



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:22 PM UTC

PDB ID : 5Q4F / pdb_00005q4f
Title : PanDDA analysis group deposition – Crystal Structure of DCLRE1A after initial refinement with no ligand modelled (structure 80)
Authors : Newman, J.A.; Aitkenhead, H.; Lee, S.Y.; Kupinska, K.; Burgess-Brown, N.; Tallon, R.; Krojer, T.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Gileadi, O.
Deposited on : 2017-05-25
Resolution : 1.97 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

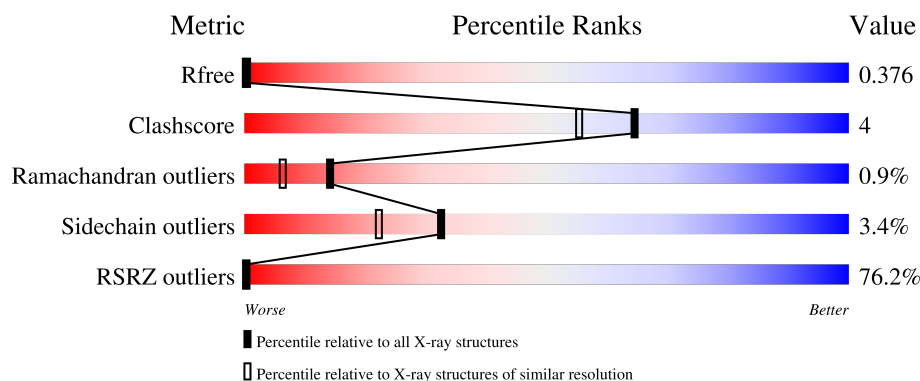
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	343	76% 85% 14% ..

2 Entry composition [i](#)

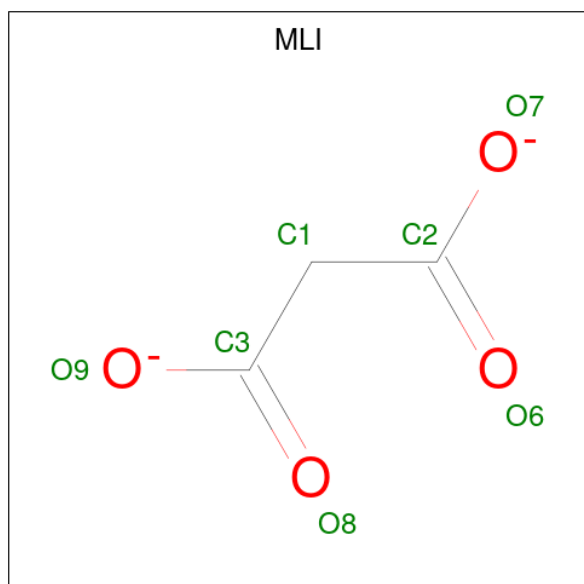
There are 4 unique types of molecules in this entry. The entry contains 3044 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DCLRE1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2726	1765	450	491	20	0	4	0

