



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:16 AM UTC

PDB ID : 2PD0 / pdb_00002pd0
Title : Protein cgd2_2020 from *Cryptosporidium parvum*
Authors : Cymborowski, M.; Chruszcz, M.; Hills, T.; Lew, J.; Melone, M.; Zhao, Y.; Artz, J.; Wernimont, A.; Edwards, A.; Sundstrom, M.; Weigelt, J.; Bochkarev, A.; Arrowsmith, C.; Hui, R.; Minor, W.; Structural Genomics Consortium (SGC)
Deposited on : 2007-03-30
Resolution : 2.30 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

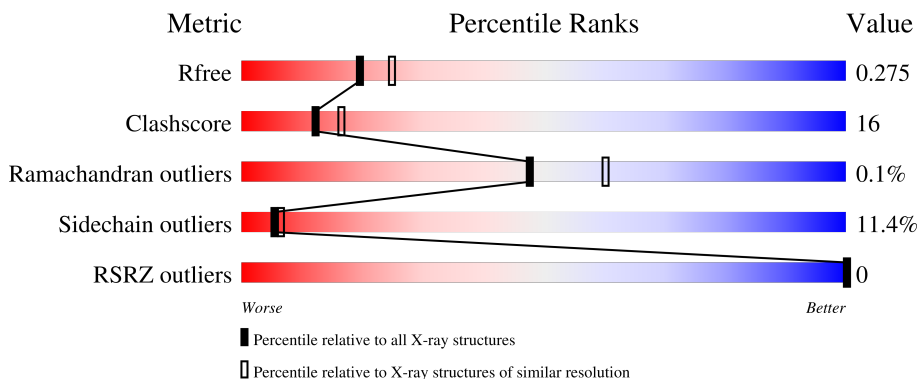
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	223	
1	B	223	
1	C	223	
1	D	223	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7306 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 Hypothetical protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	205	1760	1126	290	338	3	3	0	10	0
1	B	205	1738	1115	288	328	4	3	0	8	0
1	C	205	1687	1083	280	319	2	3	0	3	0
1	D	203	1645	1058	271	311	2	3	0	1	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	cloning artifact	UNP Q5CTR0
A	-17	GLY	-	cloning artifact	UNP Q5CTR0
A	-16	SER	-	cloning artifact	UNP Q5CTR0
A	-15	SER	-	cloning artifact	UNP Q5CTR0
A	-14	HIS	-	cloning artifact	UNP Q5CTR0
A	-13	HIS	-	cloning artifact	UNP Q5CTR0
A	-12	HIS	-	cloning artifact	UNP Q5CTR0
A	-11	HIS	-	cloning artifact	UNP Q5CTR0
A	-10	HIS	-	cloning artifact	UNP Q5CTR0
A	-9	HIS	-	cloning artifact	UNP Q5CTR0
A	-8	SER	-	cloning artifact	UNP Q5CTR0
A	-7	SER	-	cloning artifact	UNP Q5CTR0
A	-6	GLY	-	cloning artifact	UNP Q5CTR0
A	-5	LEU	-	cloning artifact	UNP Q5CTR0
A	-4	VAL	-	cloning artifact	UNP Q5CTR0
A	-3	PRO	-	cloning artifact	UNP Q5CTR0
A	-2	ARG	-	cloning artifact	UNP Q5CTR0
A	-1	GLY	-	cloning artifact	UNP Q5CTR0
A	0	SER	-	cloning artifact	UNP Q5CTR0
A	25	MSE	MET	modified residue	UNP Q5CTR0
A	131	MSE	MET	modified residue	UNP Q5CTR0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	164	MSE	MET	modified residue	UNP Q5CTR0
B	-18	MET	-	cloning artifact	UNP Q5CTR0
B	-17	GLY	-	cloning artifact	UNP Q5CTR0
B	-16	SER	-	cloning artifact	UNP Q5CTR0
B	-15	SER	-	cloning artifact	UNP Q5CTR0
B	-14	HIS	-	cloning artifact	UNP Q5CTR0
B	-13	HIS	-	cloning artifact	UNP Q5CTR0
B	-12	HIS	-	cloning artifact	UNP Q5CTR0
B	-11	HIS	-	cloning artifact	UNP Q5CTR0
B	-10	HIS	-	cloning artifact	UNP Q5CTR0
B	-9	HIS	-	cloning artifact	UNP Q5CTR0
B	-8	SER	-	cloning artifact	UNP Q5CTR0
B	-7	SER	-	cloning artifact	UNP Q5CTR0
B	-6	GLY	-	cloning artifact	UNP Q5CTR0
B	-5	LEU	-	cloning artifact	UNP Q5CTR0
B	-4	VAL	-	cloning artifact	UNP Q5CTR0
B	-3	PRO	-	cloning artifact	UNP Q5CTR0
B	-2	ARG	-	cloning artifact	UNP Q5CTR0
B	-1	GLY	-	cloning artifact	UNP Q5CTR0
B	0	SER	-	cloning artifact	UNP Q5CTR0
B	25	MSE	MET	modified residue	UNP Q5CTR0
B	131	MSE	MET	modified residue	UNP Q5CTR0
B	164	MSE	MET	modified residue	UNP Q5CTR0
C	-18	MET	-	cloning artifact	UNP Q5CTR0
C	-17	GLY	-	cloning artifact	UNP Q5CTR0
C	-16	SER	-	cloning artifact	UNP Q5CTR0
C	-15	SER	-	cloning artifact	UNP Q5CTR0
C	-14	HIS	-	cloning artifact	UNP Q5CTR0
C	-13	HIS	-	cloning artifact	UNP Q5CTR0
C	-12	HIS	-	cloning artifact	UNP Q5CTR0
C	-11	HIS	-	cloning artifact	UNP Q5CTR0
C	-10	HIS	-	cloning artifact	UNP Q5CTR0
C	-9	HIS	-	cloning artifact	UNP Q5CTR0
C	-8	SER	-	cloning artifact	UNP Q5CTR0
C	-7	SER	-	cloning artifact	UNP Q5CTR0
C	-6	GLY	-	cloning artifact	UNP Q5CTR0
C	-5	LEU	-	cloning artifact	UNP Q5CTR0
C	-4	VAL	-	cloning artifact	UNP Q5CTR0
C	-3	PRO	-	cloning artifact	UNP Q5CTR0
C	-2	ARG	-	cloning artifact	UNP Q5CTR0
C	-1	GLY	-	cloning artifact	UNP Q5CTR0
C	0	SER	-	cloning artifact	UNP Q5CTR0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	25	MSE	MET	modified residue	UNP Q5CTR0
C	131	MSE	MET	modified residue	UNP Q5CTR0
C	164	MSE	MET	modified residue	UNP Q5CTR0
D	-18	MET	-	cloning artifact	UNP Q5CTR0
D	-17	GLY	-	cloning artifact	UNP Q5CTR0
D	-16	SER	-	cloning artifact	UNP Q5CTR0
D	-15	SER	-	cloning artifact	UNP Q5CTR0
D	-14	HIS	-	cloning artifact	UNP Q5CTR0
D	-13	HIS	-	cloning artifact	UNP Q5CTR0
D	-12	HIS	-	cloning artifact	UNP Q5CTR0
D	-11	HIS	-	cloning artifact	UNP Q5CTR0
D	-10	HIS	-	cloning artifact	UNP Q5CTR0
D	-9	HIS	-	cloning artifact	UNP Q5CTR0
D	-8	SER	-	cloning artifact	UNP Q5CTR0
D	-7	SER	-	cloning artifact	UNP Q5CTR0
D	-6	GLY	-	cloning artifact	UNP Q5CTR0
D	-5	LEU	-	cloning artifact	UNP Q5CTR0
D	-4	VAL	-	cloning artifact	UNP Q5CTR0
D	-3	PRO	-	cloning artifact	UNP Q5CTR0
D	-2	ARG	-	cloning artifact	UNP Q5CTR0
D	-1	GLY	-	cloning artifact	UNP Q5CTR0
D	0	SER	-	cloning artifact	UNP Q5CTR0
D	25	MSE	MET	modified residue	UNP Q5CTR0
D	131	MSE	MET	modified residue	UNP Q5CTR0
D	164	MSE	MET	modified residue	UNP Q5CTR0

