



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 04:51 AM EDT

PDB ID : 2QJM  
Title : Crystal structure of the K271E mutant of Mannonate dehydratase from Novosphingobium aromaticivorans complexed with Mg and D-mannonate  
Authors : Fedorov, A.A.; Fedorov, E.V.; Rakus, J.F.; Vick, J.E.; Gerlt, J.A.; Almo, S.C.  
Deposited on : 2007-07-08  
Resolution : 2.20 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

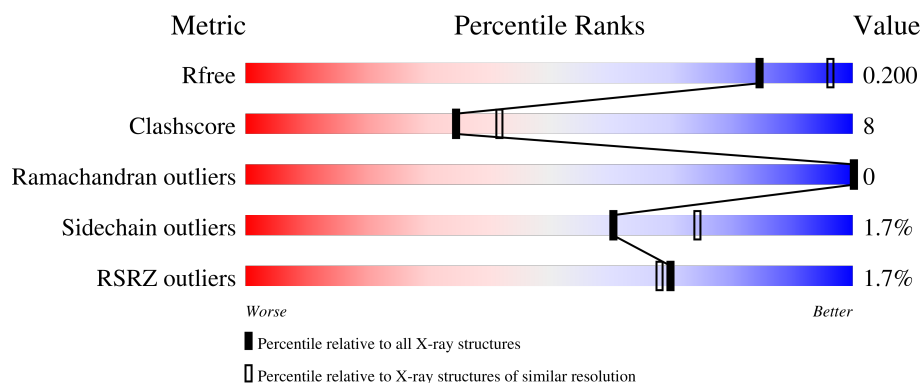
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	402	<div> <div>0%</div> <div>79%</div> <div>16%</div> <div>.</div> </div>
1	B	402	<div> <div>0%</div> <div>80%</div> <div>15%</div> <div>.</div> </div>
1	C	402	<div> <div>2%</div> <div>76%</div> <div>19%</div> <div>.</div> </div>
1	D	402	<div> <div>2%</div> <div>78%</div> <div>17%</div> <div>..</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12923 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 Mandelate racemase/muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3053	1951	528	557	17			
1	B	385	Total	C	N	O	S	0	0	0
			3058	1954	529	558	17			
1	C	384	Total	C	N	O	S	0	0	0
			3053	1951	528	557	17			
1	D	385	Total	C	N	O	S	0	0	0
			3058	1954	529	558	17			

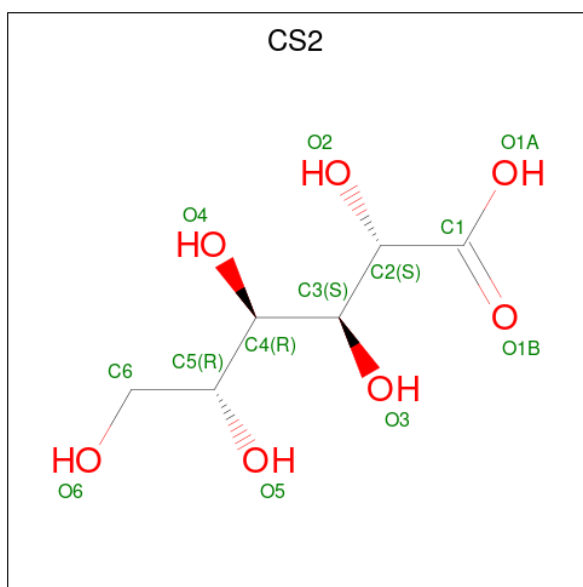
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	GLU	LYS	engineered mutation	UNP A4XF23
B	271	GLU	LYS	engineered mutation	UNP A4XF23
C	271	GLU	LYS	engineered mutation	UNP A4XF23
D	271	GLU	LYS	engineered mutation	UNP A4XF23

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is D-MANNONIC ACID (three-letter code: CS2) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		

