



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:32 AM UTC

PDB ID : 4GV7 / pdb_00004gv7
Title : Human ARTD1 (PARP1) - Catalytic domain in complex with inhibitor ME0328
Authors : Karlberg, T.; Thorsell, A.G.; Lindgren, A.E.G.; Ekblad, T.; Spjut, S.; Andersson, C.D.; Weigelt, J.; Linusson, A.; Elofsson, M.; Schuler, H.
Deposited on : 2012-08-30
Resolution : 2.89 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

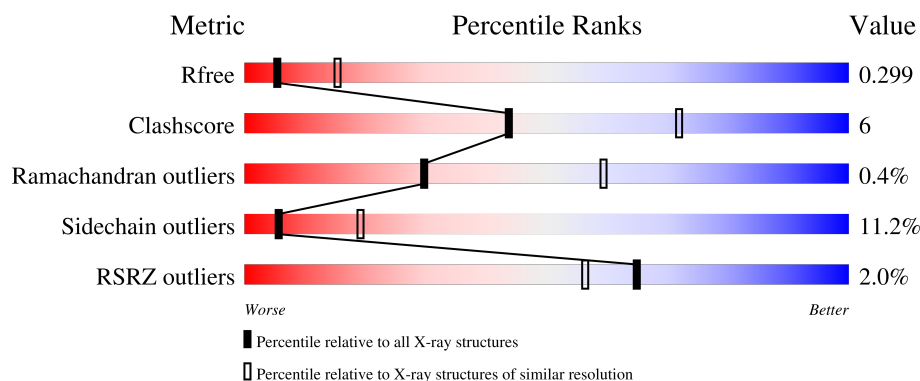
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	358	 75% 20% . .
1	B	358	 74% 21% . .
1	C	358	 65% 29% . .
1	D	358	 70% 24% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10988 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 Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2735	1740	462	522	11			
1	B	348	Total	C	N	O	S	0	0	0
			2735	1740	462	522	11			
1	C	348	Total	C	N	O	S	0	0	0
			2735	1740	462	522	11			
1	D	348	Total	C	N	O	S	0	0	0
			2735	1740	462	522	11			

There are 36 discrepancies between the modelled and reference sequences:

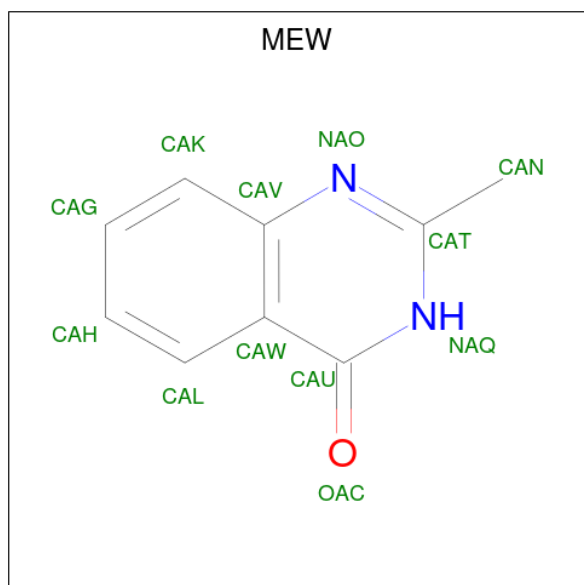
Chain	Residue	Modelled	Actual	Comment	Reference
A	661	MET	-	expression tag	UNP P09874
A	762	ALA	VAL	SEE REMARK 999	UNP P09874
A	1012	ALA	-	expression tag	UNP P09874
A	1013	HIS	-	expression tag	UNP P09874
A	1014	HIS	-	expression tag	UNP P09874
A	1015	HIS	-	expression tag	UNP P09874
A	1016	HIS	-	expression tag	UNP P09874
A	1017	HIS	-	expression tag	UNP P09874
A	1018	HIS	-	expression tag	UNP P09874
B	661	MET	-	expression tag	UNP P09874
B	762	ALA	VAL	SEE REMARK 999	UNP P09874
B	1012	ALA	-	expression tag	UNP P09874
B	1013	HIS	-	expression tag	UNP P09874
B	1014	HIS	-	expression tag	UNP P09874
B	1015	HIS	-	expression tag	UNP P09874
B	1016	HIS	-	expression tag	UNP P09874
B	1017	HIS	-	expression tag	UNP P09874
B	1018	HIS	-	expression tag	UNP P09874
C	661	MET	-	expression tag	UNP P09874
C	762	ALA	VAL	SEE REMARK 999	UNP P09874
C	1012	ALA	-	expression tag	UNP P09874

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1013	HIS	-	expression tag	UNP P09874
C	1014	HIS	-	expression tag	UNP P09874
C	1015	HIS	-	expression tag	UNP P09874
C	1016	HIS	-	expression tag	UNP P09874
C	1017	HIS	-	expression tag	UNP P09874
C	1018	HIS	-	expression tag	UNP P09874
D	661	MET	-	expression tag	UNP P09874
D	762	ALA	VAL	SEE REMARK 999	UNP P09874
D	1012	ALA	-	expression tag	UNP P09874
D	1013	HIS	-	expression tag	UNP P09874
D	1014	HIS	-	expression tag	UNP P09874
D	1015	HIS	-	expression tag	UNP P09874
D	1016	HIS	-	expression tag	UNP P09874
D	1017	HIS	-	expression tag	UNP P09874
D	1018	HIS	-	expression tag	UNP P09874

- Molecule 2 is 2-methylquinazolin-4(3H)-one (CCD ID: MEW) (formula: C₉H₈N₂O).