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is water.

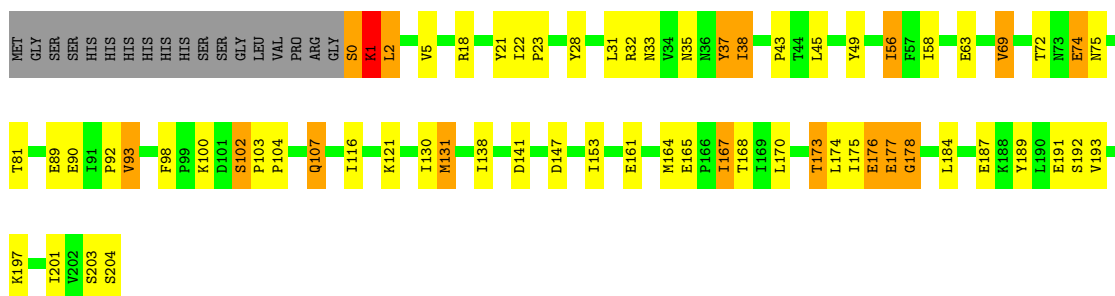
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total	O	0	0
			123	123		
3	B	130	Total	O	0	0
			130	130		
3	C	76	Total	O	0	0
			76	76		
3	D	99	Total	O	0	0
			99	99		

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.

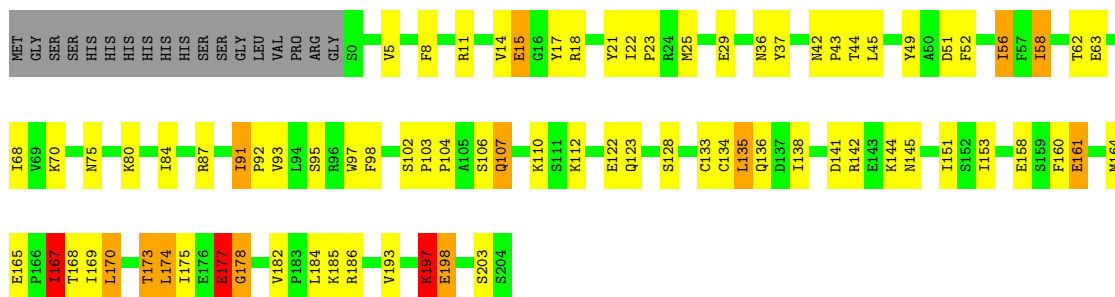
- Molecule 1: Hypothetical protein

Chain A: 



