



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 03:40 PM UTC

PDB ID : 3UOM / pdb_00003uom
Title : Ca²⁺ complex of Human skeletal calsequestrin
Authors : Sanchez, E.J.; Lewis, K.M.; Danna, B.R.; Nissen, M.S.; Kang, C.H.
Deposited on : 2011-11-16
Resolution : 2.02 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)
Xtrriage (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

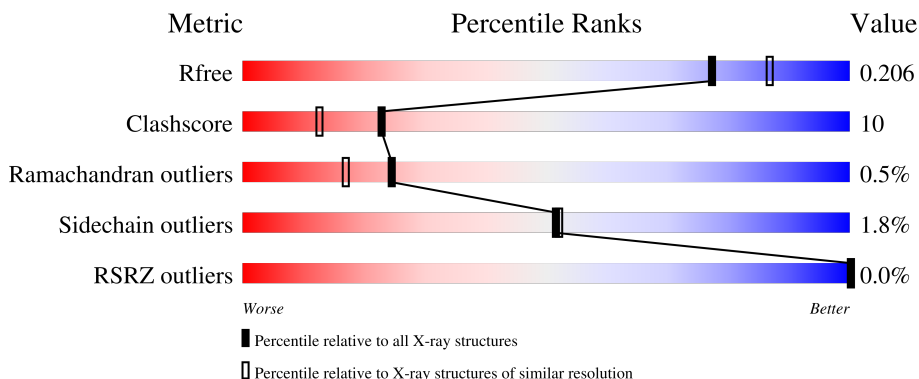
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	362	84% 11% ..
1	B	362	83% 13% ..
1	C	362	82% 14% ..
1	D	362	82% 14% ..
1	E	362	86% 10% ..

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Mol	Chain	Length	Quality of chain
1	F	362	 87% 9% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MRD	B	402	-	-	X	-
2	MRD	B	404	-	-	X	-
2	MRD	B	407	-	-	X	-
2	MRD	C	402	-	-	X	-
2	MRD	E	402	-	-	X	-
2	MRD	F	502	-	-	X	-
3	MPD	A	402	-	-	X	-
3	MPD	B	406	-	-	X	-

2 Entry composition [i](#)

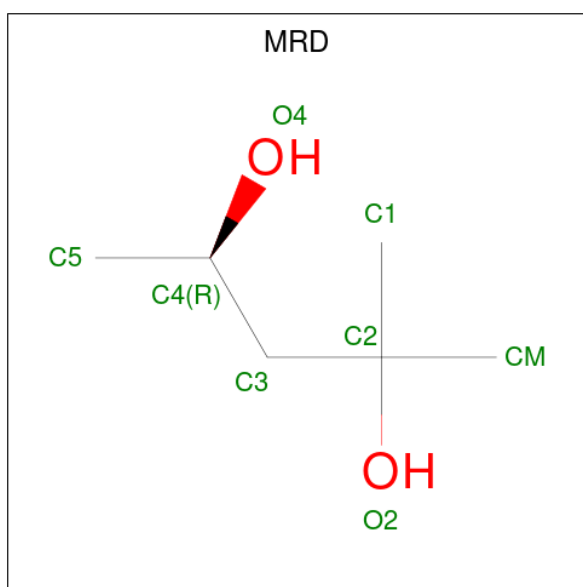
There are 5 unique types of molecules in this entry. The entry contains 18955 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Calsequestrin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	352	Total 2891	C 1854	N 429	O 601	S 7	0	6	0
1	B	350	Total 2889	C 1854	N 429	O 598	S 8	0	8	0
1	C	351	Total 2898	C 1860	N 430	O 601	S 7	0	8	0
1	D	350	Total 2872	C 1840	N 429	O 596	S 7	0	5	0
1	E	351	Total 2884	C 1851	N 427	O 599	S 7	0	6	0
1	F	350	Total 2884	C 1850	N 429	O 598	S 7	0	7	0