- Molecule 2 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	7	3	4	0	0

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		

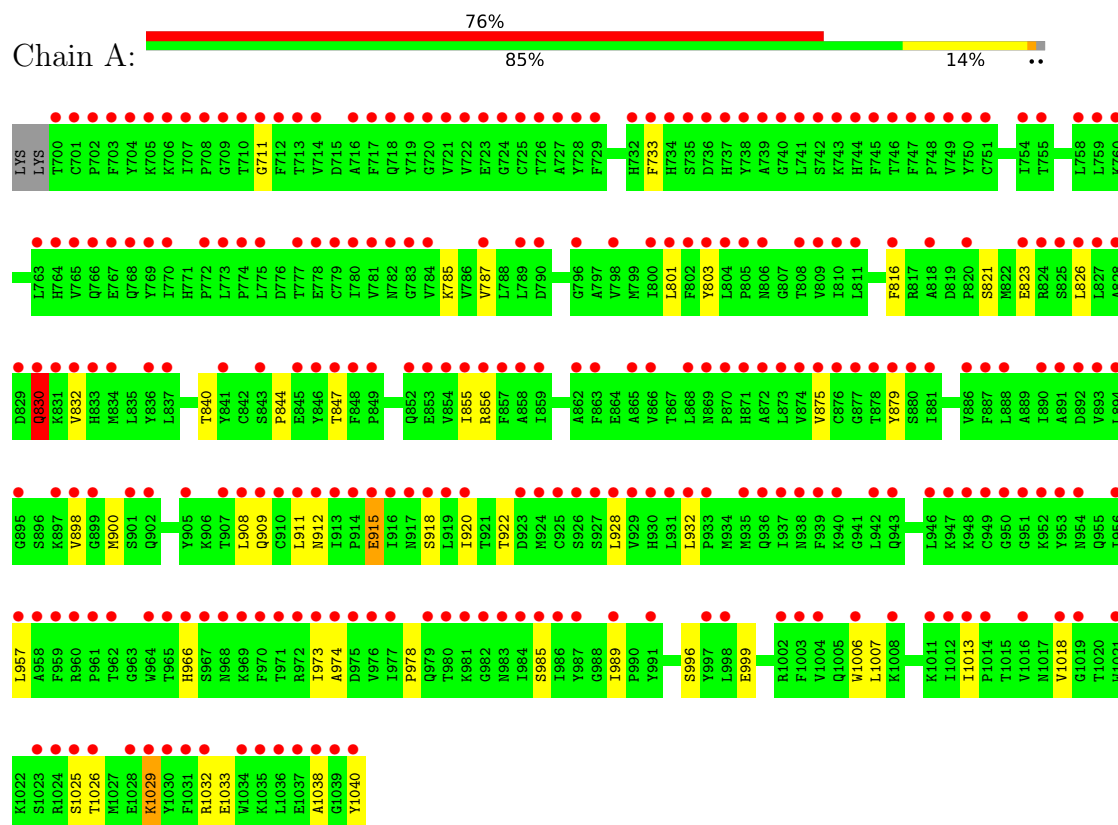
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	310	Total 310	O 310	0	0

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: DCLRE1A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.28Å 57.44Å 115.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.56 – 1.97 57.56 – 1.97	Depositor EDS
% Data completeness (in resolution range)	94.8 (57.56-1.97) 94.8 (57.56-1.97)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.322 , 0.368 0.328 , 0.376	Depositor DCC
R_{free} test set	1260 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	2.5	Xtriage
Anisotropy	3.797	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.69	EDS
Total number of atoms	3044	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% 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: MLI, NI

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	1.23	3/2802 (0.1%)	1.31	12/3809 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	898	VAL	C-O	-8.28	1.14	1.24
1	A	840	THR	C-O	-7.65	1.15	1.24
1	A	816	PHE	C-O	-5.64	1.17	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	999	GLU	CA-C-N	6.46	128.83	120.44
1	A	999	GLU	C-N-CA	6.46	128.83	120.44
1	A	830	GLN	N-CA-C	6.14	117.48	108.14
1	A	733	PHE	N-CA-C	6.12	119.11	109.39
1	A	911	LEU	N-CA-C	5.92	119.47	112.72
1	A	1013	ILE	N-CA-C	5.62	113.61	107.60
1	A	996	SER	N-CA-C	-5.39	103.79	110.41
1	A	989	ILE	CA-C-N	5.30	126.47	119.84
1	A	989	ILE	C-N-CA	5.30	126.47	119.84
1	A	821	SER	N-CA-C	5.23	118.76	112.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	816	PHE	N-CA-C	5.09	116.98	108.99
1	A	844	PRO	N-CA-C	5.01	120.13	113.86

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	978	PRO	Peptide

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	2726	0	2676	21	0
2	A	7	0	2	0	0
3	A	1	0	0	0	0
4	A	310	0	0	10	2
All	All	3044	0	2678	21	2

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 4.