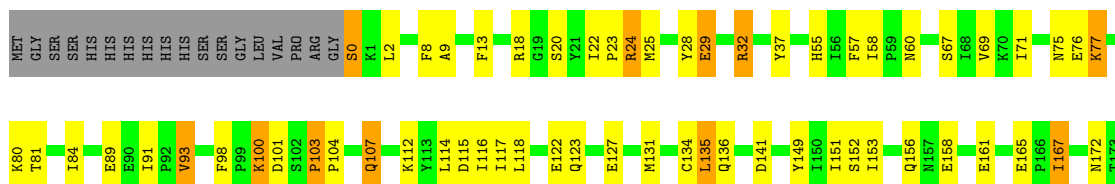
- Molecule 1: Hypothetical protein

Chain B: 



- Molecule 1: Hypothetical protein

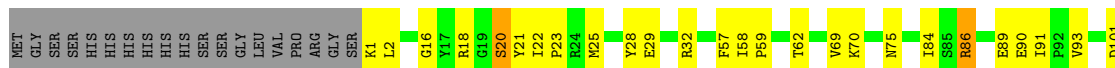
Chain C: 





- Molecule 1: Hypothetical protein

Chain D: 61% 25% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.53Å 68.52Å 79.57Å 69.29° 75.14° 93.73°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.30) 98.1 (20.00-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.69 (at 2.30Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.220 , 0.280 0.224 , 0.275	Depositor DCC
R_{free} test set	2091 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtrriage
Anisotropy	0.047	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7306	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.17% 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: MES

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	1.11	9/1796 (0.5%)	1.10	6/2420 (0.2%)
1	B	1.25	9/1773 (0.5%)	1.21	6/2391 (0.3%)
1	C	1.10	1/1722 (0.1%)	1.08	3/2325 (0.1%)
1	D	1.17	6/1680 (0.4%)	1.15	6/2272 (0.3%)
All	All	1.16	25/6971 (0.4%)	1.14	21/9408 (0.2%)

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	5
1	B	0	2
1	C	0	4
1	D	0	1
All	All	0	12

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	131	MSE	SE-CE	-14.26	1.52	1.95
1	D	93	VAL	C-O	-9.80	1.14	1.24
1	B	93	VAL	C-O	-7.92	1.15	1.23
1	D	91	ILE	C-O	-7.37	1.16	1.25
1	B	68	ILE	C-O	-6.45	1.17	1.24
1	B	91	ILE	C-O	-6.36	1.16	1.24
1	B	92	PRO	C-O	-6.07	1.16	1.23
1	B	182	VAL	C-O	-6.03	1.16	1.24
1	D	20	SER	C-O	-5.91	1.17	1.23
1	D	116	ILE	CA-CB	5.85	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	VAL	C-N	-5.84	1.25	1.33
1	D	84	ILE	CA-CB	5.61	1.61	1.54
1	A	2	LEU	C-O	-5.43	1.16	1.23
1	A	175	ILE	C-O	-5.41	1.17	1.24
1	A	33	ASN	C-O	-5.37	1.17	1.24
1	B	70	LYS	C-O	-5.30	1.17	1.23
1	A	35	ASN	C-O	-5.29	1.17	1.24
1	D	190	LEU	C-O	-5.29	1.17	1.24
1	A	37	TYR	C-O	-5.28	1.18	1.24
1	B	197	LYS	C-O	-5.21	1.17	1.24
1	A	38	ILE	C-N	5.18	1.40	1.33
1	B	197	LYS	N-CA	-5.15	1.39	1.46
1	A	72	THR	CA-CB	5.08	1.62	1.53
1	A	138	ILE	C-O	-5.08	1.18	1.24
1	B	17	TYR	C-O	-5.06	1.17	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	167	ILE	CB-CA-C	-8.99	100.00	112.14
1	A	31	LEU	N-CA-C	7.89	119.88	111.28
1	D	91	ILE	N-CA-C	7.84	117.59	108.96
1	C	103	PRO	N-CA-C	7.71	120.11	110.70
1	D	194	GLU	N-CA-C	7.26	120.12	111.33
1	B	177	GLU	N-CA-C	6.67	121.36	112.30
1	A	103	PRO	N-CA-C	6.47	118.59	110.70
1	D	103	PRO	N-CA-C	6.32	118.41	110.70
1	B	15	GLU	N-CA-C	6.18	119.44	110.42
1	A	35	ASN	N-CA-C	6.17	118.81	111.71
1	B	103	PRO	N-CA-C	6.13	118.18	110.70
1	C	177	GLU	N-CA-C	6.08	120.72	112.88
1	B	178	GLY	O-C-N	-6.03	119.55	123.35
1	A	38	ILE	O-C-N	5.91	127.70	121.91
1	A	102	SER	CA-C-N	5.54	126.08	120.38
1	A	102	SER	C-N-CA	5.54	126.08	120.38
1	B	167	ILE	CB-CA-C	-5.38	103.82	112.16
1	D	167	ILE	N-CA-CB	5.29	117.74	110.54
1	B	178	GLY	N-CA-C	5.26	121.71	111.34
1	D	192	SER	N-CA-C	5.17	116.99	111.36
1	C	9	ALA	N-CA-C	5.04	118.53	112.38