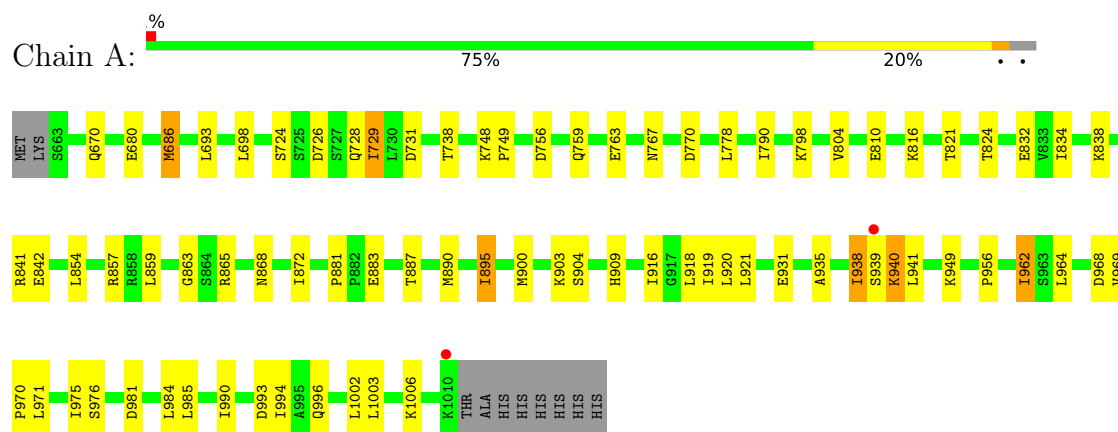


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	9	2	1		
2	B	1	Total	C	N	O	0	0
			12	9	2	1		
2	C	1	Total	C	N	O	0	0
			12	9	2	1		
2	D	1	Total	C	N	O	0	0
			12	9	2	1		

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.

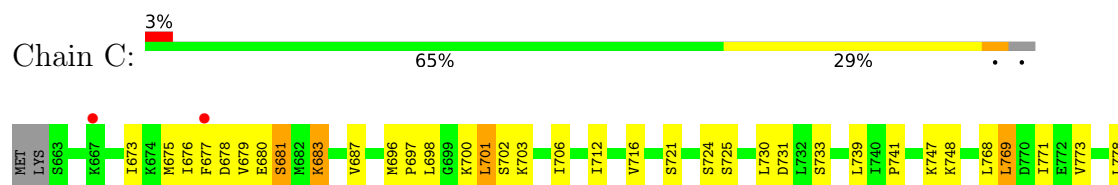
• Molecule 1: Poly [ADP-ribose] polymerase 1