- Molecule 2 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



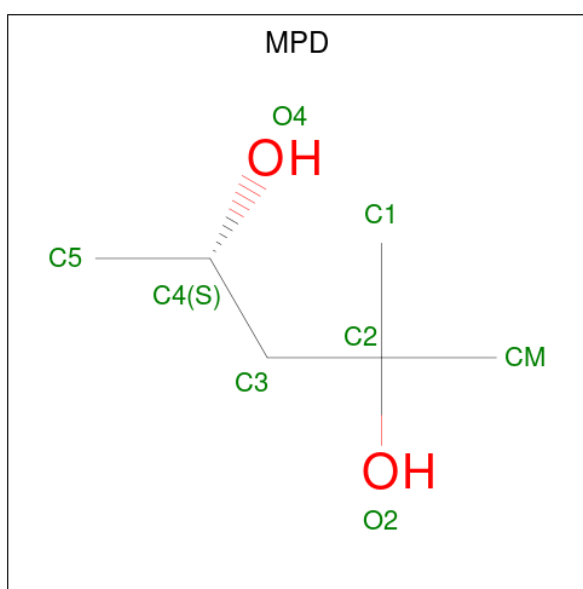
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	D	1	Total	C	O	0	0
			8	6	2		
2	D	1	Total	C	O	0	0
			8	6	2		
2	D	1	Total	C	O	0	0
			8	6	2		
2	D	1	Total	C	O	0	0
			8	6	2		
2	D	1	Total	C	O	0	0
			8	6	2		
2	D	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	F	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			8	6	2		
2	F	1	Total	C	O	0	0
			8	6	2		
2	F	1	Total	C	O	0	0
			8	6	2		
2	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	E	1	Total C O 8 6 2	0	0
3	F	1	Total C O 8 6 2	0	0
3	F	1	Total C O 8 6 2	0	0
3	F	1	Total C O 8 6 2	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total Ca 14 14	0	0
4	B	15	Total Ca 16 16	1	1
4	C	15	Total Ca 15 15	0	0
4	D	15	Total Ca 15 15	0	0
4	E	13	Total Ca 13 13	0	0
4	F	14	Total Ca 14 14	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	198	Total O 198 198	0	0
5	B	184	Total O 184 184	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	214	Total 214	O 214	0	0
5	D	207	Total 207	O 207	0	0
5	E	213	Total 213	O 213	0	0
5	F	198	Total 198	O 198	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	89.80Å 89.79Å 119.16Å 90.13° 89.90° 60.05°	Depositor
Resolution (Å)	38.90 – 2.02 38.90 – 2.02	Depositor EDS
% Data completeness (in resolution range)	91.8 (38.90-2.02) 91.1 (38.90-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.182 , 0.213 0.179 , 0.206	Depositor DCC
R_{free} test set	2005 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for k,-h+k,l 0.012 for h-k,h,l 0.448 for -h+k,-h,l 0.448 for -k,h-k,l 0.459 for -h+k,k,-l 0.467 for h,h-k,-l 0.013 for -h,-k,l 0.448 for -k,-h,-l 0.013 for k,h,-l 0.013 for h-k,-k,-l 0.013 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18955	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: MRD, MPD, CA

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	1/2971 (0.0%)	0.72	2/4032 (0.0%)
1	B	0.49	0/2978	0.72	0/4040
1	C	0.54	0/2987	0.72	1/4053 (0.0%)
1	D	0.54	0/2952	0.71	1/4006 (0.0%)
1	E	0.49	0/2967	0.71	0/4027
1	F	0.60	3/2970 (0.1%)	0.82	9/4030 (0.2%)
All	All	0.53	4/17825 (0.0%)	0.74	13/24188 (0.1%)

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	F	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	102[A]	GLU	C-N	-9.63	1.21	1.33
1	F	102[B]	GLU	C-N	-9.63	1.21	1.33
1	F	124	GLU	C-N	-9.35	1.20	1.33
1	A	127	VAL	C-O	-5.13	1.18	1.24

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	123	LEU	CA-C-N	9.71	135.09	120.82
1	F	123	LEU	C-N-CA	9.71	135.09	120.82
1	F	102[A]	GLU	O-C-N	-9.57	110.34	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	102[B]	GLU	O-C-N	-9.57	110.34	122.20
1	F	102[A]	GLU	CA-C-O	-7.22	113.44	121.89

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	102[A]	GLU	Mainchain
1	F	102[B]	GLU	Mainchain

5.2 Too-close contacts [i](#)

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	2891	0	2717	56	1
1	B	2889	0	2724	55	0
1	C	2898	0	2734	76	0
1	D	2872	0	2698	55	0
1	E	2884	0	2715	50	1
1	F	2884	0	2717	48	2
2	A	16	0	28	3	0
2	B	24	0	40	23	0
2	C	32	0	56	15	0
2	D	56	0	98	12	0
2	E	40	0	70	15	0
2	F	40	0	70	14	0
3	A	40	0	70	16	0
3	B	32	0	56	14	0
3	C	24	0	42	4	0
3	E	8	0	14	3	0
3	F	24	0	42	2	0
4	A	14	0	0	0	0
4	B	16	0	0	0	0
4	C	15	0	0	0	0
4	D	15	0	0	0	0
4	E	13	0	0	0	0
4	F	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	198	0	0	13	2
5	B	184	0	0	10	1
5	C	214	0	0	13	1
5	D	207	0	0	8	1
5	E	213	0	0	6	0
5	F	198	0	0	10	1
All	All	18955	0	16891	359	5

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 10.