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	0	SER	Peptide
1	A	1	LYS	Peptide
1	A	131	MSE	Peptide
1	A	177	GLU	Peptide
1	A	178	GLY	Peptide
1	B	177	GLU	Peptide
1	B	178	GLY	Peptide
1	C	0	SER	Peptide
1	C	177	GLU	Peptide
1	C	178	GLY	Peptide
1	C	180	SER	Peptide
1	D	177	GLU	Peptide

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	1760	0	1729	52	0
1	B	1738	0	1716	50	0
1	C	1687	0	1650	68	0
1	D	1645	0	1594	49	0
2	A	12	0	12	0	0
2	B	12	0	12	3	0
2	C	12	0	12	2	0
2	D	12	0	12	1	0
3	A	123	0	0	8	0
3	B	130	0	0	7	0
3	C	76	0	0	11	0
3	D	99	0	0	14	0
All	All	7306	0	6737	212	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 16.

All (212) 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:93:VAL:HG11	1:A:167[B]:ILE:HG12	1.28	1.15
1:A:56[A]:ILE:HD11	1:A:58:ILE:CG2	1.79	1.12
1:A:56[A]:ILE:HD11	1:A:58:ILE:HG23	1.28	1.11
1:D:1:LYS:CB	1:D:2:LEU:HA	1.82	1.10
1:C:135:LEU:N	1:C:135:LEU:HD23	1.71	1.05
1:C:84:ILE:HG23	3:C:547:HOH:O	1.63	0.95
1:C:135:LEU:N	1:C:135:LEU:CD2	2.30	0.94
1:A:93:VAL:CG1	1:A:167[B]:ILE:HG12	2.00	0.91
1:B:18:ARG:HG2	1:B:18:ARG:HH21	1.36	0.90
1:A:56[A]:ILE:CD1	1:A:58:ILE:HG23	2.04	0.87
1:C:134:CYS:C	1:C:135:LEU:CD2	2.50	0.85
1:C:134:CYS:C	1:C:135:LEU:HD23	2.03	0.84
1:C:20:SER:HA	3:C:510:HOH:O	1.78	0.82
1:A:74:GLU:HG2	1:A:75:ASN:N	1.94	0.82
1:B:161[A]:GLU:HG3	3:B:559:HOH:O	1.80	0.82
1:C:134:CYS:O	1:C:135:LEU:HD22	1.76	0.82
1:B:22[A]:ILE:CD1	1:B:153:ILE:HD13	2.10	0.80
1:C:167[A]:ILE:HD13	3:C:578:HOH:O	1.82	0.80
3:A:521:HOH:O	1:C:167[A]:ILE:HG12	1.82	0.79
1:A:193:VAL:O	1:A:197[A]:LYS:HG3	1.81	0.79
1:D:171:ARG:HD3	3:D:534:HOH:O	1.82	0.78
1:D:86:ARG:HD3	1:D:90:GLU:OE1	1.84	0.78
1:D:1:LYS:CB	1:D:2:LEU:CA	2.62	0.77
1:D:58:ILE:HD12	1:D:116:ILE:HD13	1.65	0.76
1:A:167[A]:ILE:HG12	3:A:531:HOH:O	1.86	0.75
1:B:22[A]:ILE:HD11	1:B:153:ILE:HD13	1.68	0.74
1:B:170:LEU:O	1:B:173:THR:HB	1.88	0.73
1:C:158:GLU:OE1	1:C:158:GLU:N	2.20	0.72
1:C:182:VAL:HG13	1:C:183:PRO:HD2	1.71	0.72
1:D:70:LYS:HE3	1:D:198:GLU:HG3	1.71	0.71
1:D:204:SER:HA	3:D:599:HOH:O	1.91	0.69
1:B:18:ARG:NH2	1:B:203:SER:OG	2.26	0.69
1:B:18:ARG:NE	3:B:611:HOH:O	2.27	0.68
1:B:51:ASP:HB3	3:B:619:HOH:O	1.93	0.68
1:C:134:CYS:C	1:C:135:LEU:HD22	2.17	0.68
1:C:182:VAL:CG1	1:C:183:PRO:HD2	2.24	0.68
1:D:86:ARG:CD	1:D:90:GLU:OE1	2.41	0.68
1:A:93:VAL:HG11	1:A:167[B]:ILE:CG1	2.16	0.67
1:C:84:ILE:HD12	3:C:547:HOH:O	1.93	0.67
1:D:57:PHE:HZ	1:D:161:GLU:HG3	1.61	0.65
1:B:42[A]:ASN:ND2	3:B:562:HOH:O	2.30	0.65
1:D:187:GLU:H	1:D:187:GLU:CD	2.06	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLU:OE1	1:A:89:GLU:N	2.31	0.64
