523 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	679	LEU	C-N	-7.85	1.22	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	825	ARG	N-CA-C	-7.16	103.55	111.36
1	C	825	ARG	N-CA-C	-7.12	103.60	111.36
1	A	825	ARG	N-CA-C	-7.08	103.64	111.36
1	B	635	LYS	N-CA-C	6.65	118.32	111.14
1	C	717	GLN	N-CA-C	6.06	119.15	111.69
1	B	852	ASP	N-CA-C	6.00	119.08	111.69
1	A	635	LYS	N-CA-C	5.99	117.61	111.14
1	C	690	ALA	N-CA-C	-5.98	104.84	111.36
1	C	852	ASP	N-CA-C	5.90	118.94	111.69
1	C	701	GLN	N-CA-C	-5.84	106.50	113.97
1	B	717	GLN	N-CA-C	5.80	118.82	111.69
1	A	690	ALA	N-CA-C	-5.79	105.05	111.36
1	A	678	ARG	N-CA-C	-5.68	106.57	112.93
1	B	690	ALA	N-CA-C	-5.62	105.07	111.14
1	A	717	GLN	N-CA-C	5.61	118.59	111.69
1	C	678	ARG	N-CA-C	-5.56	106.71	112.93
1	C	679	LEU	N-CA-C	5.50	119.03	110.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	680	ALA	N-CA-C	5.48	122.47	110.80
1	B	670	SER	CA-C-O	5.47	124.82	118.97
1	B	701	GLN	N-CA-C	-5.42	107.21	113.88
1	C	680	ALA	N-CA-C	5.34	122.17	110.80
1	A	886	ILE	N-CA-C	-5.33	105.82	113.07
1	C	635	LYS	N-CA-C	5.32	116.88	111.14
1	A	701	GLN	N-CA-C	-5.24	107.44	113.88
1	B	637	PHE	N-CA-C	5.24	118.50	108.97
1	C	637	PHE	N-CA-C	5.22	118.47	108.97
1	A	680	ALA	N-CA-C	5.16	121.78	110.80
1	B	886	ILE	N-CA-C	-5.12	106.11	113.07
1	A	803	SER	N-CA-C	5.07	117.78	111.24
1	A	722	ILE	N-CA-C	-5.06	105.78	110.53
1	C	670	SER	CA-C-O	5.01	124.33	118.97

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	2030	0	1953	72	0
1	B	2030	0	1953	73	0
1	C	2030	0	1953	76	0
2	A	18	0	0	3	0
2	B	18	0	0	3	0
2	C	18	0	0	3	0
All	All	6144	0	5859	221	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 18.

All (221) 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:717:GLN:HE21	1:A:717:GLN:HA	1.15	1.09
1:B:717:GLN:HA	1:B:717:GLN:HE21	1.20	1.05
1:C:717:GLN:HA	1:C:717:GLN:HE21	1.15	1.03
1:C:649:ARG:HH12	1:C:653:GLU:HG2	1.24	1.01
1:A:649:ARG:HH12	1:A:653:GLU:HG2	1.27	0.98
1:B:649:ARG:HH12	1:B:653:GLU:HG2	1.29	0.97
1:B:639:ASN:H	1:B:643:HIS:HD2	1.15	0.94
1:A:639:ASN:H	1:A:643:HIS:HD2	1.18	0.91
1:C:639:ASN:H	1:C:643:HIS:HD2	1.20	0.89
1:B:881:HIS:O	1:B:885:LEU:HG	1.73	0.88
1:B:671:LYS:HE3	1:B:675:ARG:HD3	1.58	0.86
1:A:671:LYS:HE3	1:A:675:ARG:HD3	1.57	0.86
1:C:671:LYS:HE3	1:C:675:ARG:HD3	1.56	0.85
1:C:881:HIS:O	1:C:885:LEU:HG	1.76	0.84