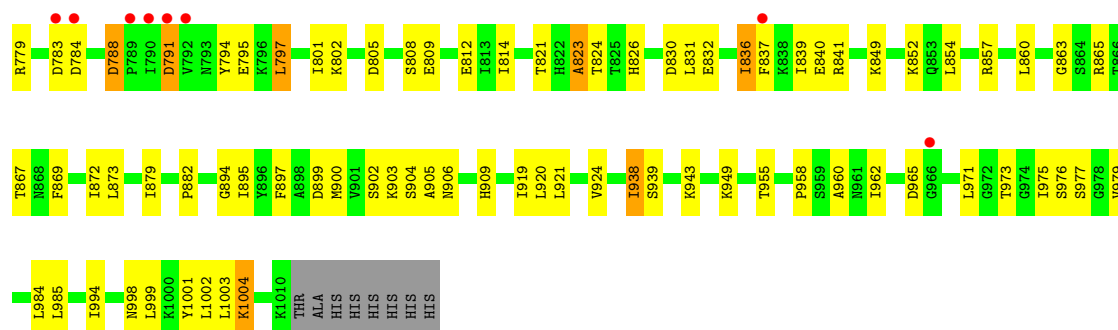


• Molecule 1: Poly [ADP-ribose] polymerase 1

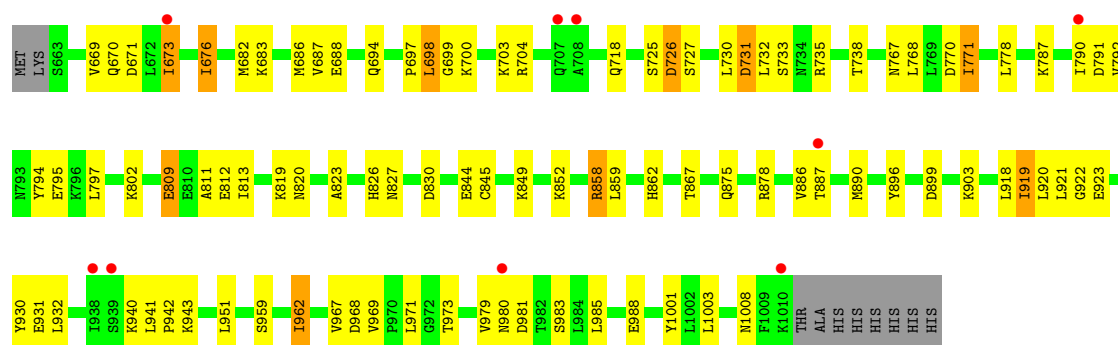


• Molecule 1: Poly [ADP-ribose] polymerase 1





• Molecule 1: Poly [ADP-ribose] polymerase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.05Å 49.43Å 183.51Å 90.00° 101.82° 90.00°	Depositor
Resolution (Å)	27.17 – 2.89 27.17 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.7 (27.17-2.89) 99.8 (27.17-2.89)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.211 , 0.286 0.226 , 0.299	Depositor DCC
R_{free} test set	1747 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10988	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: MEW

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	0.89	0/2787	1.36	7/3762 (0.2%)
1	B	0.94	3/2787 (0.1%)	1.37	15/3762 (0.4%)
1	C	0.89	0/2787	1.40	19/3762 (0.5%)
1	D	0.92	0/2787	1.40	23/3762 (0.6%)
All	All	0.91	3/11148 (0.0%)	1.38	64/15048 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	855	HIS	CG-ND1	-6.66	1.30	1.38
1	B	924	VAL	C-O	-5.53	1.18	1.24
1	B	855	HIS	CD2-NE2	-5.22	1.32	1.37

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	702	SER	CA-C-N	7.06	130.05	120.38
1	C	702	SER	C-N-CA	7.06	130.05	120.38
1	C	809	GLU	CA-C-N	6.19	128.48	120.44
1	C	809	GLU	C-N-CA	6.19	128.48	120.44
1	D	819	LYS	CA-C-N	6.14	128.51	120.28
1	D	819	LYS	C-N-CA	6.14	128.51	120.28
1	C	783	ASP	CA-CB-CG	6.13	118.73	112.60
1	C	784	ASP	CA-CB-CG	6.11	118.71	112.60
1	D	820	ASN	N-CA-C	6.00	117.83	111.28
1	D	726	ASP	CA-CB-CG	5.99	118.58	112.60
1	B	787	LYS	CA-C-N	5.96	128.68	120.39
1	B	787	LYS	C-N-CA	5.96	128.68	120.39
1	B	961	ASN	CA-CB-CG	5.94	118.54	112.60
1	B	899	ASP	CA-CB-CG	5.83	118.43	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	940	LYS	N-CA-C	5.82	118.87	107.57
1	C	882	PRO	CA-C-N	5.79	128.61	120.28
1	C	882	PRO	C-N-CA	5.79	128.61	120.28
1	B	901	VAL	CA-C-N	5.78	128.34	120.54