1:A:100:LYS:HB3	1:A:204:SER:HB3	1.80	0.63
1:D:21:TYR:HB2	3:D:599:HOH:O	1.99	0.63
1:D:58:ILE:HG22	1:D:59:PRO:O	1.97	0.63
1:C:100:LYS:HA	1:C:100:LYS:HE3	1.80	0.62
1:D:185:LYS:HE2	3:D:577:HOH:O	1.99	0.61
1:C:134:CYS:O	1:C:135:LEU:CD2	2.46	0.61
1:D:21:TYR:CE1	1:D:23:PRO:HB3	2.36	0.61
1:C:84:ILE:CD1	3:C:547:HOH:O	2.49	0.61
1:C:172:ASN:O	1:C:181:GLY:CA	2.49	0.61
1:B:145:ASN:ND2	3:B:627:HOH:O	2.34	0.60
1:A:102:SER:OG	1:A:104:PRO:HD2	2.02	0.60
1:C:123:GLN:NE2	1:C:180:SER:O	2.34	0.60
1:B:18:ARG:HG2	1:B:18:ARG:NH2	2.14	0.59
1:A:170:LEU:HD23	1:A:184:LEU:CD1	2.33	0.59
1:C:165:GLU:HB3	1:C:167[A]:ILE:HG13	1.82	0.59
1:D:167:ILE:HG12	3:D:507:HOH:O	2.02	0.59
1:B:128:SER:HA	1:B:133:CYS:SG	2.43	0.59
1:A:18:ARG:NH1	3:A:620:HOH:O	2.36	0.58
1:A:191:GLU:HG2	1:B:160:PHE:CD1	2.38	0.58
1:C:167[A]:ILE:HG23	3:C:575:HOH:O	2.03	0.58
1:C:172:ASN:O	1:C:182:VAL:N	2.35	0.58
1:C:100:LYS:HD2	1:C:204:SER:HB3	1.85	0.58
1:A:92:PRO:HG2	1:C:193:VAL:HG21	1.85	0.58
1:A:164:MSE:O	1:A:192:SER:OG	2.21	0.58
1:A:197[B]:LYS:HG2	3:C:565:HOH:O	2.04	0.57
1:C:25:MSE:HG3	1:C:29:GLU:HG2	1.85	0.57
1:D:169:ILE:HG22	1:D:184:LEU:HD12	1.86	0.57
1:A:58:ILE:HD11	1:A:116:ILE:HD11	1.85	0.57
1:B:186:ARG:HD2	1:D:177:GLU:OE2	2.04	0.57
1:C:180:SER:H	1:C:181:GLY:HA2	1.69	0.56
1:A:32[B]:ARG:NH1	1:A:141:ASP:OD1	2.39	0.55
1:D:204:SER:C	3:D:599:HOH:O	2.48	0.55
1:D:170:LEU:O	1:D:173:THR:HB	2.06	0.55
1:C:28:TYR:HE2	1:C:32:ARG:NH1	2.04	0.54
1:C:37:TYR:HE1	3:C:573:HOH:O	1.89	0.54
1:B:43:PRO:HG2	1:B:56[A]:ILE:HG21	1.88	0.54
1:A:23:PRO:HG2	1:A:63[B]:GLU:HB2	1.88	0.54
1:B:18:ARG:HH21	1:B:18:ARG:CG	2.13	0.54
1:A:49:TYR:CG	1:A:164:MSE:HE1	2.43	0.53
1:A:56[A]:ILE:CD1	1:A:58:ILE:CG2	2.69	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:PRO:C	1:C:24[A]:ARG:HG2	2.34	0.52
1:D:86:ARG:NH1	1:D:90:GLU:OE2	2.40	0.52
1:A:18:ARG:HD3	1:A:203:SER:OG	2.10	0.52
1:B:185:LYS:HE3	3:B:613:HOH:O	2.09	0.52
1:A:81:THR:HG21	1:C:81:THR:CG2	2.40	0.52
1:A:22:ILE:HD11	1:A:153:ILE:HG21	1.92	0.52
1:B:25:MSE:HE1	1:B:62:THR:HG22	1.92	0.51
1:D:101[A]:ASP:OD1	1:D:101[A]:ASP:N	2.40	0.51
1:B:173:THR:HG22	1:B:174:LEU:HG	1.93	0.51
1:B:49:TYR:CG	1:B:164:MSE:HE1	2.46	0.51
1:A:21:TYR:CE1	1:A:23:PRO:HB3	2.46	0.51
1:B:102:SER:HB2	1:B:104:PRO:HD2	1.91	0.51
1:B:36:ASN:OD1	1:B:142:ARG:NH1	2.43	0.51
1:C:127:GLU:OE1	2:C:504:MES:C7	2.58	0.50
1:B:175[B]:ILE:C	1:B:177:GLU:H	2.18	0.50
1:C:57:PHE:HZ	1:C:161[A]:GLU:HG3	1.75	0.50
1:B:84:ILE:HG13	3:B:611:HOH:O	2.12	0.50
1:D:177:GLU:H	1:D:178:GLY:HA2	1.77	0.50
1:A:187:GLU:O	1:A:191:GLU:HG3	2.11	0.49