All (21) 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:830:GLN:HB2	4:A:1441:HOH:O	1.63	0.96
1:A:909:GLN:NE2	4:A:1202:HOH:O	2.12	0.82
1:A:847:THR:HA	4:A:1425:HOH:O	1.87	0.74
1:A:1033[B]:GLU:OE2	4:A:1201:HOH:O	2.06	0.72
1:A:1029:LYS:HB2	4:A:1203:HOH:O	1.90	0.71
1:A:915:GLU:O	1:A:918:SER:OG	2.13	0.67
1:A:1029:LYS:CB	4:A:1203:HOH:O	2.44	0.66
1:A:1018:VAL:HG22	4:A:1339:HOH:O	2.00	0.61
1:A:1032:ARG:HG2	4:A:1306:HOH:O	2.10	0.49
1:A:823:GLU:HG2	1:A:1006:TRP:CD2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:LYS:HB3	1:A:803:TYR:HB2	1.96	0.47
1:A:787:VAL:HG11	1:A:826:LEU:HD12	1.98	0.46
1:A:900:MET:HE3	1:A:920:ILE:HB	1.97	0.46
1:A:875:VAL:HG11	1:A:932:LEU:HD12	1.96	0.46
1:A:711:GLY:N	4:A:1205:HOH:O	2.30	0.45
1:A:1029:LYS:HB3	4:A:1203:HOH:O	2.14	0.43
1:A:832:VAL:HG21	1:A:1007:LEU:HD11	2.00	0.43
1:A:1038:ALA:HB3	1:A:1040:TYR:CE2	2.55	0.42
1:A:855:ILE:O	1:A:856:ARG:C	2.63	0.41
1:A:900:MET:HE1	1:A:908:LEU:HD12	2.03	0.41
1:A:973:ILE:HG23	1:A:974:ALA:N	2.36	0.40

All (2) 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)
4:A:1243:HOH:O	4:A:1248:HOH:O[3_545]	1.88	0.32
4:A:1326:HOH:O	4:A:1385:HOH:O[1_655]	2.17	0.03

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	343/343 (100%)	325 (95%)	15 (4%)	3 (1%)	14 6

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	966	HIS
1	A	912	ASN
1	A	915	GLU

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	299/305 (98%)	289 (97%)	10 (3%)	33	23

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	801	LEU
1	A	830	GLN
1	A	879	TYR
1	A	922	THR
1	A	928	LEU
1	A	957	LEU
1	A	985	SER
1	A	1025	SER
1	A	1026	THR
1	A	1029	LYS

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

Mol	Chain	Res	Type
1	A	734	HIS
1	A	833	HIS
1	A	851	GLN
1	A	909	GLN
1	A	966	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
2	MLI	A	1101	3	6,6,6	1.48	1 (16%)	7,7,7	0.50	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
2	MLI	A	1101	3	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	MLI	O9-C3	-2.24	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	MLI	C2-C1-C3-O9
2	A	1101	MLI	C3-C1-C2-O6
2	A	1101	MLI	C2-C1-C3-O8
2	A	1101	MLI	C3-C1-C2-O7

There are no ring outliers.

No monomer is involved in short contacts.

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	341/343 (99%)	2.99	260 (76%) 0 0	9, 25, 47, 90	4 (1%)