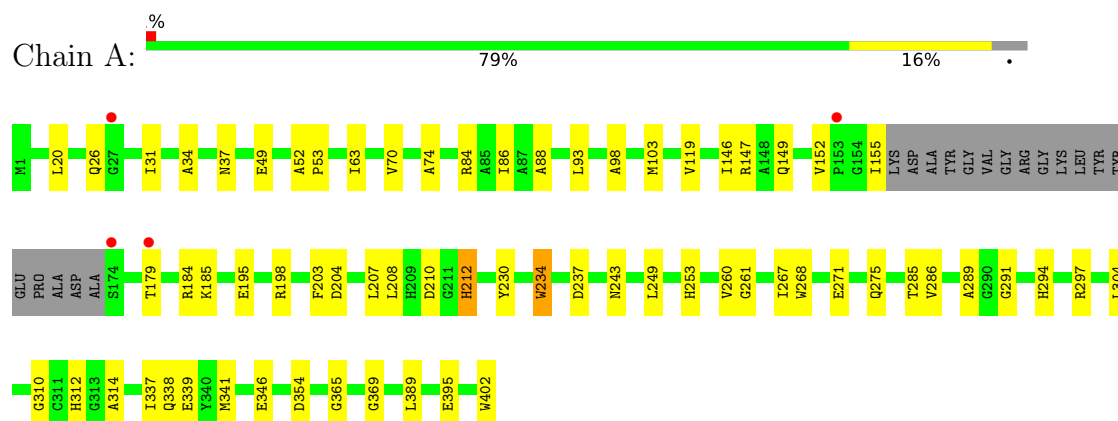
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	164	Total	O	0	0
			164	164		
4	B	177	Total	O	0	0
			177	177		
4	C	159	Total	O	0	0
			159	159		
4	D	145	Total	O	0	0
			145	145		

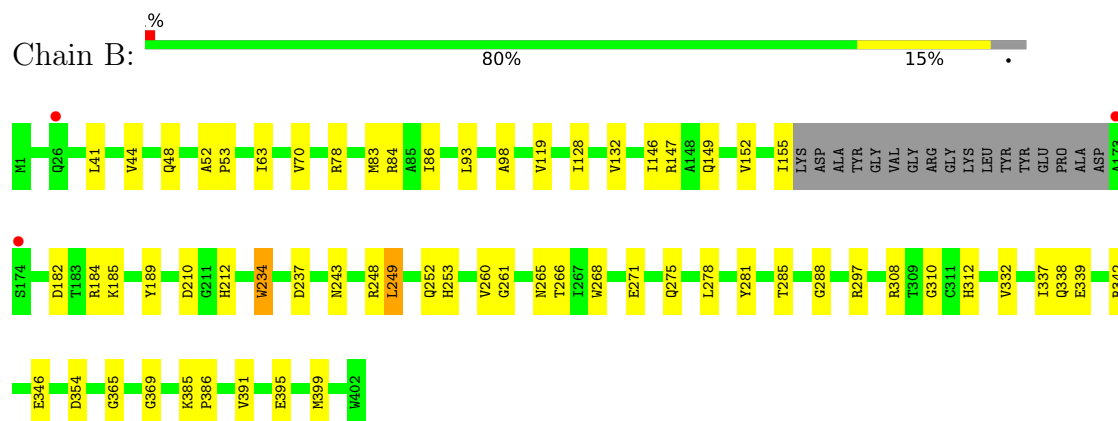
### 3 Residue-property plots

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.

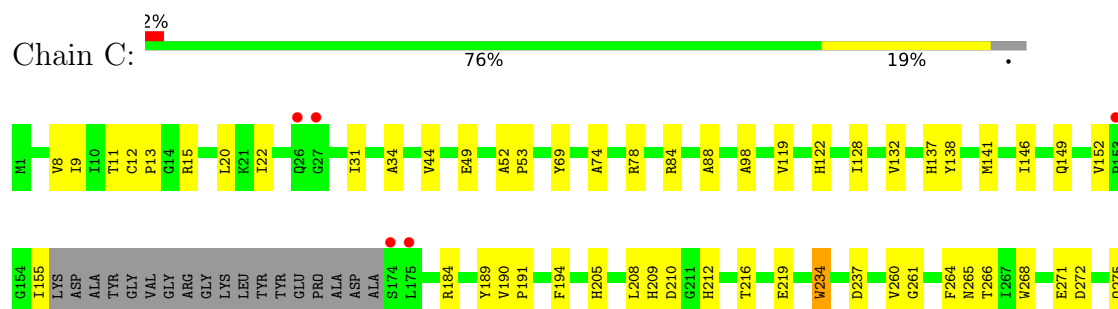
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

