



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 11:21 AM BST

PDB ID : 3DES  
Title : Crystal structure of dipeptide epimerase from *Thermotoga maritima* complexed with L-Ala-L-Phe dipeptide  
Authors : Fedorov, A.A.; Fedorov, E.V.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.  
Deposited on : 2008-06-10  
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](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 : 2.14.4.dev1  
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) : 2.14.4.dev1

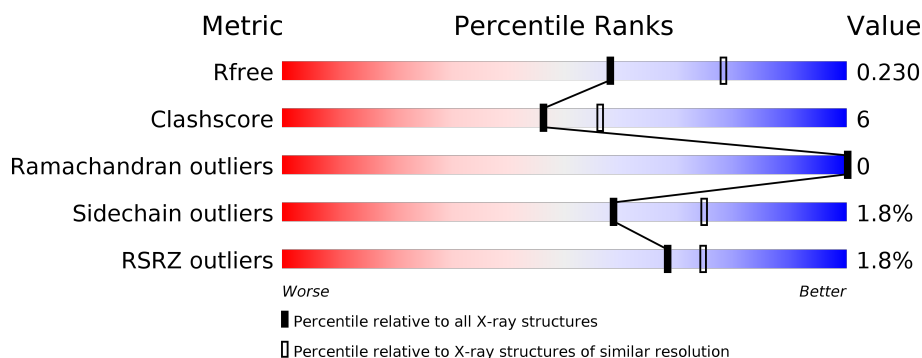
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 on 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	345	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 0%, yellow 12%, green 86%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>86%</span> <span>12%</span> <span>..</span> </div> </div>
1	B	345	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 0%, yellow 14%, green 84%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>84%</span> <span>14%</span> <span>..</span> </div> </div>
1	C	345	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 0%, yellow 14%, green 84%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>84%</span> <span>14%</span> <span>..</span> </div> </div>
1	D	345	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 0%, yellow 12%, green 85%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>85%</span> <span>12%</span> <span>..</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11266 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 Muconate cycloisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2687	1705	461	511	10			
1	B	341	Total	C	N	O	S	0	0	0
			2687	1705	461	511	10			
1	C	341	Total	C	N	O	S	0	0	0
			2687	1705	461	511	10			
1	D	341	Total	C	N	O	S	0	0	0
			2687	1705	461	511	10			

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

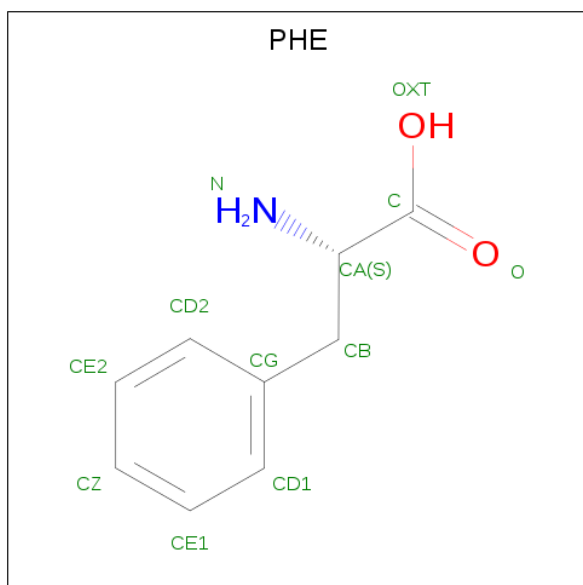
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ALANINE (three-letter code: ALA) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	3	1	1		
3	B	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	D	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 4 is PHENYLALANINE (three-letter code: PHE) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>).