1	B	901	VAL	C-N-CA	5.78	128.34	120.54
1	C	703	LYS	CA-C-N	5.76	128.27	120.44
1	C	703	LYS	C-N-CA	5.76	128.27	120.44
1	D	771	ILE	N-CA-C	-5.72	104.94	110.72
1	A	984	LEU	CA-C-N	5.72	127.88	120.44
1	A	984	LEU	C-N-CA	5.72	127.88	120.44
1	D	811	ALA	CA-C-N	5.69	127.84	120.44
1	D	811	ALA	C-N-CA	5.69	127.84	120.44
1	C	823	ALA	CA-C-N	5.64	131.85	121.70
1	C	823	ALA	C-N-CA	5.64	131.85	121.70
1	C	938	ILE	N-CA-C	5.63	115.71	110.42
1	D	812	GLU	CA-C-N	5.53	128.28	120.42
1	D	812	GLU	C-N-CA	5.53	128.28	120.42
1	D	768	LEU	CA-C-N	5.48	127.56	120.44
1	D	768	LEU	C-N-CA	5.48	127.56	120.44
1	D	959	SER	N-CA-C	-5.47	107.17	112.97
1	D	725	SER	CA-C-N	5.42	128.32	120.79
1	D	725	SER	C-N-CA	5.42	128.32	120.79
1	C	791	ASP	CA-CB-CG	5.34	117.94	112.60
1	D	809	GLU	CA-C-N	5.33	127.68	120.44
1	D	809	GLU	C-N-CA	5.33	127.68	120.44
1	B	726	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	895	ILE	N-CA-CB	5.29	116.49	110.72
1	D	673	ILE	CA-C-N	5.27	127.34	120.28
1	D	673	ILE	C-N-CA	5.27	127.34	120.28
1	B	912	GLN	CA-C-N	5.26	125.79	120.00
1	B	912	GLN	C-N-CA	5.26	125.79	120.00
1	D	738	THR	N-CA-C	-5.24	105.63	112.23
1	C	683	LYS	CA-C-N	5.24	127.56	120.65
1	C	683	LYS	C-N-CA	5.24	127.56	120.65
1	B	1007	PHE	CA-CB-CG	5.23	119.03	113.80
1	A	824	THR	CA-C-N	5.20	127.25	120.28
1	A	824	THR	C-N-CA	5.20	127.25	120.28
1	A	726	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	671	ASP	CA-C-N	5.20	127.19	120.44
1	B	671	ASP	C-N-CA	5.20	127.19	120.44
1	B	758	VAL	N-CA-CB	5.17	116.60	110.55
1	C	899	ASP	CA-CB-CG	5.14	117.74	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	795	GLU	CA-C-N	5.11	127.84	120.38
1	C	795	GLU	C-N-CA	5.11	127.84	120.38
1	B	678	ASP	CA-C-N	5.06	127.61	120.42
1	B	678	ASP	C-N-CA	5.06	127.61	120.42
1	D	671	ASP	CA-CB-CG	5.04	117.64	112.60
1	D	899	ASP	CA-CB-CG	5.03	117.62	112.60
1	D	980	ASN	CA-C-N	5.02	130.50	121.66
1	D	980	ASN	C-N-CA	5.02	130.50	121.66