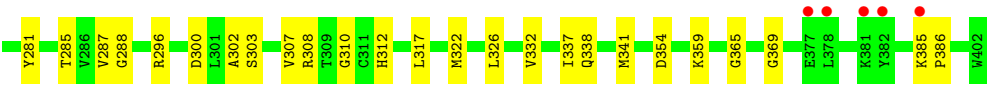


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

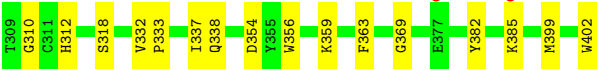
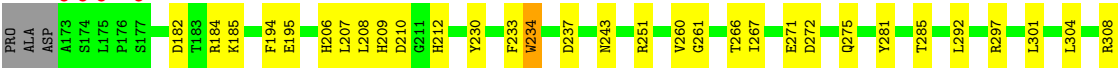
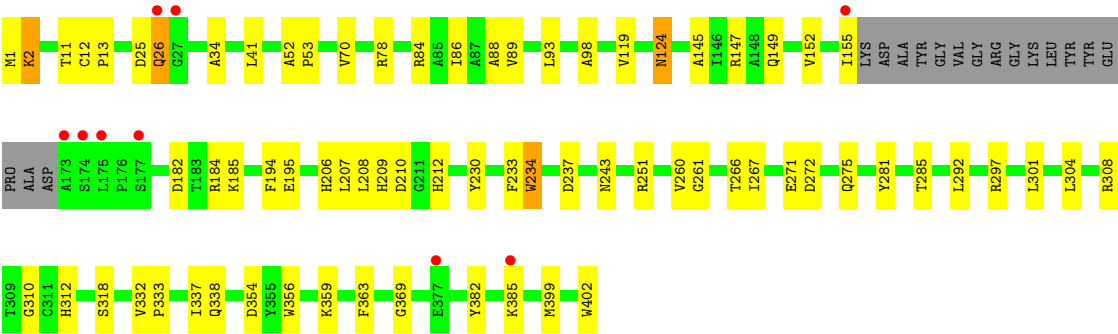
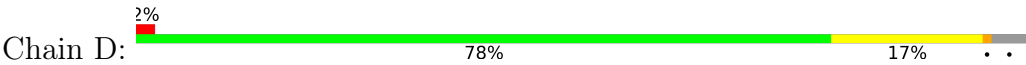


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme





● Molecule 1: Mandelate racemase/muconate lactonizing enzyme



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.25Å 165.31Å 166.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 38.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (25.00-2.20) 96.3 (38.20-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.76 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.168 , 0.206 0.165 , 0.200	Depositor DCC
$R_{free}$ test set	4089 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 45.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12923	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, CS2

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	0.33	0/3136	0.61	0/4267
1	B	0.33	0/3141	0.61	0/4274
1	C	0.31	0/3136	0.59	0/4267
1	D	0.32	0/3141	0.60	0/4274
All	All	0.32	0/12554	0.61	0/17082

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3053	0	2966	57	0
1	B	3058	0	2971	47	0
1	C	3053	0	2966	54	1
1	D	3058	0	2971	58	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	13	0	11	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	11	2	0
3	C	13	0	11	2	0
3	D	13	0	11	0	0
4	A	164	0	0	5	0
4	B	177	0	0	3	0
4	C	159	0	0	2	0
4	D	145	0	0	1	0
All	All	12923	0	11918	201	1

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 8.