The worst 5 of 359 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)
2:C:406:MRD:H1C1	2:C:406:MRD:C5	1.49	1.37
2:B:407:MRD:C5	2:B:407:MRD:H1C1	1.51	1.33
2:C:406:MRD:H5C3	2:C:406:MRD:C1	1.55	1.22
2:B:407:MRD:H5C3	2:B:407:MRD:C1	1.79	1.12
1:A:58:LEU:N	1:A:58:LEU:HD23	1.62	1.11

All (5) 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)
1:F:102[A]:GLU:OE2	5:A:609:HOH:O[1_654]	1.39	0.81
5:B:624:HOH:O	5:C:648:HOH:O[1_455]	1.68	0.52
1:E:102[B]:GLU:OE1	5:D:626:HOH:O[1_565]	1.98	0.22
1:F:101:ASP:OD1	5:A:549:HOH:O[1_654]	2.11	0.09
1:A:101:ASP:OD1	5:F:671:HOH:O[1_546]	2.19	0.01

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	356/362 (98%)	346 (97%)	8 (2%)	2 (1%)	21	12
1	B	356/362 (98%)	349 (98%)	5 (1%)	2 (1%)	21	12
1	C	357/362 (99%)	349 (98%)	5 (1%)	3 (1%)	16	8
1	D	353/362 (98%)	344 (98%)	8 (2%)	1 (0%)	36	31
1	E	355/362 (98%)	350 (99%)	5 (1%)	0	100	100
1	F	355/362 (98%)	349 (98%)	4 (1%)	2 (1%)	21	12
All	All	2132/2172 (98%)	2087 (98%)	35 (2%)	10 (0%)	24	17

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	351	ILE
1	A	352	ASN
1	B	352	ASN
1	C	5	ASP
1	D	351	ILE

5.3.2 Protein sidechains [i](#)

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	317/324 (98%)	310 (98%)	7 (2%)	45	45
1	B	318/324 (98%)	308 (97%)	10 (3%)	35	31
1	C	319/324 (98%)	314 (98%)	5 (2%)	55	56
1	D	315/324 (97%)	308 (98%)	7 (2%)	45	45
1	E	317/324 (98%)	311 (98%)	6 (2%)	50	50
1	F	317/324 (98%)	315 (99%)	2 (1%)	78	79
All	All	1903/1944 (98%)	1866 (98%)	37 (2%)	51	50

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	351	ILE

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Mol	Chain	Res	Type
1	F	58	LEU
1	E	5	ASP
1	E	128	GLU
1	B	124	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	316	ASN
1	F	25	ASN
1	F	38	HIS
1	D	316	ASN
1	E	25	ASN

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](#)