1:C:649:ARG:NH1	1:C:653:GLU:HG2	1.93	0.83
1:A:717:GLN:HE21	1:A:717:GLN:CA	1.90	0.83
1:C:717:GLN:HE21	1:C:717:GLN:CA	1.92	0.83
1:A:881:HIS:O	1:A:885:LEU:HG	1.80	0.82
1:A:649:ARG:NH1	1:A:653:GLU:HG2	1.97	0.79
1:B:649:ARG:NH1	1:B:653:GLU:HG2	1.97	0.78
1:C:879:ASP:OD1	1:C:882:LYS:HG3	1.83	0.78
1:A:717:GLN:HA	1:A:717:GLN:NE2	1.96	0.78
1:C:735:THR:HG22	1:C:736:SER:H	1.49	0.77
1:B:717:GLN:HE21	1:B:717:GLN:CA	1.95	0.77
1:A:879:ASP:OD1	1:A:882:LYS:HG3	1.84	0.76
1:C:717:GLN:HA	1:C:717:GLN:NE2	1.98	0.76
1:B:879:ASP:OD1	1:B:882:LYS:HG3	1.85	0.75
1:B:730:PRO:HD2	1:B:733:GLN:CG	2.16	0.75
1:C:639:ASN:H	1:C:643:HIS:CD2	2.06	0.73
1:B:717:GLN:HA	1:B:717:GLN:NE2	2.01	0.73
1:B:735:THR:HG22	1:B:736:SER:H	1.53	0.73
1:B:639:ASN:H	1:B:643:HIS:CD2	2.05	0.73
1:C:730:PRO:HD2	1:C:733:GLN:CG	2.19	0.72
1:A:677:LEU:HD11	1:A:826:LEU:HD21	1.72	0.72
1:A:730:PRO:HD2	1:A:733:GLN:CG	2.21	0.71
1:A:735:THR:HG22	1:A:736:SER:H	1.56	0.70
1:A:650:ASP:HA	2:A:999:TBR:BR6	2.46	0.70
1:B:650:ASP:HA	2:B:1000:TBR:BR6	2.45	0.70
1:C:677:LEU:HD11	1:C:826:LEU:HD21	1.73	0.69
1:C:730:PRO:HD2	1:C:733:GLN:HG2	1.72	0.69
1:B:730:PRO:HD2	1:B:733:GLN:HG2	1.74	0.69
1:C:763:ASP:OD1	1:C:784:ARG:NH2	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:LEU:HD11	1:B:826:LEU:HD21	1.76	0.68
1:C:650:ASP:HA	2:C:1001:TBR:BR6	2.48	0.68
1:A:730:PRO:HD2	1:A:733:GLN:HG2	1.76	0.67
1:A:702:THR:HG22	1:A:705:ASP:CG	2.19	0.67
1:C:702:THR:HG22	1:C:705:ASP:CG	2.19	0.66
1:A:639:ASN:H	1:A:643:HIS:CD2	2.07	0.66
1:C:735:THR:HG22	1:C:736:SER:N	2.11	0.65
1:A:702:THR:HG23	1:A:705:ASP:H	1.61	0.65
1:A:717:GLN:HE22	1:A:721:ASN:HD22	1.43	0.65
1:B:702:THR:HG22	1:B:705:ASP:CG	2.22	0.65
1:C:849:PHE:HZ	1:C:859:MET:CE	2.10	0.64
1:C:640:ALA:H	1:C:643:HIS:CD2	2.16	0.64
1:C:702:THR:HG23	1:C:705:ASP:H	1.62	0.64
1:A:849:PHE:HZ	1:A:859:MET:CE	2.12	0.63
1:C:717:GLN:HE22	1:C:721:ASN:HD22	1.45	0.63
1:B:763:ASP:OD1	1:B:784:ARG:NH2	2.31	0.63
1:C:775:THR:HG23	1:C:844:MET:HE2	1.81	0.63
1:B:717:GLN:HE22	1:B:721:ASN:HD22	1.47	0.62
1:A:763:ASP:OD1	1:A:784:ARG:NH2	2.33	0.62
1:B:735:THR:HG22	1:B:736:SER:N	2.15	0.61
1:A:775:THR:HG23	1:A:844:MET:HE2	1.83	0.61
1:B:673:VAL:O	1:B:677:LEU:HB2	2.00	0.60
1:B:702:THR:HG23	1:B:705:ASP:H	1.65	0.60
1:B:849:PHE:HZ	1:B:859:MET:CE	2.14	0.60