All (201) 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:149:GLN:HE22	1:A:210:ASP:H	1.11	0.99
1:B:149:GLN:HE22	1:B:210:ASP:H	1.05	0.95
1:C:149:GLN:HE22	1:C:210:ASP:H	1.08	0.94
1:D:149:GLN:HE22	1:D:210:ASP:H	1.16	0.93
1:A:275:GLN:HE21	1:D:275:GLN:HE21	1.15	0.92
1:A:275:GLN:HE21	1:D:275:GLN:NE2	1.67	0.92
1:C:98:ALA:HB3	1:C:369:GLY:HA2	1.62	0.81
1:A:267:ILE:HD13	1:D:304:LEU:HD21	1.63	0.81
1:A:304:LEU:HD21	1:D:267:ILE:HD13	1.65	0.76
1:A:52:ALA:HB3	1:A:53:PRO:HD3	1.72	0.72
1:C:138:TYR:HA	1:C:141:MET:HE3	1.74	0.70
1:D:52:ALA:HB3	1:D:53:PRO:HD3	1.73	0.70
1:A:98:ALA:HB3	1:A:369:GLY:HA2	1.75	0.69
1:C:152:VAL:HB	1:C:155:ILE:HD12	1.75	0.69
1:D:98:ALA:HB3	1:D:369:GLY:HA2	1.75	0.69
1:C:52:ALA:HB3	1:C:53:PRO:HD3	1.78	0.66
1:A:268:TRP:CZ3	1:B:243:ASN:HB2	2.31	0.65
1:D:2:LYS:HB3	1:D:2:LYS:NZ	2.13	0.64
1:B:98:ALA:HB3	1:B:369:GLY:HA2	1.81	0.62
1:B:249:LEU:HB2	4:B:2084:HOH:O	2.00	0.61
1:B:149:GLN:NE2	1:B:210:ASP:H	1.88	0.61
1:C:271:GLU:HG3	1:C:272:ASP:N	2.16	0.60
1:D:124:ASN:C	1:D:124:ASN:HD22	2.04	0.60
1:A:285:THR:CG2	1:A:312:HIS:HB3	2.32	0.58
1:C:268:TRP:CZ3	1:D:243:ASN:HB2	2.39	0.58
1:B:312:HIS:HE1	3:B:2002:CS2:H3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ASN:HB2	1:B:268:TRP:CZ3	2.39	0.58
1:B:152:VAL:HB	1:B:155:ILE:HD12	1.86	0.58
1:C:149:GLN:NE2	1:C:210:ASP:H	1.91	0.57
1:B:395:GLU:HG3	4:B:2127:HOH:O	2.04	0.57
1:B:78:ARG:HG2	1:B:266:THR:HG21	1.87	0.57
1:B:70:VAL:CG1	1:B:86:ILE:HG12	2.35	0.57
1:D:152:VAL:HB	1:D:155:ILE:HD12	1.86	0.57
1:A:198:ARG:NH1	1:A:203:PHE:HA	2.20	0.57
1:A:275:GLN:NE2	1:D:275:GLN:HE21	1.93	0.56
1:B:184:ARG:O	1:B:184:ARG:HD3	2.06	0.56
1:B:52:ALA:HB3	1:B:53:PRO:HD3	1.88	0.56
1:D:149:GLN:NE2	1:D:210:ASP:H	1.96	0.56
1:D:208:LEU:HD12	1:D:208:LEU:N	2.21	0.56
1:A:149:GLN:NE2	1:A:210:ASP:H	1.93	0.56
1:C:359:LYS:HB3	4:C:2111:HOH:O	2.05	0.56
1:C:146:ILE:HD12	1:C:146:ILE:N	2.22	0.55
1:C:69:TYR:HA	1:D:399:MET:CE	2.37	0.55
1:A:147:ARG:HG2	1:A:149:GLN:HE21	1.71	0.54
1:D:2:LYS:HG2	1:D:25:ASP:OD2	2.07	0.54
1:C:9:ILE:N	1:C:9:ILE:HD12	2.23	0.54
1:A:152:VAL:HB	1:A:155:ILE:HG13	1.90	0.54
1:A:70:VAL:CG1	1:A:86:ILE:HG12	2.38	0.53
1:B:354:ASP:CG	1:B:365:GLY:HA3	2.29	0.53
1:B:271:GLU:HG2	1:B:275:GLN:OE1	2.08	0.53
1:A:354:ASP:CG	1:A:365:GLY:HA3	2.30	0.53
1:A:49:GLU:HB3	1:B:41:LEU:HD12	1.91	0.52
1:C:49:GLU:HB3	1:D:41:LEU:HD12	1.90	0.52
1:C:234:TRP:C	1:C:234:TRP:CD1	2.83	0.52
1:C:312:HIS:HE1	3:C:2003:CS2:H3	1.74	0.52
1:B:285:THR:CG2	1:B:312:HIS:HB3	2.39	0.52
1:B:70:VAL:HG12	1:B:86:ILE:HG12	1.92	0.52
1:A:70:VAL:HG12	1:A:86:ILE:HG12	1.92	0.51
1:D:147:ARG:HG2	1:D:149:GLN:HE21	1.76	0.51
1:A:346:GLU:H	1:A:346:GLU:CD	2.14	0.51
1:D:34:ALA:HB2	1:D:88:ALA:HB2	1.92	0.51
1:A:297:ARG:NH1	4:A:2097:HOH:O	2.43	0.51
1:A:34:ALA:HB2	1:A:88:ALA:HB2	1.92	0.51
1:B:149:GLN:HE22	1:B:210:ASP:N	1.89	0.51
1:B:310:GLY:HA2	1:B:337:ILE:O	2.11	0.51
1:C:78:ARG:HG2	1:C:266:THR:HG21	1.92	0.51