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	2735	0	2771	39	0
1	B	2735	0	2771	22	0
1	C	2735	0	2771	40	0
1	D	2735	0	2771	35	0
2	A	12	0	8	1	0
2	B	12	0	8	0	0
2	C	12	0	8	1	0
2	D	12	0	8	0	0
All	All	10988	0	11116	134	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 6.

All (134) 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:940:LYS:O	1:A:940:LYS:HG3	1.55	1.02
1:D:823:ALA:HB3	1:D:826:HIS:HD2	1.39	0.86
1:D:830:ASP:HB2	1:D:1008:ASN:HB2	1.70	0.73
1:D:823:ALA:HB3	1:D:826:HIS:CD2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:ILE:HD11	1:A:1006:LYS:HB2	1.74	0.69
1:A:865:ARG:HD3	1:A:909:HIS:HB2	1.76	0.68
1:B:834:ILE:HD11	1:B:1006:LYS:HB2	1.75	0.68
1:C:919:ILE:HG22	1:C:1003:LEU:HB2	1.75	0.68
1:D:919:ILE:HG22	1:D:1003:LEU:HB2	1.77	0.66
1:B:890:MET:HE1	1:B:983:SER:HB2	1.77	0.65
1:B:859:LEU:HG	1:B:921:LEU:HD22	1.79	0.64
1:B:832:GLU:HB3	1:B:1006:LYS:HB3	1.77	0.64
1:A:686:MET:HE3	1:A:693:LEU:HD11	1.81	0.62
1:C:697:PRO:HD2	1:C:700:LYS:HB2	1.81	0.62
1:A:759:GLN:HG3	1:A:887:THR:HG22	1.83	0.60
1:D:697:PRO:HD2	1:D:700:LYS:HB2	1.85	0.59
1:C:955:THR:HG22	1:C:977:SER:HB2	1.83	0.59
1:A:938:ILE:O	1:A:940:LYS:N	2.30	0.59
1:D:903:LYS:HZ3	1:D:988:GLU:HG2	1.66	0.58
1:C:712:ILE:O	1:C:716:VAL:HG23	2.04	0.58
1:D:670:GLN:HG2	1:D:790:ILE:HG21	1.86	0.58
1:B:668:PRO:HG2	1:B:803:VAL:HG21	1.86	0.57
1:C:679:VAL:HG12	1:C:683:LYS:HE2	1.86	0.57
1:D:727:SER:O	1:D:731:ASP:HB2	2.04	0.57
1:B:854:LEU:O	1:B:857:ARG:HD3	2.05	0.56
1:A:686:MET:CB	1:A:693:LEU:HD11	2.36	0.56
1:A:903:LYS:HE2	2:A:1101:MEW:H6	1.88	0.56
1:B:826:HIS:ND1	1:B:902:SER:HB3	2.20	0.56
1:A:956:PRO:HG2	1:A:970:PRO:HB2	1.89	0.55
1:C:788:ASP:HB3	1:C:791:ASP:HB2	1.87	0.55
1:A:798:LYS:O	1:A:842:GLU:HB2	2.06	0.55
1:C:769:LEU:O	1:C:773:VAL:HG23	2.08	0.55
1:C:860:LEU:HD12	1:C:924:VAL:CG2	2.37	0.54
1:A:938:ILE:C	1:A:940:LYS:H	2.14	0.54
1:C:860:LEU:HD12	1:C:924:VAL:HG21	1.89	0.54
1:A:854:LEU:O	1:A:857:ARG:HD3	2.08	0.54
1:B:697:PRO:HD2	1:B:700:LYS:HB2	1.88	0.54
1:B:706:ILE:HG23	1:B:765:LEU:HD22	1.90	0.54
1:A:832:GLU:HB3	1:A:1006:LYS:HB3	1.90	0.53
1:B:844:GLU:HG2	1:B:998:ASN:HD22	1.74	0.53
1:B:993:ASP:HB3	1:B:996:GLN:HG3	1.92	0.52
1:D:669:VAL:O	1:D:673:ILE:HG12	2.09	0.52
1:A:919:ILE:HG22	1:A:1003:LEU:HB2	1.92	0.52
1:C:696:MET:HB2	1:C:741:PRO:HD2	1.92	0.52
1:D:923:GLU:OE2	1:D:967:VAL:CG2	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:725:SER:HB3	1:D:827:ASN:OD1	2.10	0.51
1:C:821:THR:HB	1:C:900:MET:HA	1.92	0.51
1:D:923:GLU:OE2	1:D:967:VAL:HG21	2.11	0.51
1:A:748:LYS:HD3	1:A:749:PRO:HD2	1.92	0.50
1:A:686:MET:HE3	1:A:693:LEU:CD1	2.40	0.50
1:B:809:GLU:O	1:B:813:ILE:HG12	2.11	0.50
1:D:903:LYS:NZ	1:D:988:GLU:HG2	2.25	0.50
1:B:687:VAL:HG22	1:B:693:LEU:HD11	1.94	0.50
1:B:801:ILE:HG13	1:B:839:ILE:HG22	1.93	0.50
1:A:940:LYS:O	1:A:940:LYS:CG	2.37	0.50
1:D:809:GLU:O	1:D:813:ILE:HG12	2.12	0.49
1:C:801:ILE:HG13	1:C:839:ILE:HG22	1.95	0.49
1:A:938:ILE:C	1:A:940:LYS:N	2.70	0.49
1:A:872:ILE:HG21	1:A:920:LEU:HD11	1.95	0.49
1:C:920:LEU:HD22	1:C:999:LEU:HD22	1.95	0.49
1:A:895:ILE:HD11	1:A:994:ILE:HG22	1.94	0.48
1:D:858:ARG:HG3	1:D:968:ASP:HB2	1.95	0.48
1:D:962:ILE:HD13	1:D:971:LEU:HD11	1.94	0.48
1:D:930:TYR:CE2	1:D:932:LEU:HD21	2.49	0.48
1:D:683:LYS:O	1:D:687:VAL:HG23	2.13	0.48
1:C:826:HIS:CD2	1:C:902:SER:OG	2.66	0.48
1:D:921:LEU:HB2	1:D:1001:TYR:HB2	1.94	0.48
1:B:828:ALA:HB2	1:D:726:ASP:HB3	1.96	0.47
1:A:962:ILE:HG22	1:A:969:VAL:HB	1.96	0.47
1:C:805:ASP:HB3	1:C:808:SER:HB3	1.96	0.47
1:A:890:MET:HG2	1:A:935:ALA:HA	1.96	0.47