1:A:640:ALA:H	1:A:643:HIS:CD2	2.19	0.60
1:B:730:PRO:HD2	1:B:733:GLN:HG3	1.83	0.60
1:C:673:VAL:O	1:C:677:LEU:HB2	2.01	0.60
1:C:659:PRO:O	1:C:663:VAL:HG23	2.02	0.59
1:B:717:GLN:NE2	1:B:721:ASN:HD22	2.01	0.59
1:A:717:GLN:NE2	1:A:721:ASN:HD22	2.00	0.59
1:B:760:LEU:HD13	1:B:868:LEU:CD2	2.34	0.58
1:B:650:ASP:OD1	2:B:1000:TBR:BR6	2.76	0.58
1:B:775:THR:HG23	1:B:844:MET:HE2	1.84	0.58
1:A:760:LEU:HD13	1:A:868:LEU:CD2	2.34	0.57
1:A:650:ASP:OD1	2:A:999:TBR:BR6	2.78	0.57
1:A:735:THR:HG22	1:A:736:SER:N	2.17	0.57
1:B:659:PRO:O	1:B:663:VAL:HG23	2.04	0.57
1:C:640:ALA:H	1:C:643:HIS:HD2	1.52	0.57
1:B:760:LEU:HD13	1:B:868:LEU:HD23	1.85	0.57
1:C:717:GLN:NE2	1:C:721:ASN:HD22	2.03	0.56
1:B:640:ALA:H	1:B:643:HIS:CD2	2.24	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:711:CYS:O	1:C:715:HIS:HD2	1.89	0.56
1:A:673:VAL:O	1:A:677:LEU:HB2	2.05	0.55
1:A:760:LEU:HD13	1:A:868:LEU:HD23	1.88	0.55
1:C:843:LYS:HE2	1:C:845:TYR:OH	2.07	0.55
1:C:862:ILE:O	1:C:866:SER:HB3	2.07	0.55
1:B:682:THR:HG23	1:B:686:GLU:OE1	2.07	0.54
1:A:862:ILE:O	1:A:866:SER:HB3	2.08	0.53
1:A:671:LYS:O	1:A:675:ARG:CB	2.56	0.53
1:B:671:LYS:O	1:B:675:ARG:CB	2.56	0.53
1:A:671:LYS:O	1:A:675:ARG:HB2	2.09	0.53
1:C:730:PRO:HD2	1:C:733:GLN:HG3	1.90	0.53
1:C:671:LYS:O	1:C:675:ARG:CB	2.57	0.52
1:B:671:LYS:O	1:B:675:ARG:HB2	2.09	0.52
1:C:671:LYS:O	1:C:675:ARG:HB2	2.09	0.52
1:C:682:THR:HG23	1:C:686:GLU:OE1	2.10	0.52
1:A:730:PRO:HD2	1:A:733:GLN:HG3	1.89	0.52
1:A:850:GLU:H	1:A:858:HIS:HD2	1.58	0.51
1:B:812:GLN:HA	1:B:812:GLN:OE1	2.10	0.51
1:A:812:GLN:OE1	1:A:812:GLN:HA	2.11	0.51
1:A:682:THR:HG23	1:A:686:GLU:OE1	2.10	0.51
1:C:760:LEU:HD13	1:C:868:LEU:HD23	1.91	0.51
1:A:856:ASN:HB3	1:A:858:HIS:ND1	2.26	0.51
1:B:711:CYS:O	1:B:715:HIS:HD2	1.93	0.51
1:A:640:ALA:H	1:A:643:HIS:HD2	1.58	0.51
1:C:760:LEU:HD13	1:C:868:LEU:CD2	2.41	0.51
1:C:812:GLN:OE1	1:C:812:GLN:HA	2.10	0.51
1:B:850:GLU:H	1:B:858:HIS:HD2	1.57	0.51
1:C:882:LYS:O	1:C:886:ILE:HG13	2.11	0.51
1:C:679:LEU:HD12	1:C:680:ALA:H	1.76	0.50
1:C:689:GLU:HG3	1:C:829:LEU:HD11	1.94	0.50
1:C:650:ASP:OD1	2:C:1001:TBR:BR6	2.85	0.50
1:A:845:TYR:CD1	1:A:845:TYR:N	2.79	0.50
1:B:845:TYR:N	1:B:845:TYR:CD1	2.80	0.50
1:C:845:TYR:N	1:C:845:TYR:CD1	2.79	0.50
1:C:849:PHE:HZ	1:C:859:MET:HE2	1.75	0.49
1:A:882:LYS:HA	1:A:885:LEU:HD12	1.94	0.49