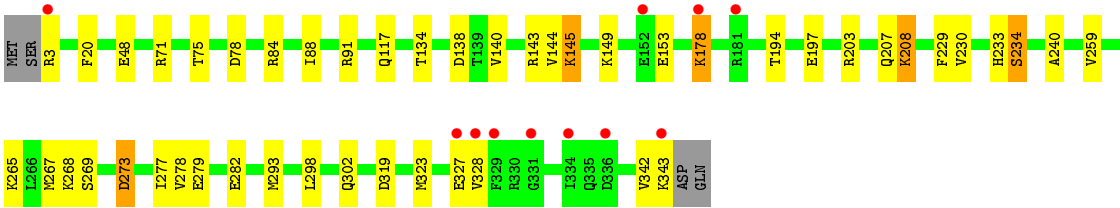


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	9	1	2		
4	B	1	Total	C	N	O	0	0
			12	9	1	2		
4	C	1	Total	C	N	O	0	0
			12	9	1	2		
4	D	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	112	Total	O	0	0
			112	112		
5	B	111	Total	O	0	0
			111	111		
5	C	125	Total	O	0	0
			125	125		
5	D	98	Total	O	0	0
			98	98		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	191.67Å 191.67Å 283.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.92 – 2.30 39.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.92-2.30) 99.9 (39.82-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.213 , 0.231 0.212 , 0.230	Depositor DCC
$R_{free}$ test set	6793 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.8	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 37.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11266	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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

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	0.35	0/2726	0.61	0/3662
1	B	0.34	0/2726	0.61	0/3662
1	C	0.36	0/2726	0.63	0/3662
1	D	0.34	0/2726	0.61	0/3662
All	All	0.35	0/10904	0.62	0/14648