1:C:683:LYS:O	1:C:687:VAL:HG23	2.14	0.47
1:C:869:PHE:HA	1:C:872:ILE:HB	1.96	0.47
1:C:678:ASP:HB3	1:C:681:SER:HB2	1.95	0.47
1:C:814:ILE:HD13	1:C:836:ILE:HG21	1.95	0.47
1:D:770:ASP:OD1	1:D:878:ARG:NH2	2.48	0.47
1:C:854:LEU:O	1:C:857:ARG:HD3	2.15	0.46
1:D:682:MET:O	1:D:686:MET:HG3	2.16	0.46
1:A:863:GLY:N	1:A:904:SER:HB3	2.30	0.45
1:B:919:ILE:HG22	1:B:1003:LEU:HB2	1.98	0.45
1:A:881:PRO:HB2	1:A:883:GLU:OE1	2.17	0.45
1:C:865:ARG:HD3	1:C:909:HIS:HB2	1.99	0.45
1:D:703:LYS:HB2	1:D:704:ARG:HH11	1.81	0.45
1:A:918:LEU:HB3	1:A:1002:LEU:HD21	1.99	0.44
1:C:701:LEU:HD21	1:C:768:LEU:HD22	1.99	0.44
1:C:673:ILE:HD11	1:C:794:TYR:HD1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:962:ILE:HD12	1:A:971:LEU:HD11	1.99	0.44
1:A:724:SER:HB2	1:A:729:ILE:HD12	1.99	0.44
1:A:670:GLN:HG2	1:A:790:ILE:HG21	1.98	0.44
1:A:931:GLU:HG2	1:A:949:LYS:HB3	2.00	0.44
1:B:848:TYR:OH	1:B:923:GLU:OE2	2.26	0.44
1:D:859:LEU:HA	1:D:922:GLY:O	2.18	0.44
1:C:903:LYS:HE2	2:C:1101:MEW:H6	2.00	0.43
1:C:869:PHE:O	1:C:873:LEU:HG	2.17	0.43
1:A:804:VAL:HG22	1:A:838:LYS:HB2	2.00	0.43
1:C:797:LEU:HD22	1:C:873:LEU:HB2	2.01	0.43
1:C:863:GLY:HA3	1:C:904:SER:O	2.18	0.43
1:C:879:ILE:HG12	1:C:894:GLY:HA2	2.01	0.43
1:B:767:ASN:HD21	1:B:865:ARG:HG3	1.83	0.43
1:D:699:GLY:O	1:D:700:LYS:HD3	2.19	0.43
1:D:918:LEU:HA	1:D:1003:LEU:O	2.19	0.43
1:D:962:ILE:HG22	1:D:969:VAL:HB	2.00	0.43
1:A:770:ASP:HB3	1:A:868:ASN:HA	2.00	0.42
1:C:902:SER:HA	1:C:905:ALA:HB3	2.01	0.42
1:A:686:MET:CE	1:A:693:LEU:HD11	2.49	0.42
1:A:821:THR:HB	1:A:900:MET:HA	2.02	0.42
1:D:862:HIS:HD2	1:D:896:TYR:O	2.01	0.42
1:D:676:ILE:HD11	1:D:797:LEU:HD11	2.01	0.42
1:D:931:GLU:HB3	1:D:951:LEU:HD11	2.02	0.42
1:C:701:LEU:HD22	1:C:706:ILE:HD11	2.01	0.42
1:C:958:PRO:C	1:C:960:ALA:H	2.28	0.42
1:C:675:MET:HE1	1:C:1004:LYS:HD2	2.01	0.42
1:C:921:LEU:HD23	1:C:921:LEU:HA	1.95	0.42
1:D:794:TYR:HA	1:D:797:LEU:HD12	2.01	0.42
1:C:680:GLU:HA	1:C:683:LYS:HE3	2.01	0.41
1:C:921:LEU:HB2	1:C:1001:TYR:HB2	2.01	0.41
1:D:862:HIS:HB3	1:D:920:LEU:HB2	2.03	0.41
1:A:895:ILE:O	1:A:990:ILE:HA	2.20	0.41
1:D:890:MET:HE1	1:D:983:SER:HB2	2.01	0.41
1:C:677:PHE:CD1	1:C:778:LEU:HD13	2.56	0.41
1:B:712:ILE:O	1:B:716:VAL:HG23	2.20	0.41
1:A:686:MET:HB2	1:A:693:LEU:HD11	2.02	0.41
1:A:863:GLY:HA3	1:A:904:SER:O	2.21	0.41
1:B:854:LEU:O	1:B:857:ARG:CD	2.69	0.41
1:C:826:HIS:CE1	1:C:906:ASN:HD21	2.39	0.41
1:C:895:ILE:HD11	1:C:994:ILE:HG22	2.02	0.41
1:C:837:PHE:HB2	1:C:1002:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:897:PHE:CE1	1:C:924:VAL:HG11	2.55	0.41
1:D:682:MET:HB3	1:D:698:LEU:HD21	2.02	0.41
1:A:724:SER:HB3	1:A:728:GLN:HG3	2.03	0.40
1:D:941:LEU:HA	1:D:942:PRO:HD3	1.98	0.40
1:B:797:LEU:HD22	1:B:873:LEU:HB2	2.04	0.40
1:A:859:LEU:HG	1:A:921:LEU:HD22	2.04	0.40
1:A:993:ASP:HB3	1:A:996:GLN:HG3	2.04	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	346/358 (97%)	325 (94%)	20 (6%)	1 (0%)	36	65
1	B	346/358 (97%)	327 (94%)	19 (6%)	0	100	100
1	C	346/358 (97%)	319 (92%)	23 (7%)	4 (1%)	10	34
1	D	346/358 (97%)	318 (92%)	27 (8%)	1 (0%)	36	65
All	All	1384/1432 (97%)	1289 (93%)	89 (6%)	6 (0%)	30	59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	939	SER
1	C	823	ALA
1	C	779	ARG
1	C	939	SER
1	D	867	THR
1	C	824	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/314 (97%)	282 (92%)	23 (8%)	12	37
1	B	305/314 (97%)	267 (88%)	38 (12%)	4	15
1	C	305/314 (97%)	263 (86%)	42 (14%)	3	12
1	D	305/314 (97%)	271 (89%)	34 (11%)	6	20
All	All	1220/1256 (97%)	1083 (89%)	137 (11%)	6	19