1:A:711:CYS:O	1:A:715:HIS:HD2	1.94	0.49
1:C:856:ASN:HB3	1:C:858:HIS:ND1	2.28	0.49
1:C:850:GLU:H	1:C:858:HIS:HD2	1.61	0.49
1:B:862:ILE:O	1:B:866:SER:HB3	2.12	0.48
1:A:689:GLU:HG3	1:A:829:LEU:HD11	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:856:ASN:HB3	1:B:858:HIS:ND1	2.29	0.48
1:C:639:ASN:HA	1:C:747:ARG:HD2	1.94	0.48
1:B:882:LYS:HA	1:B:885:LEU:HD12	1.94	0.48
1:C:883:SER:O	1:C:887:ALA:HB2	2.14	0.48
1:B:692:GLN:OE1	1:B:833:LEU:HD23	2.14	0.47
1:C:692:GLN:OE1	1:C:833:LEU:HD23	2.14	0.47
1:A:849:PHE:HZ	1:A:859:MET:HE2	1.77	0.47
1:B:883:SER:O	1:B:887:ALA:HB2	2.14	0.47
1:A:659:PRO:O	1:A:663:VAL:HG23	2.15	0.47
1:A:752:LEU:HD13	1:A:872:ASN:OD1	2.15	0.47
1:A:863:VAL:HG21	1:A:880:ARG:HA	1.97	0.47
1:B:689:GLU:HG3	1:B:829:LEU:HD11	1.96	0.47
1:A:850:GLU:H	1:A:858:HIS:CD2	2.33	0.47
1:A:692:GLN:OE1	1:A:833:LEU:HD23	2.15	0.46
1:A:843:LYS:HE2	1:A:845:TYR:OH	2.14	0.46
1:A:775:THR:HG22	1:A:776:TYR:CD2	2.51	0.46
1:B:849:PHE:HZ	1:B:859:MET:HE2	1.80	0.46
1:A:650:ASP:CG	2:A:999:TBR:BR6	3.14	0.46
1:A:883:SER:O	1:A:887:ALA:HB2	2.16	0.46
1:C:876:SER:HA	1:C:877:PRO:HD3	1.82	0.46
1:A:717:GLN:CA	1:A:717:GLN:NE2	2.63	0.45
1:B:650:ASP:CG	2:B:1000:TBR:BR6	3.14	0.45
1:B:850:GLU:H	1:B:858:HIS:CD2	2.33	0.45
1:C:863:VAL:HG21	1:C:880:ARG:HA	1.98	0.45
1:A:702:THR:HG23	1:A:705:ASP:N	2.29	0.45
1:B:858:HIS:O	1:B:862:ILE:HG12	2.17	0.45
1:A:775:THR:HG23	1:A:844:MET:CE	2.47	0.45
1:C:647:TRP:CE3	1:C:869:ARG:HD2	2.52	0.45
1:B:639:ASN:HA	1:B:747:ARG:HD2	1.99	0.45
1:A:644:THR:HG23	1:A:866:SER:HA	1.99	0.44
1:B:679:LEU:HD12	1:B:680:ALA:H	1.82	0.44
1:C:850:GLU:H	1:C:858:HIS:CD2	2.36	0.44
1:A:858:HIS:O	1:A:862:ILE:HG12	2.18	0.44
1:B:644:THR:CG2	1:B:866:SER:OG	2.66	0.44
1:A:856:ASN:HB3	1:A:858:HIS:H	1.83	0.44
1:C:887:ALA:C	1:C:889:LYS:H	2.25	0.44
1:B:775:THR:HG22	1:B:776:TYR:CD2	2.53	0.43
1:C:702:THR:HG23	1:C:705:ASP:N	2.31	0.43
1:A:639:ASN:HA	1:A:747:ARG:HD2	1.99	0.43
1:B:775:THR:HG23	1:B:844:MET:CE	2.46	0.43
1:B:856:ASN:HB3	1:B:858:HIS:H	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:647:TRP:CD2	1:C:869:ARG:HD2	2.53	0.43
1:C:651:GLU:HG3	1:C:655:LEU:CD1	2.49	0.43
1:B:863:VAL:HG21	1:B:880:ARG:HA	2.00	0.43
1:A:762:LEU:HD23	1:A:762:LEU:HA	1.85	0.43
1:C:644:THR:HG23	1:C:866:SER:HA	2.01	0.43
1:C:689:GLU:CG	1:C:829:LEU:HD11	2.49	0.43
1:A:679:LEU:HD12	1:A:680:ALA:H	1.84	0.43