Of 129 ligands modelled in this entry, 87 are monoatomic - leaving 42 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	MRD	E	402	-	7,7,7	0.37	0	9,10,10	0.26	0
3	MPD	C	405	-	7,7,7	0.31	0	9,10,10	0.31	0
2	MRD	F	501	-	7,7,7	0.28	0	9,10,10	0.19	0
3	MPD	F	504	-	7,7,7	0.31	0	9,10,10	0.25	0
2	MRD	F	506	-	7,7,7	0.30	0	9,10,10	0.18	0
2	MRD	F	502	-	7,7,7	0.33	0	9,10,10	0.30	0
2	MRD	C	402	-	7,7,7	0.42	0	9,10,10	0.40	0
2	MRD	D	405	-	7,7,7	0.31	0	9,10,10	0.22	0
2	MRD	D	404	-	7,7,7	0.32	0	9,10,10	0.26	0
3	MPD	A	403	-	7,7,7	0.28	0	9,10,10	0.33	0
3	MPD	B	401	-	7,7,7	0.33	0	9,10,10	0.41	0
3	MPD	B	405	-	7,7,7	0.29	0	9,10,10	0.35	0
2	MRD	D	403	-	7,7,7	0.31	0	9,10,10	0.35	0
2	MRD	D	407	-	7,7,7	0.33	0	9,10,10	0.29	0
2	MRD	A	401	-	7,7,7	0.29	0	9,10,10	0.23	0
2	MRD	C	407	-	7,7,7	0.32	0	9,10,10	0.24	0
2	MRD	E	404	-	7,7,7	0.30	0	9,10,10	0.33	0
3	MPD	F	503	-	7,7,7	0.29	0	9,10,10	0.33	0
3	MPD	F	505	-	7,7,7	0.31	0	9,10,10	0.28	0
2	MRD	D	401	-	7,7,7	0.31	0	9,10,10	0.29	0
3	MPD	C	403	-	7,7,7	0.33	0	9,10,10	0.19	0
2	MRD	E	406	-	7,7,7	0.33	0	9,10,10	0.32	0
2	MRD	F	508	-	7,7,7	0.36	0	9,10,10	0.38	0
2	MRD	A	407	-	7,7,7	0.50	0	9,10,10	0.50	0
2	MRD	E	401	-	7,7,7	0.29	0	9,10,10	0.23	0
2	MRD	D	406	-	7,7,7	0.37	0	9,10,10	0.50	0
3	MPD	A	405	-	7,7,7	0.32	0	9,10,10	0.22	0
3	MPD	B	406	-	7,7,7	1.09	1 (14%)	9,10,10	0.82	0
2	MRD	B	402	-	7,7,7	0.40	0	9,10,10	0.50	0
2	MRD	F	507	-	7,7,7	0.30	0	9,10,10	0.48	0
3	MPD	E	405	-	7,7,7	0.31	0	9,10,10	0.44	0
3	MPD	A	402	-	7,7,7	0.30	0	9,10,10	0.25	0
3	MPD	C	404	-	7,7,7	0.31	0	9,10,10	0.27	0
2	MRD	D	402	-	7,7,7	0.40	0	9,10,10	0.41	0
2	MRD	E	403	-	7,7,7	0.32	0	9,10,10	0.26	0
2	MRD	B	407	-	7,7,7	0.30	0	9,10,10	0.21	0
2	MRD	C	406	-	7,7,7	0.61	0	9,10,10	0.45	0
3	MPD	B	403	-	7,7,7	0.43	0	9,10,10	0.36	0
2	MRD	B	404	-	7,7,7	0.31	0	9,10,10	0.21	0
2	MRD	C	401	-	7,7,7	0.30	0	9,10,10	0.27	0
3	MPD	A	406	-	7,7,7	0.29	0	9,10,10	0.23	0
3	MPD	A	404	-	7,7,7	0.29	0	9,10,10	0.30	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	MRD	E	402	-	-	5/5/5/5	-
3	MPD	C	405	-	-	4/5/5/5	-
2	MRD	F	501	-	-	0/5/5/5	-
3	MPD	F	504	-	-	3/5/5/5	-
2	MRD	F	506	-	-	3/5/5/5	-
2	MRD	F	502	-	-	3/5/5/5	-
2	MRD	C	402	-	-	2/5/5/5	-
2	MRD	D	405	-	-	5/5/5/5	-
2	MRD	D	404	-	-	3/5/5/5	-
3	MPD	A	403	-	-	2/5/5/5	-
3	MPD	B	401	-	-	0/5/5/5	-
3	MPD	B	405	-	-	3/5/5/5	-
2	MRD	D	403	-	-	2/5/5/5	-
2	MRD	D	407	-	-	3/5/5/5	-
2	MRD	A	401	-	-	0/5/5/5	-
2	MRD	C	407	-	-	3/5/5/5	-
2	MRD	E	404	-	-	1/5/5/5	-
3	MPD	F	503	-	-	3/5/5/5	-
3	MPD	F	505	-	-	3/5/5/5	-
2	MRD	D	401	-	-	0/5/5/5	-
3	MPD	C	403	-	-	0/5/5/5	-
2	MRD	E	406	-	-	2/5/5/5	-
2	MRD	F	508	-	-	4/5/5/5	-
2	MRD	A	407	-	-	3/5/5/5	-
2	MRD	E	401	-	-	0/5/5/5	-
2	MRD	D	406	-	-	5/5/5/5	-
3	MPD	A	405	-	-	3/5/5/5	-
3	MPD	B	406	-	-	4/5/5/5	-
2	MRD	B	402	-	-	5/5/5/5	-
2	MRD	F	507	-	-	5/5/5/5	-
3	MPD	E	405	-	-	2/5/5/5	-
3	MPD	A	402	-	-	0/5/5/5	-
3	MPD	C	404	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MRD	D	402	-	-	2/5/5/5	-
2	MRD	E	403	-	-	2/5/5/5	-
2	MRD	B	407	-	-	3/5/5/5	-
2	MRD	C	406	-	-	4/5/5/5	-
3	MPD	B	403	-	-	1/5/5/5	-
2	MRD	B	404	-	-	3/5/5/5	-
2	MRD	C	401	-	-	0/5/5/5	-
3	MPD	A	406	-	-	3/5/5/5	-
3	MPD	A	404	-	-	5/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	406	MPD	O2-C2	-2.46	1.38	1.44