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	680	GLU
1	A	686	MET
1	A	698	LEU
1	A	729	ILE
1	A	731	ASP
1	A	738	THR
1	A	756	ASP
1	A	763	GLU
1	A	767	ASN
1	A	778	LEU
1	A	810	GLU
1	A	816	LYS
1	A	841	ARG
1	A	916	ILE
1	A	938	ILE
1	A	941	LEU
1	A	962	ILE
1	A	964	LEU
1	A	968	ASP
1	A	975	ILE
1	A	976	SER
1	A	981	ASP
1	A	985	LEU
1	B	667	LYS

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Mol	Chain	Res	Type
1	B	693	LEU
1	B	700	LYS
1	B	703	LYS
1	B	717	GLN
1	B	722	GLN
1	B	728	GLN
1	B	729	ILE
1	B	732	LEU
1	B	740	ILE
1	B	748	LYS
1	B	757	SER
1	B	758	VAL
1	B	763	GLU
1	B	769	LEU
1	B	791	ASP
1	B	805	ASP
1	B	830	ASP
1	B	838	LYS
1	B	852	LYS
1	B	864	SER
1	B	865	ARG
1	B	875	GLN
1	B	890	MET
1	B	923	GLU
1	B	938	ILE
1	B	940	LYS
1	B	959	SER
1	B	963	SER
1	B	964	LEU
1	B	968	ASP
1	B	980	ASN
1	B	981	ASP
1	B	983	SER
1	B	984	LEU
1	B	985	LEU
1	B	991	VAL
1	B	1004	LYS
1	C	676	ILE
1	C	681	SER
1	C	698	LEU
1	C	701	LEU
1	C	721	SER

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Mol	Chain	Res	Type
1	C	724	SER
1	C	725	SER
1	C	730	LEU
1	C	731	ASP
1	C	733	SER
1	C	739	LEU
1	C	747	LYS
1	C	748	LYS
1	C	769	LEU
1	C	771	ILE
1	C	788	ASP
1	C	797	LEU
1	C	802	LYS
1	C	812	GLU
1	C	830	ASP
1	C	831	LEU
1	C	832	GLU
1	C	836	ILE
1	C	840	GLU
1	C	841	ARG
1	C	849	LYS
1	C	852	LYS
1	C	867	THR
1	C	938	ILE
1	C	943	LYS
1	C	949	LYS
1	C	962	ILE
1	C	965	ASP
1	C	971	LEU
1	C	973	THR
1	C	975	ILE
1	C	976	SER
1	C	979	VAL
1	C	984	LEU
1	C	985	LEU
1	C	998	ASN
1	C	1004	LYS
1	D	676	ILE
1	D	688	GLU
1	D	694	GLN
1	D	698	LEU
1	D	718	GLN

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Mol	Chain	Res	Type
1	D	730	LEU
1	D	731	ASP
1	D	732	LEU
1	D	733	SER
1	D	735	ARG
1	D	767	ASN
1	D	771	ILE
1	D	778	LEU
1	D	787	LYS
1	D	791	ASP
1	D	792	VAL
1	D	795	GLU
1	D	802	LYS
1	D	844	GLU
1	D	845	CYS
1	D	849	LYS
1	D	852	LYS
1	D	858	ARG
1	D	875	GLN
1	D	886	VAL
1	D	887	THR
1	D	919	ILE
1	D	940	LYS
1	D	943	LYS
1	D	962	ILE
1	D	973	THR
1	D	979	VAL
1	D	981	ASP
1	D	985	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	722	GLN
1	A	820	ASN
1	A	856	ASN
1	A	868	ASN
1	B	670	GLN
1	B	717	GLN
1	B	722	GLN
1	B	767	ASN
1	B	793	ASN

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Mol	Chain	Res	Type
1	B	868	ASN
1	C	705	GLN
1	C	754	ASN
1	C	822	HIS
1	C	826	HIS
1	C	906	ASN
1	D	705	GLN
1	D	734	ASN
1	D	754	ASN
1	D	759	GLN
1	D	820	ASN
1	D	846	GLN
1	D	906	ASN
1	D	937	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEW	B	1101	-	13,13,13	2.25	2 (15%)	18,18,18	2.56	6 (33%)
2	MEW	D	1101	-	13,13,13	2.16	4 (30%)	18,18,18	2.47	9 (50%)
2	MEW	C	1101	-	13,13,13	2.25	5 (38%)	18,18,18	2.97	8 (44%)
2	MEW	A	1101	-	13,13,13	1.91	2 (15%)	18,18,18	2.75	8 (44%)