1:D:237:ASP:OD1	1:D:260:VAL:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:O	1:A:31:ILE:HA	2.11	0.50
1:D:70:VAL:HG12	1:D:86:ILE:HG12	1.92	0.50
1:D:2:LYS:HB3	1:D:2:LYS:HZ3	1.77	0.50
1:B:297:ARG:HG2	1:B:297:ARG:HH11	1.76	0.49
1:A:275:GLN:NE2	1:D:275:GLN:NE2	2.48	0.49
1:C:271:GLU:HG3	1:C:272:ASP:H	1.78	0.49
1:C:34:ALA:HB2	1:C:88:ALA:HB2	1.95	0.49
1:A:249:LEU:HD13	1:A:249:LEU:O	2.13	0.49
1:D:207:LEU:C	1:D:208:LEU:HD12	2.33	0.49
1:B:385:LYS:HD2	1:B:386:PRO:HD2	1.95	0.49
1:D:12:CYS:SG	1:D:385:LYS:HE3	2.53	0.49
1:D:194:PHE:CZ	1:D:209:HIS:HB2	2.47	0.49
1:A:234:TRP:C	1:A:234:TRP:CD1	2.86	0.48
1:A:286:VAL:HG13	1:A:291:GLY:HA2	1.95	0.48
1:D:78:ARG:HG2	1:D:266:THR:HG21	1.95	0.48
1:B:237:ASP:OD1	1:B:260:VAL:HA	2.13	0.48
1:D:119:VAL:HA	1:D:338:GLN:O	2.13	0.48
1:C:128:ILE:HG13	1:C:189:TYR:CZ	2.49	0.48
1:B:146:ILE:HD12	1:B:146:ILE:N	2.29	0.48
1:C:194:PHE:CZ	1:C:209:HIS:HB2	2.48	0.48
1:C:285:THR:CG2	1:C:312:HIS:HB3	2.44	0.48
1:C:302:ALA:HB1	1:C:307:VAL:HB	1.94	0.47
1:A:179:THR:HG21	4:A:2124:HOH:O	2.14	0.47
1:C:296:ARG:NH2	4:C:2131:HOH:O	2.48	0.47
1:B:44:VAL:O	1:B:48:GLN:HB2	2.14	0.47
1:B:234:TRP:C	1:B:234:TRP:CD1	2.88	0.47
1:B:249:LEU:HD11	1:D:251:ARG:CZ	2.45	0.47
1:D:260:VAL:HG22	1:D:261:GLY:N	2.29	0.47
1:A:354:ASP:OD2	1:A:365:GLY:HA3	2.14	0.47
1:B:63:ILE:HG12	1:B:93:LEU:HB3	1.97	0.47
1:B:281:TYR:HA	1:B:308:ARG:O	2.15	0.47
1:C:354:ASP:CG	1:C:365:GLY:HA3	2.34	0.47
1:A:26:GLN:CD	1:A:26:GLN:O	2.54	0.46
1:A:155:ILE:HD11	1:A:185:LYS:HB2	1.97	0.46
1:D:70:VAL:CG1	1:D:86:ILE:HG12	2.45	0.46
1:D:281:TYR:HA	1:D:308:ARG:O	2.14	0.46
1:A:285:THR:HG23	1:A:312:HIS:HB3	1.97	0.46
1:D:124:ASN:HA	1:D:149:GLN:O	2.15	0.46
1:C:20:LEU:HD21	1:C:22:ILE:HD11	1.97	0.46
1:A:37:ASN:ND2	1:A:389:LEU:HD21	2.30	0.46
1:C:8:VAL:HG11	1:C:44:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:VAL:HA	1:B:338:GLN:O	2.16	0.46
1:D:234:TRP:CD1	1:D:234:TRP:C	2.89	0.45
1:D:297:ARG:HG3	1:D:297:ARG:HH11	1.80	0.45
1:C:74:ALA:HB2	4:D:2051:HOH:O	2.16	0.45
1:D:182:ASP:OD2	1:D:185:LYS:HG3	2.16	0.45
1:A:208:LEU:HD12	1:A:208:LEU:N	2.32	0.45
1:D:310:GLY:HA2	1:D:337:ILE:O	2.17	0.45
1:B:182:ASP:OD2	1:B:185:LYS:HG3	2.17	0.45
1:B:248:ARG:HE	1:B:278:LEU:HD21	1.81	0.45
1:A:312:HIS:HE1	3:A:2001:CS2:H3	1.81	0.45
1:C:237:ASP:OD1	1:C:260:VAL:HA	2.16	0.45
1:A:253:HIS:HD2	4:A:2066:HOH:O	1.99	0.44
1:A:310:GLY:HA2	1:A:337:ILE:O	2.16	0.44
1:B:265:ASN:HA	1:B:288:GLY:O	2.17	0.44
1:C:261:GLY:HA2	1:C:264:PHE:CD2	2.51	0.44
1:B:260:VAL:HG22	1:B:261:GLY:N	2.32	0.44
1:D:212:HIS:ND1	1:D:402:TRP:OXT	2.46	0.44
1:A:152:VAL:HB	1:A:155:ILE:CG1	2.47	0.44
1:B:83:MET:HG3	1:B:265:ASN:HB2	1.99	0.44
1:B:285:THR:HG23	1:B:312:HIS:HB3	1.99	0.44
1:C:119:VAL:HA	1:C:338:GLN:O	2.18	0.44
1:D:285:THR:CG2	1:D:312:HIS:HB3	2.48	0.44
1:A:119:VAL:HA	1:A:338:GLN:O	2.18	0.44
1:C:208:LEU:N	1:C:208:LEU:HD12	2.33	0.44
1:C:122:HIS:CE1	1:C:341:MET:HG3	2.52	0.44