There are no bond angle outliers.

There are no chirality outliers.

5 of 104 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	407	MRD	C2-C3-C4-O4
2	B	402	MRD	C1-C2-C3-C4
2	B	402	MRD	C2-C3-C4-O4
2	B	402	MRD	C2-C3-C4-C5
2	B	404	MRD	C2-C3-C4-O4

There are no ring outliers.

31 monomers are involved in 121 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	402	MRD	10	0
3	C	405	MPD	3	0
2	F	502	MRD	6	0
2	C	402	MRD	10	0
2	D	405	MRD	2	0
2	D	404	MRD	1	0
3	A	403	MPD	2	0
3	B	401	MPD	1	0
3	B	405	MPD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	403	MRD	3	0
2	C	407	MRD	2	0
2	E	404	MRD	2	0
3	F	505	MPD	2	0
3	C	403	MPD	1	0
2	E	406	MRD	1	0
2	F	508	MRD	4	0
2	A	407	MRD	3	0
2	D	406	MRD	1	0
3	B	406	MPD	8	0
2	B	402	MRD	7	0
2	F	507	MRD	4	0
3	E	405	MPD	3	0
3	A	402	MPD	8	0
2	D	402	MRD	5	0
2	E	403	MRD	2	0
2	B	407	MRD	8	0
2	C	406	MRD	3	0
3	B	403	MPD	4	0
2	B	404	MRD	8	0
3	A	406	MPD	2	0
3	A	404	MPD	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	352/362 (97%)	-1.09	1 (0%) 90 90	16, 36, 77, 101	6 (1%)
1	B	350/362 (96%)	-1.09	0 100 100	16, 35, 75, 97	8 (2%)
1	C	351/362 (96%)	-1.10	0 100 100	15, 35, 76, 109	8 (2%)
1	D	350/362 (96%)	-1.11	0 100 100	19, 36, 75, 99	5 (1%)
1	E	351/362 (96%)	-1.11	0 100 100	17, 36, 76, 102	6 (1%)
1	F	350/362 (96%)	-1.10	0 100 100	17, 35, 72, 99	7 (2%)
All	All	2104/2172 (96%)	-1.10	1 (0%) 100 100	15, 36, 77, 109	40 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	THR	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CA	E	411	1/1	0.90	0.06	35,35,35,35	1
4	CA	F	514	1/1	0.94	0.06	32,32,32,32	1
2	MRD	C	402	8/8	0.95	0.09	50,55,64,82	0
2	MRD	C	407	8/8	0.95	0.08	67,73,75,78	0
4	CA	D	413	1/1	0.96	0.05	32,32,32,32	1
2	MRD	C	406	8/8	0.96	0.09	26,59,65,65	0
2	MRD	E	406	8/8	0.96	0.07	50,57,64,67	0
2	MRD	F	508	8/8	0.97	0.06	62,66,68,71	0
3	MPD	A	402	8/8	0.97	0.07	37,54,62,65	0
3	MPD	B	403	8/8	0.97	0.07	43,54,62,68	0
3	MPD	C	404	8/8	0.97	0.07	48,57,65,75	0
3	MPD	C	405	8/8	0.97	0.10	54,61,65,69	0
3	MPD	E	405	8/8	0.97	0.07	49,57,62,63	0
3	MPD	F	505	8/8	0.97	0.07	51,58,66,68	0
4	CA	A	412	1/1	0.97	0.05	60,60,60,60	0
2	MRD	D	407	8/8	0.97	0.08	60,69,74,76	0
2	MRD	D	402	8/8	0.97	0.08	47,57,68,75	0
2	MRD	F	506	8/8	0.97	0.06	44,57,67,69	0
4	CA	F	515	1/1	0.97	0.23	62,62,62,62	0