1:A:81:THR:CG2	1:C:81:THR:HG21	2.43	0.49
1:C:103:PRO:O	1:C:107:GLN:NE2	2.43	0.49
1:D:20:SER:HA	3:D:523:HOH:O	2.13	0.49
1:D:173:THR:HG22	1:D:174:LEU:HG	1.95	0.49
1:C:69:VAL:HG13	1:C:98:PHE:CE2	2.47	0.48
1:A:107:GLN:HB2	3:A:615:HOH:O	2.12	0.48
1:B:56[B]:ILE:HD12	1:B:58:ILE:CD1	2.43	0.48
1:C:180:SER:N	1:C:181:GLY:HA2	2.28	0.48
1:D:131:MSE:SE	1:D:178:GLY:HA3	2.63	0.48
1:D:25:MSE:HG3	1:D:29:GLU:HG2	1.96	0.48
1:A:121:LYS:HD2	3:A:613:HOH:O	2.13	0.48
1:A:176:GLU:HG2	1:A:177:GLU:HG2	1.93	0.48
1:B:80:LYS:HD3	1:B:97:TRP:CZ2	2.49	0.48
1:C:194:GLU:OE1	1:C:194:GLU:HA	2.14	0.47
1:B:87:ARG:HH21	2:B:503:MES:H31	1.80	0.47
1:C:55:HIS:HD1	1:C:115:ASP:CG	2.23	0.47
1:D:177:GLU:N	1:D:178:GLY:HA2	2.29	0.47
1:A:90:GLU:HA	3:A:612:HOH:O	2.14	0.47
1:C:22:ILE:HD11	1:C:153:ILE:HD13	1.96	0.47
1:A:189:TYR:CE1	1:C:91:ILE:HD12	2.50	0.47
1:B:8:PHE:CD2	2:B:503:MES:H32	2.50	0.47
1:B:52:PHE:CD1	1:B:123:GLN:HG2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ILE:HG13	1:C:198:GLU:C	2.40	0.47
1:B:23:PRO:HG2	1:B:63:GLU:HB2	1.96	0.47
1:B:37:TYR:CD2	1:B:58:ILE:HG12	2.49	0.47
1:C:107:GLN:H	1:C:107:GLN:HG2	1.56	0.46
1:D:175:ILE:O	1:D:175:ILE:HG13	2.15	0.46
1:A:58:ILE:CD1	1:A:116:ILE:HD11	2.45	0.46
1:D:22:ILE:HD12	1:D:153:ILE:HD13	1.96	0.46
1:D:86:ARG:NH2	2:D:501:MES:O3S	2.48	0.46
1:B:135:LEU:N	1:B:135:LEU:CD2	2.78	0.46
1:C:75:ASN:HB2	1:C:104:PRO:HG3	1.97	0.46
1:D:182:VAL:CG1	3:D:577:HOH:O	2.64	0.46
1:B:141:ASP:HA	1:B:144:LYS:HE2	1.97	0.46
1:C:8:PHE:CG	2:C:504:MES:H32	2.51	0.46
1:B:15:GLU:HG3	1:B:21:TYR:CE1	2.52	0.45
1:B:167:ILE:HD12	1:B:168:THR:N	2.31	0.45
1:B:25:MSE:HG2	1:B:29:GLU:HB3	1.98	0.45
1:C:180:SER:N	1:C:181:GLY:CA	2.79	0.45
1:D:16:GLY:HA2	1:D:204:SER:OG	2.17	0.45
1:B:75:ASN:HB2	1:B:104:PRO:HG3	1.98	0.45
1:C:13:PHE:CZ	1:C:22:ILE:HD13	2.52	0.45
1:B:87:ARG:NH2	2:B:503:MES:H31	2.31	0.45
1:B:167:ILE:HD12	1:B:168:THR:H	1.80	0.45
1:A:0:SER:O	1:A:147:ASP:HB2	2.17	0.45
1:C:172:ASN:O	1:C:181:GLY:HA3	2.17	0.45
1:C:93:VAL:CG1	1:C:167[A]:ILE:HG21	2.47	0.45
1:A:167[A]:ILE:HG21	3:A:611:HOH:O	2.17	0.45
1:D:86:ARG:HD2	1:D:90:GLU:OE1	2.16	0.44
1:A:69:VAL:HG22	1:A:98:PHE:CE2	2.53	0.44
1:C:60:ASN:OD1	1:C:114:LEU:HD11	2.18	0.44
1:C:167[B]:ILE:HD13	3:C:575:HOH:O	2.17	0.44
1:C:77:LYS:CB	1:C:77:LYS:NZ	2.81	0.44
1:D:182:VAL:HG13	3:D:577:HOH:O	2.17	0.44
1:B:193:VAL:O	1:B:197:LYS:HB3	2.18	0.44
1:C:84:ILE:HG23	1:C:84:ILE:HD12	1.62	0.44
1:D:57:PHE:CZ	1:D:161:GLU:HG3	2.48	0.44
1:C:117:ILE:HB	1:C:152:SER:HB3	2.00	0.43
1:C:167[A]:ILE:HG12	3:C:505:HOH:O	2.17	0.43
1:B:164:MSE:HG3	1:B:168:THR:HB	2.00	0.43