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	2687	0	2723	32	0
1	B	2687	0	2723	37	0
1	C	2687	0	2723	35	0
1	D	2687	0	2723	33	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	5	0	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	4	1	0
3	C	5	0	4	0	0
3	D	5	0	4	1	0
4	A	12	0	9	2	0
4	B	12	0	9	1	0
4	C	12	0	9	0	0
4	D	12	0	9	2	0
5	A	112	0	0	0	0
5	B	111	0	0	3	0
5	C	125	0	0	1	0
5	D	98	0	0	0	0
All	All	11266	0	10944	137	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (137) 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:B:71:ARG:O	1:B:75:THR:HG23	1.85	0.77
1:B:31:ARG:HG3	1:B:31:ARG:HH11	1.52	0.72
1:C:31:ARG:HG3	1:C:31:ARG:HH11	1.55	0.70
1:B:149:LYS:O	1:B:153:GLU:HG3	1.93	0.67
1:B:230:VAL:O	1:B:234:SER:HB3	1.95	0.67
1:D:230:VAL:O	1:D:234:SER:HB3	1.95	0.66
1:D:265:LYS:HB2	1:D:268:LYS:HE2	1.77	0.65
1:D:208:LYS:HE3	1:D:208:LYS:HA	1.78	0.64
1:C:149:LYS:O	1:C:153:GLU:HG3	1.97	0.64
1:A:204:ALA:O	1:A:208:LYS:HE2	1.97	0.63
1:C:138:ASP:O	1:C:143:ARG:HD2	1.98	0.63
1:A:265:LYS:HB2	1:A:268:LYS:HE2	1.82	0.61
1:B:174:GLU:OE1	1:B:208:LYS:HG3	2.01	0.60
1:B:300:ILE:HD11	1:B:320:SER:HB3	1.84	0.60
1:D:134:THR:HG1	3:D:411:ALA:N	1.98	0.60
1:B:225:GLU:HG3	5:B:437:HOH:O	2.02	0.60
1:B:90:ASP:OD1	1:B:99:LYS:HE3	2.01	0.60
1:D:278:VAL:O	1:D:282:GLU:HG3	2.02	0.59
1:C:3:ARG:HA	1:C:78:ASP:HA	1.83	0.58
1:B:194:THR:OG1	1:B:197:GLU:HG3	2.03	0.58
1:C:48:GLU:H	1:C:302:GLN:NE2	2.01	0.58
1:C:333:PHE:N	1:C:343:LYS:HE3	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ARG:HB3	1:A:181:ARG:NH1	2.20	0.57
1:D:203:ARG:O	1:D:207:GLN:HG2	2.04	0.56
1:B:295:GLU:HB2	1:B:300:ILE:HD12	1.87	0.56
1:C:229:PHE:O	1:C:233:HIS:HD2	1.89	0.56
1:B:31:ARG:NH1	1:B:31:ARG:HG3	2.21	0.55
1:A:7:VAL:HG21	1:A:74:ILE:HD11	1.89	0.55
1:A:129:ILE:HG13	1:A:340:MET:HE3	1.89	0.54
1:D:279:GLU:HA	1:D:279:GLU:OE1	2.08	0.54
1:C:343:LYS:H	1:C:343:LYS:HD2	1.73	0.54
1:B:104:PHE:CD2	1:B:302:GLN:HG2	2.42	0.54
1:C:278:VAL:O	1:C:282:GLU:HG3	2.08	0.54
1:A:229:PHE:O	1:A:233:HIS:HD2	1.91	0.53
1:D:138:ASP:O	1:D:143:ARG:HD2	2.08	0.53
1:B:251:MET:HE2	1:B:255:LYS:HE3	1.91	0.53
1:D:194:THR:OG1	1:D:197:GLU:HG3	2.09	0.53
1:D:48:GLU:H	1:D:302:GLN:NE2	2.06	0.52
1:A:265:LYS:HZ3	4:A:412:PHE:HA	1.73	0.52
1:C:230:VAL:O	1:C:234:SER:HB3	2.09	0.52
1:A:138:ASP:O	1:A:143:ARG:HD2	2.10	0.52
1:A:336:ASP:HB3	1:A:341:ARG:HH22	1.75	0.52
1:B:75:THR:HG21	5:B:432:HOH:O	2.09	0.52
1:A:90:ASP:OD1	1:A:99:LYS:HE3	2.09	0.51
1:B:295:GLU:HB2	1:B:300:ILE:CD1	2.40	0.51
1:A:31:ARG:HG3	1:A:31:ARG:HH11	1.76	0.51
1:C:225:GLU:HG3	5:C:525:HOH:O	2.11	0.50
1:D:178:LYS:HB3	1:D:178:LYS:NZ	2.25	0.50
1:A:278:VAL:O	1:A:282:GLU:HG3	2.10	0.50
1:C:265:LYS:HB2	1:C:268:LYS:HE2	1.94	0.49
1:C:343:LYS:N	1:C:343:LYS:HD2	2.26	0.49
1:D:229:PHE:O	1:D:233:HIS:HD2	1.96	0.48
1:C:321:HIS:NE2	1:C:335:GLN:NE2	2.59	0.48
1:D:208:LYS:CA	1:D:208:LYS:HE3	2.42	0.48
1:D:269:SER:HB3	1:D:273:ASP:HB2	1.94	0.48
1:D:3:ARG:HA	1:D:78:ASP:HA	1.94	0.48
1:B:155:PHE:CD1	1:B:338:PRO:HB3	2.48	0.48
1:B:229:PHE:O	1:B:233:HIS:HD2	1.96	0.48
1:C:90:ASP:OD1	1:C:99:LYS:HE3	2.13	0.48
1:D:48:GLU:HB2	1:D:298:LEU:HD12	1.96	0.48
1:A:174:GLU:OE1	1:A:208:LYS:HE3	2.14	0.47
1:B:138:ASP:O	1:B:143:ARG:HD2	2.14	0.47