1:A:74:ALA:HB2	4:A:2032:HOH:O	2.17	0.43
1:A:184:ARG:O	1:A:184:ARG:HD3	2.17	0.43
1:A:195:GLU:HB2	1:A:230:TYR:CZ	2.53	0.43
1:C:281:TYR:HA	1:C:308:ARG:O	2.19	0.43
1:D:89:VAL:O	1:D:93:LEU:HG	2.19	0.43
1:B:128:ILE:HG13	1:B:189:TYR:CZ	2.53	0.43
1:C:322:MET:O	1:C:326:LEU:HG	2.19	0.43
1:B:128:ILE:O	1:B:132:VAL:HG23	2.18	0.43
1:D:195:GLU:HA	1:D:230:TYR:CE1	2.53	0.43
1:C:12:CYS:HA	1:C:15:ARG:O	2.19	0.43
1:C:137:HIS:O	1:C:141:MET:HG3	2.18	0.43
1:C:312:HIS:CE1	3:C:2003:CS2:H3	2.52	0.43
1:A:212:HIS:ND1	1:A:402:TRP:OXT	2.51	0.43
1:B:249:LEU:HD11	1:D:251:ARG:NH2	2.33	0.43
1:C:184:ARG:O	1:C:184:ARG:HD3	2.19	0.43
1:D:184:ARG:O	1:D:184:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:VAL:HB	1:B:399:MET:CE	2.49	0.42
1:B:342:ARG:HH11	1:B:342:ARG:HG3	1.84	0.42
1:A:195:GLU:HA	1:A:230:TYR:CE1	2.54	0.42
1:D:354:ASP:OD2	1:D:354:ASP:C	2.58	0.42
1:C:11:THR:OG1	1:C:13:PRO:HD3	2.20	0.42
1:C:285:THR:HG23	1:C:312:HIS:HB3	2.01	0.42
1:C:332:VAL:O	1:C:332:VAL:HG13	2.19	0.42
1:D:292:LEU:HD22	1:D:292:LEU:H	1.84	0.42
1:D:292:LEU:HD22	1:D:292:LEU:N	2.35	0.42
1:C:8:VAL:C	1:C:9:ILE:HD12	2.40	0.42
1:A:346:GLU:CD	1:A:346:GLU:N	2.72	0.42
1:A:63:ILE:HG12	1:A:93:LEU:HB3	2.01	0.42
1:C:260:VAL:HG22	1:C:261:GLY:N	2.34	0.42
1:A:237:ASP:OD1	1:A:260:VAL:HA	2.18	0.42
1:C:128:ILE:O	1:C:132:VAL:HG23	2.20	0.42
1:C:149:GLN:HE22	1:C:210:ASP:N	1.92	0.42
1:A:207:LEU:C	1:A:208:LEU:HD12	2.41	0.42
1:A:249:LEU:HD13	1:A:249:LEU:C	2.40	0.42
1:A:339:GLU:OE2	3:A:2001:CS2:O1A	2.38	0.42
1:B:339:GLU:OE2	3:B:2002:CS2:O1A	2.37	0.42
1:C:20:LEU:O	1:C:31:ILE:HA	2.20	0.42
1:C:190:VAL:HB	1:C:191:PRO:HD3	2.01	0.42
1:C:265:ASN:HA	1:C:288:GLY:O	2.19	0.42
1:D:1:MET:HB3	1:D:26:GLN:NE2	2.35	0.42
1:D:208:LEU:HG	1:D:233:PHE:HB3	2.01	0.42
1:D:208:LEU:HD23	1:D:234:TRP:CE2	2.55	0.42
1:A:289:ALA:O	1:A:294:HIS:HB3	2.19	0.41
1:C:385:LYS:HA	1:C:386:PRO:HD2	1.91	0.41
1:C:287:VAL:HG11	1:C:317:LEU:HG	2.02	0.41
1:C:310:GLY:HA2	1:C:337:ILE:O	2.20	0.41
1:B:83:MET:CG	1:B:265:ASN:HB2	2.50	0.41
1:B:147:ARG:HG2	1:B:149:GLN:HE21	1.85	0.41
1:D:332:VAL:O	1:D:332:VAL:HG13	2.20	0.41
1:A:149:GLN:HE22	1:A:210:ASP:N	1.95	0.41
1:D:359:LYS:O	1:D:359:LYS:HG2	2.20	0.41
1:A:304:LEU:HD11	1:D:301:LEU:HD22	2.03	0.41
1:A:314:ALA:HA	1:A:341:MET:SD	2.61	0.41
1:A:395:GLU:HG3	4:A:2071:HOH:O	2.20	0.41
1:C:234:TRP:C	1:C:234:TRP:HD1	2.24	0.41
1:C:300:ASP:O	1:C:303:SER:HB3	2.21	0.41
1:A:146:ILE:HD12	1:A:146:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:VAL:HG22	1:A:261:GLY:N	2.35	0.41
1:D:356:TRP:CE2	1:D:363:PHE:HB2	2.56	0.41
1:B:253:HIS:HD2	4:B:2136:HOH:O	2.03	0.41
1:D:271:GLU:HG3	1:D:272:ASP:H	1.86	0.41
1:D:11:THR:OG1	1:D:13:PRO:HD3	2.21	0.40
1:D:145:ALA:HA	1:D:206:HIS:HB2	2.03	0.40
1:D:332:VAL:HA	1:D:333:PRO:HD2	1.98	0.40
1:B:332:VAL:O	1:B:332:VAL:HG13	2.20	0.40
1:B:346:GLU:H	1:B:346:GLU:CD	2.24	0.40
1:D:13:PRO:HB3	1:D:382:TYR:CD2	2.57	0.40
1:C:216:THR:OG1	1:C:219:GLU:HG3	2.21	0.40