2	MRD	B	404	8/8	0.98	0.07	52,63,68,69	0
2	MRD	F	507	8/8	0.98	0.06	62,72,78,79	0
2	MRD	C	401	8/8	0.98	0.05	36,40,43,44	0
2	MRD	D	403	8/8	0.98	0.06	50,59,66,68	0
3	MPD	A	403	8/8	0.98	0.08	46,57,65,69	0
3	MPD	A	404	8/8	0.98	0.07	52,58,66,67	0
3	MPD	A	405	8/8	0.98	0.05	47,59,66,69	0
3	MPD	B	401	8/8	0.98	0.06	36,44,49,59	0
2	MRD	D	404	8/8	0.98	0.08	52,65,68,75	0
3	MPD	B	405	8/8	0.98	0.07	51,58,67,69	0
3	MPD	B	406	8/8	0.98	0.09	54,63,72,72	0
3	MPD	C	403	8/8	0.98	0.06	43,56,64,74	0
2	MRD	D	405	8/8	0.98	0.07	52,62,69,71	0
2	MRD	D	406	8/8	0.98	0.06	57,60,64,65	0
2	MRD	A	407	8/8	0.98	0.07	64,69,73,75	0
3	MPD	F	503	8/8	0.98	0.06	48,57,61,64	0
3	MPD	F	504	8/8	0.98	0.06	51,62,67,74	0
2	MRD	E	401	8/8	0.98	0.05	37,42,46,48	0
4	CA	A	409	1/1	0.98	0.14	57,57,57,57	0
2	MRD	E	402	8/8	0.98	0.05	45,58,69,73	0
4	CA	A	413	1/1	0.98	0.14	61,61,61,61	0
4	CA	B	408	1/1	0.98	0.08	50,50,50,50	0
4	CA	B	411	1/1	0.98	0.09	57,57,57,57	0
4	CA	B	414	1/1	0.98	0.03	54,54,54,54	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	B	415	1/1	0.98	0.20	59,59,59,59	0
4	CA	C	413	1/1	0.98	0.19	64,64,64,64	0
4	CA	C	421	1/1	0.98	0.08	49,49,49,49	0
4	CA	D	408	1/1	0.98	0.08	49,49,49,49	0
2	MRD	E	403	8/8	0.98	0.06	50,57,62,64	0
2	MRD	E	404	8/8	0.98	0.08	60,66,73,76	0
4	CA	E	412	1/1	0.98	0.14	63,63,63,63	0
2	MRD	B	402	8/8	0.98	0.07	40,52,65,69	0
2	MRD	F	502	8/8	0.98	0.07	52,62,72,74	0
2	MRD	D	401	8/8	0.99	0.03	33,41,42,47	0
4	CA	B	412	1/1	0.99	0.08	63,63,63,63	0
4	CA	A	408	1/1	0.99	0.10	51,51,51,51	0
2	MRD	A	401	8/8	0.99	0.04	34,41,46,47	0
4	CA	B	418	1/1	0.99	0.03	37,37,37,37	0
4	CA	B	409[A]	1/1	-	-	57,57,57,57	1
4	CA	B	409[B]	1/1	-	-	57,57,57,57	1
4	CA	B	422	1/1	0.99	0.03	32,32,32,32	0
4	CA	C	408	1/1	0.99	0.07	53,53,53,53	0
4	CA	C	409	1/1	0.99	0.10	54,54,54,54	0
4	CA	C	410	1/1	0.99	0.06	56,56,56,56	0
4	CA	C	412	1/1	0.99	0.09	42,42,42,42	0
4	CA	A	410	1/1	0.99	0.07	56,56,56,56	0
4	CA	C	418	1/1	0.99	0.04	35,35,35,35	0
4	CA	C	419	1/1	0.99	0.03	32,32,32,32	0
4	CA	C	420	1/1	0.99	0.04	32,32,32,32	0
2	MRD	B	407	8/8	0.99	0.06	59,71,77,81	0
4	CA	C	422	1/1	0.99	0.11	57,57,57,57	1
2	MRD	F	501	8/8	0.99	0.05	37,45,48,51	0
4	CA	D	409	1/1	0.99	0.08	52,52,52,52	0
4	CA	D	410	1/1	0.99	0.07	56,56,56,56	0
4	CA	D	411	1/1	0.99	0.06	60,60,60,60	0
4	CA	A	414	1/1	0.99	0.03	61,61,61,61	0