1:C:724:GLN:O	1:C:727:HIS:HB3	2.19	0.43
1:C:775:THR:HG22	1:C:776:TYR:CD2	2.54	0.43
1:C:702:THR:HG22	1:C:705:ASP:OD2	2.19	0.43
1:C:775:THR:HG23	1:C:844:MET:CE	2.47	0.43
1:A:689:GLU:CG	1:A:829:LEU:HD11	2.49	0.42
1:A:810:SER:O	1:A:812:GLN:N	2.51	0.42
1:C:849:PHE:CZ	1:C:859:MET:HE2	2.54	0.42
1:A:718:TYR:HA	1:A:872:ASN:HD21	1.84	0.42
1:B:843:LYS:HE2	1:B:845:TYR:OH	2.19	0.42
1:C:858:HIS:O	1:C:862:ILE:HG12	2.19	0.42
1:B:810:SER:O	1:B:812:GLN:N	2.50	0.42
1:C:685:LEU:HD23	1:C:685:LEU:HA	1.89	0.42
1:C:638:PRO:HD2	1:C:873:TYR:CE2	2.54	0.42
1:C:810:SER:O	1:C:812:GLN:N	2.52	0.42
1:C:640:ALA:N	1:C:643:HIS:CD2	2.87	0.42
1:B:886:ILE:HG22	1:B:886:ILE:O	2.19	0.42
1:C:717:GLN:CA	1:C:717:GLN:NE2	2.65	0.42
1:B:752:LEU:HD13	1:B:872:ASN:OD1	2.20	0.41
1:C:644:THR:HG22	1:C:645:LEU:N	2.35	0.41
1:A:638:PRO:HD2	1:A:873:TYR:CE2	2.56	0.41
1:B:644:THR:HG23	1:B:866:SER:HA	2.02	0.41
1:B:689:GLU:CG	1:B:829:LEU:HD11	2.50	0.41
1:A:629:ILE:O	1:A:630:PRO:C	2.62	0.41
1:C:849:PHE:CZ	1:C:859:MET:CE	2.97	0.41
1:B:644:THR:HG22	1:B:866:SER:OG	2.21	0.41
1:C:683:GLN:O	1:C:684:PRO:C	2.64	0.41
1:A:849:PHE:CZ	1:A:859:MET:HE2	2.56	0.41
1:B:640:ALA:H	1:B:643:HIS:HD2	1.67	0.41
1:C:685:LEU:HD23	1:C:826:LEU:HD12	2.02	0.41
1:B:629:ILE:O	1:B:630:PRO:C	2.63	0.41
1:B:702:THR:HG23	1:B:705:ASP:N	2.32	0.41
1:B:882:LYS:O	1:B:886:ILE:HG13	2.21	0.41
1:B:687:VAL:HG12	1:B:688:LEU:N	2.36	0.40
1:B:849:PHE:CZ	1:B:859:MET:CE	3.00	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:ARG:HG3	1:A:698:GLN:HG3	2.03	0.40
1:A:647:TRP:CE3	1:A:869:ARG:HD2	2.56	0.40
1:A:796:VAL:HA	1:A:797:PRO:HD3	1.97	0.40
1:B:671:LYS:O	1:B:671:LYS:HG3	2.21	0.40
1:B:683:GLN:O	1:B:684:PRO:C	2.65	0.40
1:B:693:ARG:HG3	1:B:698:GLN:HG3	2.03	0.40
1:B:724:GLN:O	1:B:727:HIS:HB3	2.21	0.40
1:A:800:THR:HA	1:A:801:PRO:HD3	1.97	0.40
1:A:849:PHE:CZ	1:A:859:MET:CE	2.99	0.40
1:C:650:ASP:CG	2:C:1001:TBR:BR6	3.20	0.40
1:C:856:ASN:HB3	1:C:858:HIS:H	1.85	0.40
1:A:644:THR:CG2	1:A:866:SER:OG	2.69	0.40
1:B:647:TRP:CD2	1:B:869:ARG:HD2	2.57	0.40
1:B:647:TRP:CE3	1:B:869:ARG:HD2	2.56	0.40
1:C:887:ALA:C	1:C:889:LYS:N	2.79	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	251/276 (91%)	232 (92%)	18 (7%)	1 (0%)	30	60
1	B	251/276 (91%)	235 (94%)	14 (6%)	2 (1%)	16	44
1	C	251/276 (91%)	233 (93%)	16 (6%)	2 (1%)	16	44