1:C:48:GLU:H	1:C:302:GLN:HE22	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:ASP:O	1:D:323:MET:HG2	2.14	0.47
1:A:194:THR:OG1	1:A:197:GLU:HG3	2.15	0.47
1:B:333:PHE:HE1	1:B:335:GLN:HE21	1.62	0.47
1:B:3:ARG:HB2	1:B:40:GLU:OE2	2.15	0.47
1:C:129:ILE:HG13	1:C:340:MET:HE3	1.97	0.47
1:D:71:ARG:O	1:D:75:THR:HG23	2.15	0.47
1:D:267:MET:CB	1:D:293:MET:HG3	2.45	0.46
1:C:131:THR:HB	1:C:340:MET:CE	2.45	0.46
1:A:132:ASP:HB2	1:A:157:VAL:O	2.15	0.46
1:B:335:GLN:HE22	1:B:340:MET:CE	2.28	0.46
1:D:149:LYS:O	1:D:153:GLU:HG3	2.16	0.46
1:D:117:GLN:HE22	1:D:342:VAL:HG22	1.79	0.46
1:B:252:ARG:O	1:B:256:GLU:HG2	2.16	0.46
1:C:332:LYS:C	1:C:343:LYS:HE3	2.36	0.46
1:A:251:MET:HE2	1:A:255:LYS:HE3	1.97	0.46
1:B:48:GLU:H	1:B:302:GLN:NE2	2.14	0.45
1:B:300:ILE:CD1	1:B:320:SER:HB3	2.46	0.45
1:C:37:ILE:HG13	1:C:37:ILE:O	2.16	0.45
1:D:265:LYS:HZ3	4:D:412:PHE:HA	1.81	0.45
1:A:155:PHE:CD1	1:A:338:PRO:HB3	2.51	0.45
1:A:264:ILE:HD11	1:A:277:ILE:HG22	1.98	0.45
1:B:184:LYS:HE2	5:B:478:HOH:O	2.15	0.45
1:B:335:GLN:HE22	1:B:340:MET:HE3	1.81	0.45
1:B:162:VAL:HB	1:B:169:ASP:CG	2.36	0.45
1:C:78:ASP:OD1	1:C:80:ARG:HG2	2.17	0.45
1:A:149:LYS:HG2	1:A:153:GLU:OE2	2.18	0.44
1:A:31:ARG:HB2	1:A:60:VAL:HG21	2.00	0.44
1:B:117:GLN:NE2	1:B:342:VAL:HG22	2.32	0.44
1:D:328:VAL:O	1:D:328:VAL:HG13	2.16	0.44
1:C:155:PHE:CD1	1:C:338:PRO:HB3	2.53	0.44
1:C:71:ARG:O	1:C:75:THR:HG23	2.18	0.44
1:D:20:PHE:HE2	4:D:412:PHE:HD1	1.65	0.44
1:D:240:ALA:HB2	1:D:259:VAL:HG11	2.00	0.44
1:B:134:THR:HG1	3:B:411:ALA:N	2.16	0.44
1:A:132:ASP:OD1	1:A:132:ASP:C	2.56	0.43
1:B:292:CYS:SG	1:B:320:SER:HB2	2.57	0.43
1:D:342:VAL:HG22	1:D:343:LYS:N	2.33	0.43
1:C:104:PHE:CE1	1:C:302:GLN:HA	2.53	0.43
1:D:84:ARG:O	1:D:88:ILE:HG12	2.17	0.43
1:B:121:LEU:HA	1:B:121:LEU:HD12	1.91	0.43
1:C:266:LEU:HD22	1:C:271:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ALA:HB3	1:B:218:PRO:HA	1.99	0.43
1:C:131:THR:HB	1:C:340:MET:HE1	2.01	0.43
1:C:194:THR:OG1	1:C:197:GLU:HG3	2.19	0.43
1:C:239:ALA:HB2	1:C:261:TYR:HB2	2.00	0.43
1:C:31:ARG:NH2	1:C:60:VAL:HG22	2.34	0.43
1:A:131:THR:HB	1:A:340:MET:HE1	2.01	0.42
1:B:335:GLN:HE21	1:B:335:GLN:HB2	1.64	0.42
1:C:342:VAL:HG22	1:C:343:LYS:N	2.35	0.42
1:C:269:SER:O	1:C:273:ASP:HB2	2.19	0.42
1:D:88:ILE:HD13	1:D:91:ARG:NH2	2.35	0.42
1:A:78:ASP:HB3	1:A:81:ASN:ND2	2.34	0.42
1:A:181:ARG:HH11	1:A:181:ARG:CB	2.33	0.42
1:A:269:SER:HB3	1:A:273:ASP:HB2	2.02	0.42
1:A:265:LYS:NZ	4:A:412:PHE:HA	2.34	0.42
1:D:267:MET:HG3	1:D:293:MET:HG3	2.02	0.42
1:D:273:ASP:O	1:D:277:ILE:HG13	2.20	0.42
1:D:140:VAL:O	1:D:144:VAL:HG23	2.20	0.41
1:D:48:GLU:H	1:D:302:GLN:HE22	1.67	0.41
1:A:181:ARG:CB	1:A:181:ARG:NH1	2.82	0.41
1:B:148:LYS:HE2	1:B:179:VAL:HG11	2.03	0.41
1:B:269:SER:HB3	1:B:273:ASP:HB2	2.03	0.41
1:A:104:PHE:CD2	1:A:302:GLN:HG2	2.56	0.41
1:A:78:ASP:HB3	1:A:81:ASN:HD22	1.85	0.41
1:B:104:PHE:CE1	1:B:302:GLN:HA	2.56	0.41
1:D:145:LYS:O	1:D:145:LYS:HE2	2.21	0.41
1:A:131:THR:HB	1:A:340:MET:CE	2.51	0.40
1:A:156:ARG:HA	1:A:156:ARG:HD3	1.93	0.40
1:B:265:LYS:HZ3	4:B:412:PHE:HA	1.86	0.40
1:C:343:LYS:H	1:C:343:LYS:CD	2.34	0.40
1:C:189:ALA:HB3	1:C:218:PRO:HA	2.03	0.40
1:C:69:ALA:O	1:C:73:MET:HG3	2.21	0.40
1:A:134:THR:HG1	3:A:411:ALA:N	2.19	0.40
1:C:264:ILE:HD11	1:C:277:ILE:HG22	2.03	0.40