1:B:112:LYS:HB3	1:B:112:LYS:HE2	1.52	0.43
1:B:174:LEU:HD21	1:D:173:THR:HG21	1.99	0.43
1:D:163:PRO:HG2	1:D:195:PHE:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ARG:HD3	1:C:203:SER:HB2	1.99	0.43
1:C:58:ILE:HD12	1:C:116:ILE:CD1	2.48	0.43
1:B:98:PHE:CD1	1:B:104:PRO:HG2	2.53	0.43
1:B:45:LEU:HD12	1:B:45:LEU:HA	1.85	0.43
1:C:28:TYR:CE2	1:C:32:ARG:NH1	2.85	0.43
1:C:122:GLU:HG3	3:C:570:HOH:O	2.17	0.43
1:C:174:LEU:O	1:C:178:GLY:HA2	2.19	0.43
1:A:167[A]:ILE:HD12	1:A:168:THR:N	2.33	0.43
1:D:177:GLU:OE1	1:D:177:GLU:HA	2.18	0.43
1:B:5:VAL:HB	1:B:138:ILE:HB	2.00	0.43
1:B:144:LYS:HA	1:B:144:LYS:HD3	1.84	0.43
1:C:55:HIS:CE1	1:C:161[A]:GLU:HG2	2.54	0.43
1:D:146:PRO:HG2	1:D:149:TYR:CZ	2.53	0.43
1:C:93:VAL:CG2	1:C:167[B]:ILE:HG12	2.49	0.42
1:A:174:LEU:O	1:A:178:GLY:HA2	2.19	0.42
1:C:71:ILE:N	1:C:198:GLU:O	2.29	0.42
1:B:107:GLN:H	1:B:107:GLN:HG2	1.62	0.42
1:A:176:GLU:HB3	3:A:560:HOH:O	2.19	0.42
1:C:93:VAL:HG21	1:C:167[B]:ILE:HG12	2.02	0.42
1:D:164:MSE:CE	3:D:580:HOH:O	2.67	0.42
1:D:204:SER:CA	3:D:599:HOH:O	2.58	0.42
1:D:75:ASN:HB2	1:D:104:PRO:HG3	2.01	0.42
1:B:197:LYS:HE3	1:B:198:GLU:OE1	2.20	0.42
1:A:23:PRO:HG2	1:A:63[B]:GLU:CB	2.49	0.42
1:A:176:GLU:O	1:A:176:GLU:HG3	2.19	0.42
1:C:118:LEU:HA	1:C:149:TYR:O	2.20	0.42
1:D:28:TYR:HE1	1:D:139:LEU:O	2.03	0.41
1:D:58:ILE:O	1:D:59:PRO:C	2.63	0.41
1:A:28:TYR:O	1:A:32[B]:ARG:HG2	2.20	0.41
1:A:38:ILE:HA	1:A:43:PRO:HD2	2.02	0.41
1:A:32[B]:ARG:CZ	1:A:32[B]:ARG:HB3	2.50	0.41
1:A:167[A]:ILE:H	1:A:167[A]:ILE:HG13	1.68	0.41
1:C:156:GLN:HB2	1:C:158:GLU:OE1	2.21	0.41
1:A:1:LYS:HB2	1:A:2:LEU:H	1.79	0.41
1:C:93:VAL:HG21	1:C:167[B]:ILE:CG1	2.51	0.41
1:D:171:ARG:NH2	3:D:526:HOH:O	2.43	0.41
1:A:37:TYR:CE2	1:A:58:ILE:HG22	2.55	0.41
1:D:70:LYS:HE3	1:D:198:GLU:CG	2.44	0.41
1:D:186:ARG:NH2	3:D:584:HOH:O	2.52	0.41
1:A:32[A]:ARG:HB3	1:A:32[A]:ARG:CZ	2.51	0.40
1:A:58:ILE:CD1	1:A:116:ILE:CD1	3.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:THR:HG22	1:A:174:LEU:HG	2.02	0.40
1:B:106:SER:OG	1:B:107:GLN:NE2	2.53	0.40
1:C:93:VAL:HG13	1:C:167[A]:ILE:HG21	2.03	0.40
1:C:151:ILE:HD12	1:C:152:SER:HB2	2.03	0.40
1:D:137:ASP:OD1	3:D:593:HOH:O	2.22	0.40
1:D:158:GLU:HB2	1:D:160:PHE:CE2	2.57	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	213/223 (96%)	205 (96%)	8 (4%)	0	100	100
1	B	211/223 (95%)	204 (97%)	7 (3%)	0	100	100
1	C	206/223 (92%)	199 (97%)	5 (2%)	2 (1%)	12	15
1	D	200/223 (90%)	197 (98%)	3 (2%)	0	100	100
All	All	830/892 (93%)	805 (97%)	23 (3%)	2 (0%)	48	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	24[A]	ARG
1	C	24[B]	ARG