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	970	PHE	10.3
1	A	703	PHE	9.5
1	A	968	ASN	7.5
1	A	969	LYS	7.4
1	A	829	ASP	7.2
1	A	704	TYR	7.0
1	A	879	TYR	6.8
1	A	706	LYS	6.7
1	A	971	THR	6.7
1	A	967	SER	6.6
1	A	769	TYR	6.5
1	A	700	THR	6.3
1	A	743	LYS	6.2
1	A	740	GLY	6.1
1	A	973	ILE	6.0
1	A	722	VAL	6.0
1	A	745	PHE	5.9
1	A	919	LEU	5.8
1	A	708	PRO	5.6
1	A	721	VAL	5.5
1	A	711	GLY	5.5
1	A	972	ARG	5.4
1	A	950	GLY	5.2
1	A	1023	SER	5.2
1	A	748	PRO	5.2
1	A	974	ALA	5.1
1	A	826	LEU	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	709	GLY	5.0
1	A	924	MET	5.0
1	A	701	CYS	4.9
1	A	726	THR	4.9
1	A	966	HIS	4.9
1	A	702	PRO	4.8
1	A	741	LEU	4.8
1	A	746	THR	4.8
1	A	965	THR	4.8
1	A	808	THR	4.8
1	A	831	LYS	4.8
1	A	763	LEU	4.7
1	A	979	GLN	4.7
1	A	710	THR	4.6
1	A	878	THR	4.6
1	A	949	CYS	4.4
1	A	935	MET	4.4
1	A	739	ALA	4.4
1	A	720	GLY	4.3
1	A	915	GLU	4.3
1	A	738	TYR	4.3
1	A	707	ILE	4.2
1	A	1040	TYR	4.2
1	A	912	ASN	4.2
1	A	765	VAL	4.1
1	A	1032	ARG	4.0
1	A	874	VAL	4.0
1	A	719	TYR	4.0
1	A	781	VAL	4.0
1	A	946	LEU	4.0
1	A	767	GLU	4.0
1	A	1021	TRP	3.9
1	A	1036	LEU	3.9
1	A	768	GLN	3.9
1	A	830	GLN	3.9
1	A	875	VAL	3.9
1	A	937	ILE	3.9
1	A	783	GLY	3.9
1	A	705	LYS	3.9
1	A	859	ILE	3.9
1	A	747	PHE	3.8
1	A	928	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1028[A]	GLU	3.8
1	A	772	PRO	3.8
1	A	742	SER	3.8
1	A	833	HIS	3.7
1	A	925	CYS	3.7
1	A	764[A]	HIS	3.7
1	A	848	PHE	3.7
1	A	1030	TYR	3.6
1	A	939	PHE	3.6
1	A	913	ILE	3.6
1	A	936	GLN	3.5
1	A	964	TRP	3.5
1	A	871	HIS	3.5
1	A	893	VAL	3.5
1	A	940	LYS	3.5
1	A	827	LEU	3.5
1	A	868	LEU	3.5
1	A	920	ILE	3.5
1	A	749	VAL	3.5
1	A	798	VAL	3.5
1	A	948	LYS	3.5
1	A	975	ASP	3.4
1	A	782	ASN	3.4
1	A	770	ILE	3.4
1	A	773	LEU	3.4
1	A	917	ASN	3.4
1	A	750	TYR	3.4
1	A	754	ILE	3.4
1	A	802	PHE	3.4
1	A	932	LEU	3.4
1	A	780	ILE	3.3
1	A	947	LYS	3.3
1	A	728	TYR	3.3
1	A	953	TYR	3.3
1	A	854	VAL	3.3
1	A	712	PHE	3.3
1	A	856	ARG	3.3
1	A	803	TYR	3.3
1	A	981	LYS	3.3
1	A	759	LEU	3.3
1	A	816	PHE	3.3
1	A	1018	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	952	LYS	3.2
1	A	1006	TRP	3.2
1	A	910	CYS	3.2
1	A	736	ASP	3.2
1	A	847	THR	3.2
1	A	976	VAL	3.2
1	A	804	LEU	3.2
1	A	894	LEU	3.2
1	A	908	LEU	3.2
1	A	914	PRO	3.1
1	A	737	HIS	3.1
1	A	897	LYS	3.1
1	A	1035	LYS	3.1
1	A	909	GLN	3.1
1	A	954	ASN	3.1
1	A	849	PRO	3.1
1	A	855	ILE	3.1
1	A	887	PHE	3.1
1	A	902	GLN	3.1
1	A	713	THR	3.1
1	A	810	ILE	3.1
1	A	916	ILE	3.1
1	A	888	LEU	3.1
1	A	857	PHE	3.1
1	A	891	ALA	3.1
1	A	836	TYR	3.0
1	A	834	MET	3.0
1	A	784	VAL	3.0
1	A	832	VAL	3.0