There are no symmetry-related clashes.

## 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	339/345 (98%)	326 (96%)	13 (4%)	0	100	100
1	B	339/345 (98%)	326 (96%)	13 (4%)	0	100	100
1	C	339/345 (98%)	327 (96%)	12 (4%)	0	100	100
1	D	339/345 (98%)	324 (96%)	15 (4%)	0	100	100
All	All	1356/1380 (98%)	1303 (96%)	53 (4%)	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	288/292 (99%)	284 (99%)	4 (1%)	67	81
1	B	288/292 (99%)	283 (98%)	5 (2%)	60	76
1	C	288/292 (99%)	282 (98%)	6 (2%)	53	70
1	D	288/292 (99%)	282 (98%)	6 (2%)	53	70
All	All	1152/1168 (99%)	1131 (98%)	21 (2%)	59	75

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

Mol	Chain	Res	Type
1	A	17	GLU
1	A	31	ARG

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Mol	Chain	Res	Type
1	A	208	LYS
1	A	273	ASP
1	B	31	ARG
1	B	39	LEU
1	B	234	SER
1	B	273	ASP
1	B	335	GLN
1	C	31	ARG
1	C	130	GLU
1	C	234	SER
1	C	273	ASP
1	C	335	GLN
1	C	343	LYS
1	D	145	LYS
1	D	178	LYS
1	D	208	LYS
1	D	234	SER
1	D	273	ASP
1	D	327	GLU

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

Mol	Chain	Res	Type
1	A	21	HIS
1	A	68	ASN
1	A	81	ASN
1	A	233	HIS
1	A	302	GLN
1	A	335	GLN
1	B	21	HIS
1	B	81	ASN
1	B	117	GLN
1	B	207	GLN
1	B	233	HIS
1	B	302	GLN
1	B	335	GLN
1	C	81	ASN
1	C	233	HIS
1	C	302	GLN
1	C	335	GLN
1	D	68	ASN
1	D	81	ASN