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	197/203 (97%)	180 (91%)	17 (9%)	10	13
1	B	193/203 (95%)	166 (86%)	27 (14%)	3	3
1	C	185/203 (91%)	161 (87%)	24 (13%)	4	4
1	D	178/203 (88%)	158 (89%)	20 (11%)	6	7
All	All	753/812 (93%)	665 (88%)	88 (12%)	5	6

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	45	LEU
1	A	56[A]	ILE
1	A	56[B]	ILE
1	A	69	VAL
1	A	74	GLU
1	A	93	VAL
1	A	107	GLN
1	A	130	ILE
1	A	131	MSE
1	A	161	GLU
1	A	165	GLU
1	A	167[A]	ILE
1	A	167[B]	ILE
1	A	173	THR
1	A	176	GLU
1	A	201	ILE
1	B	11	ARG
1	B	14	VAL
1	B	44	THR
1	B	56[A]	ILE
1	B	56[B]	ILE
1	B	58	ILE
1	B	91	ILE
1	B	95	SER
1	B	107	GLN
1	B	110	LYS
1	B	122	GLU
1	B	134	CYS
1	B	135	LEU

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Mol	Chain	Res	Type
1	B	136	GLN
1	B	151	ILE
1	B	158	GLU
1	B	161[A]	GLU
1	B	161[B]	GLU
1	B	165	GLU
1	B	167	ILE
1	B	169	ILE
1	B	170	LEU
1	B	173	THR
1	B	174	LEU
1	B	184	LEU
1	B	197	LYS
1	B	198	GLU
1	C	0	SER
1	C	2	LEU
1	C	29	GLU
1	C	32	ARG
1	C	67	SER
1	C	76	GLU
1	C	77	LYS
1	C	80	LYS
1	C	89	GLU
1	C	93	VAL
1	C	100	LYS
1	C	101	ASP
1	C	107	GLN
1	C	112	LYS
1	C	135	LEU
1	C	136	GLN
1	C	141	ASP
1	C	167[A]	ILE
1	C	167[B]	ILE
1	C	176	GLU
1	C	186	ARG
1	C	192	SER
1	C	194	GLU
1	C	201	ILE
1	D	18	ARG
1	D	32	ARG
1	D	62	THR
1	D	69	VAL

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Mol	Chain	Res	Type
1	D	86	ARG
1	D	89	GLU
1	D	107	GLN
1	D	116	ILE
1	D	125	GLU
1	D	130	ILE
1	D	151	ILE
1	D	158	GLU
1	D	167	ILE
1	D	173	THR
1	D	175	ILE
1	D	176	GLU
1	D	177	GLU
1	D	188	LYS
1	D	190	LEU
1	D	194	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	B	107	GLN
1	D	60	ASN
1	D	157	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](#)

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	MES	C	504	-	12,12,12	2.08	1 (8%)	15,16,16	2.34	6 (40%)
2	MES	A	502	-	12,12,12	2.16	1 (8%)	15,16,16	2.47	7 (46%)
2	MES	B	503	-	12,12,12	2.43	1 (8%)	15,16,16	2.21	4 (26%)
2	MES	D	501	-	12,12,12	1.56	1 (8%)	15,16,16	2.48	4 (26%)

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	MES	C	504	-	-	1/6/14/14	0/1/1/1
2	MES	A	502	-	-	4/6/14/14	0/1/1/1
2	MES	B	503	-	-	4/6/14/14	0/1/1/1
2	MES	D	501	-	-	4/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	503	MES	C8-S	-7.84	1.66	1.77
2	C	504	MES	C8-S	-6.78	1.68	1.77
2	A	502	MES	C8-S	-6.74	1.68	1.77
2	D	501	MES	C8-S	-4.70	1.71	1.77

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	MES	C5-N4-C3	6.81	123.51	108.84
2	A	502	MES	C5-N4-C3	6.62	123.09	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	504	MES	C5-N4-C3	6.00	121.77	108.84
2	B	503	MES	C5-N4-C3	5.90	121.56	108.84
2	A	502	MES	O1S-S-C8	3.35	111.79	106.73
2	D	501	MES	C7-N4-C5	3.22	119.82	111.24
2	D	501	MES	O2S-S-C8	3.17	111.52	106.73
2	B	503	MES	C7-N4-C5	3.09	119.46	111.24
2	C	504	MES	C7-N4-C5	3.03	119.32	111.24
2	B	503	MES	C7-N4-C3	2.90	118.97	111.24
2	C	504	MES	C7-N4-C3	2.88	118.91	111.24
2	A	502	MES	C7-N4-C3	2.87	118.89	111.24
2	C	504	MES	O2S-S-C8	2.67	110.76	106.73
2	A	502	MES	C7-N4-C5	2.54	118.00	111.24
2	B	503	MES	O3S-S-C8	2.51	110.92	106.00
2	C	504	MES	C6-C5-N4	-2.49	106.34	110.12
2	D	501	MES	O3S-S-C8	2.47	110.84	106.00
2	A	502	MES	C6-C5-N4	2.38	113.74	110.12
2	A	502	MES	O2S-S-O1S	-2.33	106.24	113.82
2	A	502	MES	O2S-S-C8	2.22	110.08	106.73
2	C	504	MES	C2-C3-N4	2.20	113.47	110.12

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	MES	C7-C8-S-O1S
2	A	502	MES	C7-C8-S-O3S
2	B	503	MES	C8-C7-N4-C3
2	D	501	MES	C8-C7-N4-C3
2	D	501	MES	C7-C8-S-O2S
2	D	501	MES	C7-C8-S-O3S
2	B	503	MES	C7-C8-S-O3S
2	A	502	MES	C8-C7-N4-C3
2	C	504	MES	C8-C7-N4-C5
2	A	502	MES	C7-C8-S-O2S
2	B	503	MES	C7-C8-S-O2S
2	D	501	MES	C7-C8-S-O1S
2	B	503	MES	C7-C8-S-O1S

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	504	MES	2	0
2	B	503	MES	3	0
2	D	501	MES	1	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	202/223 (90%)	-1.47	0 100 100	8, 25, 41, 59	10 (4%)
1	B	202/223 (90%)	-1.48	0 100 100	9, 24, 38, 53	8 (3%)
1	C	202/223 (90%)	-1.45	0 100 100	9, 29, 46, 61	3 (1%)
1	D	200/223 (89%)	-1.44	0 100 100	16, 30, 44, 63	1 (0%)
All	All	806/892 (90%)	-1.46	0 100 100	8, 27, 44, 63	22 (2%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	MES	B	503	12/12	0.98	0.05	39,41,43,43	0
2	MES	A	502	12/12	0.99	0.03	31,37,49,50	0
2	MES	C	504	12/12	0.99	0.04	54,56,57,59	0
2	MES	D	501	12/12	0.99	0.03	36,38,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.