All (1) 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:C:275:GLN:NE2	1:C:275:GLN:NE2[3_555]	2.09	0.11

## 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	380/402 (94%)	360 (95%)	20 (5%)	0	100	100
1	B	381/402 (95%)	363 (95%)	18 (5%)	0	100	100
1	C	380/402 (94%)	359 (94%)	21 (6%)	0	100	100
1	D	381/402 (95%)	360 (94%)	21 (6%)	0	100	100
All	All	1522/1608 (95%)	1442 (95%)	80 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	314/326 (96%)	308 (98%)	6 (2%)	57	71
1	B	314/326 (96%)	309 (98%)	5 (2%)	62	76
1	C	314/326 (96%)	310 (99%)	4 (1%)	69	81
1	D	314/326 (96%)	308 (98%)	6 (2%)	57	71
All	All	1256/1304 (96%)	1235 (98%)	21 (2%)	60	74

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	103	MET
1	A	204	ASP
1	A	212	HIS
1	A	234	TRP
1	A	271	GLU
1	B	84	ARG
1	B	212	HIS
1	B	234	TRP
1	B	249	LEU
1	B	252	GLN
1	C	84	ARG
1	C	205	HIS
1	C	212	HIS
1	C	234	TRP
1	D	2	LYS
1	D	26	GLN
1	D	84	ARG
1	D	124	ASN
1	D	234	TRP
1	D	318	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
1	A	149	GLN
1	A	253	HIS
1	A	312	HIS
1	A	338	GLN
1	A	343	HIS
1	B	149	GLN
1	B	252	GLN
1	B	253	HIS
1	B	312	HIS
1	B	343	HIS
1	C	149	GLN
1	C	312	HIS
1	C	343	HIS
1	D	124	ASN
1	D	149	GLN
1	D	253	HIS
1	D	275	GLN
1	D	312	HIS
1	D	343	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z  > 2$
3	CS2	D	2004	2	9,12,12	0.74	0	12,16,16	0.85	0
3	CS2	B	2002	2	9,12,12	0.90	0	12,16,16	0.96	1 (8%)
3	CS2	C	2003	2	9,12,12	0.88	0	12,16,16	0.98	1 (8%)
3	CS2	A	2001	2	9,12,12	0.83	0	12,16,16	0.90	1 (8%)