1	A	1038	ALA	3.0
1	A	723	GLU	3.0
1	A	1029	LYS	3.0
1	A	895	GLY	3.0
1	A	714	VAL	2.9
1	A	733	PHE	2.9
1	A	863	PHE	2.9
1	A	989	ILE	2.9
1	A	801	LEU	2.9
1	A	997	TYR	2.9
1	A	778	GLU	2.9
1	A	729	PHE	2.9
1	A	901	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	984	ILE	2.9
1	A	846	TYR	2.9
1	A	744	HIS	2.9
1	A	872	ALA	2.9
1	A	1037	GLU	2.9
1	A	1012	ILE	2.9
1	A	806	ASN	2.8
1	A	809	VAL	2.8
1	A	774	PRO	2.8
1	A	841	TYR	2.8
1	A	918	SER	2.8
1	A	800	ILE	2.8
1	A	942	LEU	2.8
1	A	724	GLY	2.8
1	A	852	GLN	2.8
1	A	870	PRO	2.8
1	A	960	ARG	2.8
1	A	735	SER	2.8
1	A	1025	SER	2.8
1	A	938	ASN	2.8
1	A	982	GLY	2.8
1	A	881	ILE	2.8
1	A	961	PRO	2.8
1	A	959	PHE	2.8
1	A	926	SER	2.7
1	A	718	GLN	2.7
1	A	1019	GLY	2.7
1	A	962	THR	2.7
1	A	977	ILE	2.7
1	A	766	GLN	2.7
1	A	929	VAL	2.7
1	A	1034	TRP	2.7
1	A	853	GLU	2.7
1	A	905	TYR	2.7
1	A	931	LEU	2.7
1	A	818	ALA	2.7
1	A	725	CYS	2.7
1	A	933	PRO	2.6
1	A	758	LEU	2.6
1	A	789	LEU	2.6
1	A	956	ILE	2.6
1	A	951	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	991	TYR	2.6
1	A	777	THR	2.6
1	A	751	CYS	2.6
1	A	880	SER	2.6
1	A	811	LEU	2.6
1	A	1039	GLY	2.6
1	A	958	ALA	2.6
1	A	820	PRO	2.6
1	A	858	ALA	2.6
1	A	911	LEU	2.5
1	A	869	ASN	2.5
1	A	732	HIS	2.5
1	A	1031	PHE	2.5
1	A	998	LEU	2.5
1	A	727	ALA	2.5
1	A	755	THR	2.5
1	A	943	GLN	2.5
1	A	790	ASP	2.5
1	A	779	CYS	2.5
1	A	987	TYR	2.4
1	A	1003	PHE	2.4
1	A	927	SER	2.4
1	A	886	VAL	2.4
1	A	985	SER	2.4
1	A	760	LYS	2.4
1	A	775	LEU	2.4
1	A	986	ILE	2.4
1	A	862	ALA	2.4
1	A	845	GLU	2.4
1	A	892	ASP	2.3
1	A	873	LEU	2.3
1	A	1011	LYS	2.3
1	A	1016	VAL	2.3
1	A	907	THR	2.3
1	A	717	PHE	2.3
1	A	865	ALA	2.3
1	A	877	GLY	2.3
1	A	1002	ARG	2.3
1	A	787	VAL	2.3
1	A	898	VAL	2.3
1	A	923	ASP	2.3
1	A	1004	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	980	THR	2.3
1	A	824	ARG	2.3
1	A	1026	THR	2.3
1	A	890	ILE	2.2
1	A	1013	ILE	2.2
1	A	734	HIS	2.2
1	A	876[A]	CYS	2.2
1	A	843	SER	2.2
1	A	899	GLY	2.2
1	A	1024	ARG	2.2
1	A	957	LEU	2.2
1	A	805	PRO	2.2
1	A	716	ALA	2.2
1	A	930	HIS	2.1
1	A	837	LEU	2.1
1	A	1014	PRO	2.1
1	A	983	ASN	2.1
1	A	796	GLY	2.1
1	A	825	SER	2.1
1	A	828	ALA	2.1
1	A	866	VAL	2.0
1	A	823	GLU	2.0
1	A	1008	LYS	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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
-----	------	-------	-----	-------	------	-----	-----------------------------	-------

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MLI	A	1101	7/7	0.59	0.25	27,30,33,35	0
3	NI	A	1102	1/1	0.97	0.06	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.