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	MEW	B	1101	-	-	-	0/2/2/2
2	MEW	D	1101	-	-	-	0/2/2/2
2	MEW	C	1101	-	-	-	0/2/2/2
2	MEW	A	1101	-	-	-	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	MEW	CAW-CAU	-7.05	1.35	1.47
2	D	1101	MEW	CAW-CAU	-5.76	1.37	1.47
2	A	1101	MEW	CAW-CAU	-5.59	1.37	1.47
2	C	1101	MEW	CAW-CAU	-5.58	1.37	1.47
2	C	1101	MEW	CAT-NAO	3.59	1.39	1.31
2	D	1101	MEW	CAT-NAO	2.86	1.38	1.31
2	C	1101	MEW	CAT-NAQ	2.48	1.43	1.36
2	D	1101	MEW	CAW-CAV	2.30	1.43	1.40
2	C	1101	MEW	CAG-CAK	2.28	1.42	1.38
2	B	1101	MEW	CAW-CAV	2.14	1.43	1.40
2	A	1101	MEW	CAT-NAO	2.12	1.36	1.31
2	D	1101	MEW	CAU-NAQ	2.11	1.41	1.37
2	C	1101	MEW	CAU-NAQ	2.04	1.40	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	MEW	CAU-NAQ-CAT	-7.55	119.77	123.87
2	C	1101	MEW	CAU-NAQ-CAT	-7.37	119.86	123.87
2	C	1101	MEW	CAW-CAU-NAQ	5.98	121.25	114.93
2	B	1101	MEW	CAU-NAQ-CAT	-5.96	120.63	123.87
2	B	1101	MEW	CAW-CAU-NAQ	5.28	120.51	114.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	MEW	CAW-CAU-NAQ	5.24	120.46	114.93
2	D	1101	MEW	CAW-CAU-NAQ	4.89	120.10	114.93
2	D	1101	MEW	CAH-CAG-CAK	3.88	125.02	120.24
2	C	1101	MEW	OAC-CAU-CAW	-3.79	116.50	123.27
2	D	1101	MEW	CAK-CAV-CAW	-3.53	115.66	119.14
2	B	1101	MEW	OAC-CAU-CAW	-3.53	116.96	123.27
2	C	1101	MEW	CAG-CAH-CAL	-3.41	116.03	120.24
2	B	1101	MEW	CAN-CAT-NAQ	3.34	123.22	116.27
2	D	1101	MEW	CAU-NAQ-CAT	-3.20	122.13	123.87
2	B	1101	MEW	CAV-NAO-CAT	3.14	121.29	118.16
2	A	1101	MEW	CAG-CAH-CAL	3.10	124.07	120.24
2	D	1101	MEW	CAG-CAH-CAL	-3.08	116.44	120.24
2	A	1101	MEW	CAV-NAO-CAT	3.06	121.21	118.16
2	D	1101	MEW	OAC-CAU-CAW	-3.04	117.85	123.27
2	A	1101	MEW	OAC-CAU-CAW	-3.02	117.87	123.27
2	D	1101	MEW	CAK-CAV-NAO	2.96	122.38	118.61
2	C	1101	MEW	NAQ-CAT-NAO	-2.89	118.58	123.15
2	C	1101	MEW	CAH-CAG-CAK	2.85	123.75	120.24
2	D	1101	MEW	NAQ-CAT-NAO	-2.66	118.94	123.15
2	D	1101	MEW	CAL-CAW-CAV	2.52	122.66	119.78
2	B	1101	MEW	NAQ-CAT-NAO	-2.49	119.21	123.15
2	A	1101	MEW	CAN-CAT-NAQ	2.43	121.32	116.27
2	C	1101	MEW	CAK-CAV-CAW	-2.39	116.79	119.14
2	C	1101	MEW	CAK-CAV-NAO	2.31	121.55	118.61
2	A	1101	MEW	NAQ-CAT-NAO	-2.19	119.69	123.15
2	A	1101	MEW	CAW-CAV-NAO	-2.04	120.36	122.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1101	MEW	1	0
2	A	1101	MEW	1	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, 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	348/358 (97%)	-0.08	2 (0%) 85 81	21, 48, 77, 112	0
1	B	348/358 (97%)	0.03	7 (2%) 65 56	25, 52, 93, 130	0
1	C	348/358 (97%)	0.40	10 (2%) 53 45	36, 66, 107, 138	0
1	D	348/358 (97%)	0.51	9 (2%) 57 48	37, 68, 97, 134	0
All	All	1392/1432 (97%)	0.21	28 (2%) 65 56	21, 60, 97, 138	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	938	ILE	3.8
1	D	887	THR	3.2
1	A	939	SER	3.1
1	D	939	SER	3.1
1	C	790	ILE	2.9
1	C	789	PRO	2.9
1	D	980	ASN	2.7
1	B	938	ILE	2.6
1	C	667	LYS	2.6
1	D	673	ILE	2.6
1	B	939	SER	2.4
1	A	1010	LYS	2.4
1	B	830	ASP	2.4
1	C	783	ASP	2.3
1	C	677	PHE	2.3
1	D	707	GLN	2.3
1	D	1010	LYS	2.3
1	D	708	ALA	2.3
1	B	780	GLY	2.3
1	C	837	PHE	2.2
1	B	964	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	887	THR	2.2
1	C	966	GLY	2.1
1	C	784	ASP	2.1
1	C	791	ASP	2.1
1	C	792	VAL	2.1
1	B	784	ASP	2.1
1	D	790	ILE	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	MEW	B	1101	12/12	0.89	0.10	35,39,40,40	0
2	MEW	C	1101	12/12	0.91	0.09	26,39,40,42	0
2	MEW	D	1101	12/12	0.91	0.08	21,30,35,38	0
2	MEW	A	1101	12/12	0.92	0.09	30,33,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.