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
3	CS2	D	2004	2	-	4/14/18/18	-
3	CS2	B	2002	2	-	4/14/18/18	-
3	CS2	C	2003	2	-	0/14/18/18	-
3	CS2	A	2001	2	-	4/14/18/18	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2003	CS2	C4-C3-C2	2.20	117.45	113.58
3	A	2001	CS2	C4-C3-C2	2.11	117.31	113.58
3	B	2002	CS2	C4-C3-C2	2.11	117.31	113.58

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	CS2	C1-C2-C3-C4
3	A	2001	CS2	O2-C2-C3-C4
3	B	2002	CS2	C1-C2-C3-C4
3	B	2002	CS2	O2-C2-C3-C4
3	A	2001	CS2	O2-C2-C3-O3
3	B	2002	CS2	O2-C2-C3-O3
3	D	2004	CS2	O2-C2-C3-C4
3	D	2004	CS2	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	2001	CS2	C1-C2-C3-O3
3	B	2002	CS2	C1-C2-C3-O3
3	D	2004	CS2	C1-C2-C3-C4
3	D	2004	CS2	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2002	CS2	2	0
3	C	2003	CS2	2	0
3	A	2001	CS2	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	384/402 (95%)	-0.40	4 (1%) 82 81	17, 25, 39, 51	0
1	B	385/402 (95%)	-0.48	3 (0%) 86 85	16, 24, 38, 53	0
1	C	384/402 (95%)	-0.23	10 (2%) 56 53	20, 30, 45, 55	0
1	D	385/402 (95%)	-0.31	9 (2%) 60 58	18, 29, 44, 57	0
All	All	1538/1608 (95%)	-0.35	26 (1%) 70 68	16, 27, 42, 57	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	173	ALA	4.8
1	A	174	SER	4.6
1	D	174	SER	3.4
1	C	174	SER	3.3
1	B	26	GLN	3.2
1	C	381	LYS	3.2
1	B	173	ALA	3.1
1	C	377	GLU	3.1
1	C	27	GLY	3.0
1	B	174	SER	2.9
1	A	153	PRO	2.9
1	C	26	GLN	2.7
1	D	377	GLU	2.6
1	C	175	LEU	2.6
1	C	385	LYS	2.6
1	D	26	GLN	2.6
1	A	27	GLY	2.5
1	D	155	ILE	2.5
1	D	385	LYS	2.5
1	D	175	LEU	2.5
1	C	382	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	179	THR	2.2
1	C	378	LEU	2.2
1	D	27	GLY	2.2
1	C	153	PRO	2.2
1	D	177	SER	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 monosaccharides 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, 95<sup>th</sup> 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	MG	C	1003	1/1	0.85	0.24	31,31,31,31	0
3	CS2	C	2003	13/13	0.91	0.14	30,35,36,40	0
2	MG	D	1004	1/1	0.93	0.17	33,33,33,33	0
3	CS2	B	2002	13/13	0.93	0.12	23,26,30,30	0
2	MG	B	1002	1/1	0.93	0.17	26,26,26,26	0
3	CS2	D	2004	13/13	0.93	0.10	28,30,33,34	0
3	CS2	A	2001	13/13	0.94	0.10	24,26,30,30	0
2	MG	A	1001	1/1	0.97	0.24	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.