All	All	753/828 (91%)	700 (93%)	48 (6%)	5 (1%)	18	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	681	GLY
1	B	681	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	681	GLY
1	C	680	ALA
1	B	680	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	223/243 (92%)	204 (92%)	19 (8%)	10	31
1	B	223/243 (92%)	205 (92%)	18 (8%)	11	33
1	C	223/243 (92%)	204 (92%)	19 (8%)	10	31
All	All	669/729 (92%)	613 (92%)	56 (8%)	10	32

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	642	GLU
1	A	644	THR
1	A	646	GLN
1	A	661	GLU
1	A	669	ASP
1	A	684	PRO
1	A	694	SER
1	A	699	ARG
1	A	717	GLN
1	A	733	GLN
1	A	760	LEU
1	A	762	LEU
1	A	775	THR
1	A	796	VAL
1	A	802	LYS
1	A	813	GLU
1	A	837	ASP
1	A	866	SER
1	A	869	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	642	GLU
1	B	644	THR
1	B	646	GLN
1	B	661	GLU
1	B	669	ASP
1	B	684	PRO
1	B	694	SER
1	B	699	ARG
1	B	717	GLN
1	B	733	GLN
1	B	760	LEU
1	B	762	LEU
1	B	775	THR
1	B	796	VAL
1	B	802	LYS
1	B	813	GLU
1	B	837	ASP
1	B	869	ARG
1	C	642	GLU
1	C	644	THR
1	C	646	GLN
1	C	661	GLU
1	C	669	ASP
1	C	684	PRO
1	C	694	SER
1	C	699	ARG
1	C	717	GLN
1	C	733	GLN
1	C	752	LEU
1	C	760	LEU
1	C	762	LEU
1	C	775	THR
1	C	796	VAL
1	C	802	LYS
1	C	813	GLU
1	C	837	ASP
1	C	869	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	643	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	646	GLN
1	A	658	GLN
1	A	665	GLN
1	A	683	GLN
1	A	713	HIS
1	A	715	HIS
1	A	717	GLN
1	A	733	GLN
1	A	750	HIS
1	A	774	GLN
1	A	858	HIS
1	A	872	ASN
1	B	643	HIS
1	B	646	GLN
1	B	658	GLN
1	B	665	GLN
1	B	683	GLN
1	B	713	HIS
1	B	715	HIS
1	B	717	GLN
1	B	733	GLN
1	B	750	HIS
1	B	858	HIS
1	C	643	HIS
1	C	646	GLN
1	C	658	GLN
1	C	665	GLN
1	C	683	GLN
1	C	713	HIS
1	C	715	HIS
1	C	717	GLN
1	C	733	GLN
1	C	750	HIS
1	C	858	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TBR	A	999	-	0,36,36	-	-	-		
2	TBR	C	1001	-	0,36,36	-	-	-		
2	TBR	B	1000	-	0,36,36	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	999	TBR	3	0
2	C	1001	TBR	3	0
2	B	1000	TBR	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	255/276 (92%)	0.52	32 (12%) 8 6	23, 70, 112, 161	0
1	B	255/276 (92%)	0.39	31 (12%) 8 6	23, 63, 103, 162	0
1	C	255/276 (92%)	1.12	47 (18%) 3 2	23, 81, 117, 162	0
All	All	765/828 (92%)	0.68	110 (14%) 6 5	23, 73, 113, 162	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	822	ASP	6.3