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Mol	Chain	Res	Type
1	D	117	GLN
1	D	233	HIS
1	D	302	GLN
1	D	335	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	ALA	D	411	4	3,4,5	0.64	0	2,4,6	0.80	0
3	ALA	C	411	4	3,4,5	0.61	0	2,4,6	0.72	0
3	ALA	B	411	4	3,4,5	0.69	0	2,4,6	0.81	0
3	ALA	A	411	4	3,4,5	0.65	0	2,4,6	0.75	0
4	PHE	D	412	3	9,12,12	0.50	0	10,15,15	0.28	0
4	PHE	B	412	3,2	9,12,12	0.48	0	10,15,15	0.27	0
4	PHE	A	412	3,2	9,12,12	0.63	0	10,15,15	0.23	0
4	PHE	C	412	3,2	9,12,12	0.57	0	10,15,15	0.24	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
3	ALA	D	411	4	-	0/0/2/4	-
3	ALA	C	411	4	-	0/0/2/4	-
3	ALA	B	411	4	-	0/0/2/4	-
3	ALA	A	411	4	-	0/0/2/4	-
4	PHE	D	412	3	-	0/4/8/8	0/1/1/1
4	PHE	B	412	3,2	-	0/4/8/8	0/1/1/1
4	PHE	A	412	3,2	-	0/4/8/8	0/1/1/1
4	PHE	C	412	3,2	-	0/4/8/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	411	ALA	1	0
3	B	411	ALA	1	0
3	A	411	ALA	1	0
4	D	412	PHE	2	0
4	B	412	PHE	1	0
4	A	412	PHE	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	341/345 (98%)	-0.37	5 (1%) 73 79	22, 31, 51, 65	0
1	B	341/345 (98%)	-0.36	5 (1%) 73 79	21, 31, 53, 70	0
1	C	341/345 (98%)	-0.44	3 (0%) 84 88	21, 29, 47, 69	0
1	D	341/345 (98%)	-0.16	11 (3%) 47 54	23, 34, 53, 71	0
All	All	1364/1380 (98%)	-0.33	24 (1%) 68 74	21, 32, 51, 71	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	GLU	4.7
1	A	343	LYS	3.4
1	D	329	PHE	3.3
1	D	181	ARG	3.1
1	C	181	ARG	3.0
1	D	343	LYS	3.0
1	C	343	LYS	2.9
1	B	181	ARG	2.9
1	A	327	GLU	2.7
1	B	328	VAL	2.7
1	D	152	GLU	2.7
1	D	331	GLY	2.6
1	A	334	ILE	2.6
1	D	178	LYS	2.6
1	A	328	VAL	2.4
1	D	327	GLU	2.4
1	A	181	ARG	2.3
1	C	327	GLU	2.2
1	D	328	VAL	2.2
1	D	336	ASP	2.2
1	B	152	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	334	ILE	2.1
1	B	17	GLU	2.1
1	D	3	ARG	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 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(Å <sup>2</sup> )	Q<0.9
2	MG	C	401	1/1	0.34	0.20	38,38,38,38	0
2	MG	A	401	1/1	0.60	0.10	34,34,34,34	0
2	MG	D	401	1/1	0.87	0.14	32,32,32,32	0
2	MG	B	401	1/1	0.91	0.09	33,33,33,33	0
4	PHE	C	412	12/12	0.96	0.10	24,25,27,28	0
3	ALA	D	411	5/6	0.96	0.10	27,27,28,29	0
4	PHE	A	412	12/12	0.97	0.10	27,29,34,35	0
3	ALA	B	411	5/6	0.97	0.10	28,30,31,31	0
4	PHE	D	412	12/12	0.97	0.10	29,30,34,35	0
4	PHE	B	412	12/12	0.97	0.07	30,32,34,35	0
3	ALA	C	411	5/6	0.99	0.11	23,23,24,24	0
3	ALA	A	411	5/6	0.99	0.15	24,26,27,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.