4	CA	D	414	1/1	0.99	0.11	55,55,55,55	0
4	CA	D	415	1/1	0.99	0.04	58,58,58,58	0
4	CA	D	417	1/1	0.99	0.05	36,36,36,36	0
4	CA	D	420	1/1	0.99	0.03	33,33,33,33	0
4	CA	E	407	1/1	0.99	0.09	52,52,52,52	0
4	CA	E	408	1/1	0.99	0.10	54,54,54,54	0
4	CA	A	419	1/1	0.99	0.02	31,31,31,31	0
4	CA	A	421	1/1	0.99	0.06	48,48,48,48	0
4	CA	E	413	1/1	0.99	0.03	58,58,58,58	0
4	CA	E	417	1/1	0.99	0.04	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	E	419	1/1	0.99	0.09	49,49,49,49	0
4	CA	F	509	1/1	0.99	0.12	49,49,49,49	0
4	CA	F	510	1/1	0.99	0.09	50,50,50,50	0
4	CA	F	511	1/1	0.99	0.11	56,56,56,56	0
4	CA	F	512	1/1	0.99	0.03	57,57,57,57	0
3	MPD	A	406	8/8	0.99	0.06	65,73,76,79	0
4	CA	B	410	1/1	0.99	0.11	51,51,51,51	0
4	CA	F	519	1/1	0.99	0.03	30,30,30,30	0
4	CA	F	520	1/1	0.99	0.05	34,34,34,34	0
4	CA	A	420	1/1	1.00	0.01	35,35,35,35	0
4	CA	D	416	1/1	1.00	0.04	54,54,54,54	0
4	CA	A	415	1/1	1.00	0.02	57,57,57,57	0
4	CA	D	418	1/1	1.00	0.02	29,29,29,29	0
4	CA	D	419	1/1	1.00	0.02	34,34,34,34	0
4	CA	C	414	1/1	1.00	0.02	65,65,65,65	0
4	CA	D	421	1/1	1.00	0.02	34,34,34,34	0
4	CA	D	422	1/1	1.00	0.03	34,34,34,34	0
4	CA	C	415	1/1	1.00	0.04	53,53,53,53	0
4	CA	C	416	1/1	1.00	0.03	37,37,37,37	0
4	CA	E	409	1/1	1.00	0.03	57,57,57,57	0
4	CA	E	410	1/1	1.00	0.05	38,38,38,38	0
4	CA	C	417	1/1	1.00	0.03	30,30,30,30	0
4	CA	B	416	1/1	1.00	0.02	66,66,66,66	0
4	CA	B	417	1/1	1.00	0.01	57,57,57,57	0
4	CA	E	414	1/1	1.00	0.03	52,52,52,52	0
4	CA	E	415	1/1	1.00	0.05	35,35,35,35	0
4	CA	E	416	1/1	1.00	0.03	30,30,30,30	0
4	CA	A	416	1/1	1.00	0.05	36,36,36,36	0
4	CA	E	418	1/1	1.00	0.01	33,33,33,33	0
4	CA	B	419	1/1	1.00	0.04	30,30,30,30	0
4	CA	B	420	1/1	1.00	0.05	32,32,32,32	0
4	CA	B	421	1/1	1.00	0.02	31,31,31,31	0
4	CA	A	417	1/1	1.00	0.02	29,29,29,29	0
4	CA	A	418	1/1	1.00	0.04	34,34,34,34	0
4	CA	F	513	1/1	1.00	0.03	41,41,41,41	0
4	CA	A	411	1/1	1.00	0.03	41,41,41,41	0
4	CA	D	412	1/1	1.00	0.04	40,40,40,40	0
4	CA	F	516	1/1	1.00	0.05	63,63,63,63	0
4	CA	F	517	1/1	1.00	0.02	55,55,55,55	0
4	CA	F	518	1/1	1.00	0.03	36,36,36,36	0
4	CA	B	413	1/1	1.00	0.03	40,40,40,40	0
4	CA	C	411	1/1	1.00	0.03	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CA	F	521	1/1	1.00	0.02	31,31,31,31	0
4	CA	F	522	1/1	1.00	0.02	34,34,34,34	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.