1	C	822	ASP	6.1
1	B	821	VAL	6.0
1	A	814	LEU	5.7
1	C	630	PRO	5.4
1	B	814	LEU	5.4
1	A	824	SER	5.3
1	C	885	LEU	5.0
1	A	679	LEU	4.7
1	B	885	LEU	4.6
1	C	676	THR	4.5
1	B	681	GLY	4.3
1	B	889	LYS	4.3
1	C	821	VAL	4.3
1	A	885	LEU	4.3
1	C	828	GLU	4.1
1	A	744	GLY	3.9
1	C	735	THR	3.9
1	A	745	PRO	3.8
1	B	671	LYS	3.7
1	B	792	GLN	3.7
1	C	881	HIS	3.7
1	C	669	ASP	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	856	ASN	3.7
1	C	650	ASP	3.6
1	C	829	LEU	3.6
1	A	821	VAL	3.5
1	C	736	SER	3.5
1	C	823	ASP	3.5
1	A	630	PRO	3.4
1	C	836	PRO	3.4
1	A	682	THR	3.3
1	C	879	ASP	3.3
1	B	630	PRO	3.3
1	A	669	ASP	3.3
1	C	854	ASP	3.3
1	B	812	GLN	3.2
1	C	875	ILE	3.2
1	C	675	ARG	3.1
1	C	850	GLU	3.1
1	C	674	GLU	3.0
1	A	736	SER	3.0
1	B	803	SER	3.0
1	C	738	GLY	3.0
1	C	672	PHE	2.9
1	B	798	GLU	2.9
1	A	889	LYS	2.8
1	B	856	ASN	2.8
1	C	811	ASP	2.8
1	C	831	ALA	2.8
1	A	792	GLN	2.7
1	C	814	LEU	2.7
1	A	633	THR	2.7
1	B	735	THR	2.7
1	A	684	PRO	2.7
1	B	674	GLU	2.7
1	A	822	ASP	2.7
1	A	683	GLN	2.7
1	C	835	SER	2.7
1	C	629	ILE	2.6
1	A	650	ASP	2.6
1	B	670	SER	2.6
1	C	682	THR	2.5
1	A	813	GLU	2.5
1	C	679	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	850	GLU	2.5
1	B	675	ARG	2.5
1	C	683	GLN	2.5
1	C	668	THR	2.5
1	C	634	LEU	2.4
1	A	735	THR	2.4
1	B	827	GLU	2.4
1	C	758	ASN	2.4
1	C	856	ASN	2.4
1	C	853	ASP	2.4
1	C	889	LYS	2.4
1	C	686	GLU	2.4
1	B	888	GLY	2.4
1	C	632	CYS	2.4
1	C	860	ASP	2.4
1	A	676	THR	2.4
1	A	686	GLU	2.3
1	A	831	ALA	2.3
1	C	824	SER	2.3
1	A	675	ARG	2.3
1	C	690	ALA	2.3
1	C	840	PRO	2.3
1	C	660	ALA	2.3
1	A	825	ARG	2.3
1	B	678	ARG	2.3
1	C	812	GLN	2.2
1	B	668	THR	2.2
1	B	824	SER	2.2
1	B	669	ASP	2.2
1	B	837	ASP	2.2
1	B	835	SER	2.2
1	C	681	GLY	2.2
1	A	828	GLU	2.2
1	B	665	GLN	2.1
1	A	829	LEU	2.1
1	C	813	GLU	2.1
1	A	632	CYS	2.1
1	A	810	SER	2.1
1	C	876	SER	2.1
1	B	823	ASP	2.1
1	B	828	GLU	2.1
1	A	804	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	650	ASP	2.0
1	A	670	SER	2.0
1	B	831	ALA	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 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
2	TBR	C	1001	18/18	0.85	0.20	86,87,88,89	18
2	TBR	B	1000	18/18	0.86	0.25	86,87,88,88	18
2	TBR	A	999	18/18	0.86	0.26	83,86,87,88	18

6.5 Other polymers [i](#)

There are no such residues in this entry.