



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:53 AM GMT

PDB ID : 1JDF  
Title : Glucarate Dehydratase from E.coli N341D mutant  
Authors : Gulick, A.M.; Hubbard, B.K.; Gerlt, J.A.; Rayment, I.  
Deposited on : 2001-06-13  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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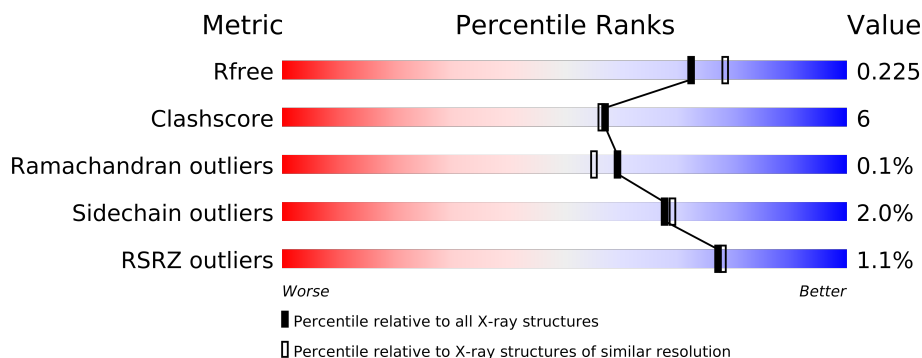
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	446	
1	B	446	
1	C	446	
1	D	446	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	IPA	A	3603	-	X
4	IPA	B	3604	-	X
4	IPA	C	3601	-	X
4	IPA	C	3607	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	IPA	D	3602	-	X
4	IPA	D	3608	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14868 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Glucarate Dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3421	2163	598	639	21			
1	B	442	Total	C	N	O	S	0	0	0
			3396	2148	593	634	21			
1	C	442	Total	C	N	O	S	0	0	0
			3417	2160	598	638	21			
1	D	442	Total	C	N	O	S	0	0	0
			3410	2157	598	634	21			

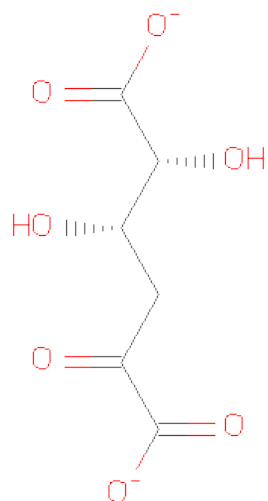
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	341	ASP	ASN	ENGINEERED	UNP P76637
B	341	ASP	ASN	ENGINEERED	UNP P76637
C	341	ASP	ASN	ENGINEERED	UNP P76637
D	341	ASP	ASN	ENGINEERED	UNP P76637

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

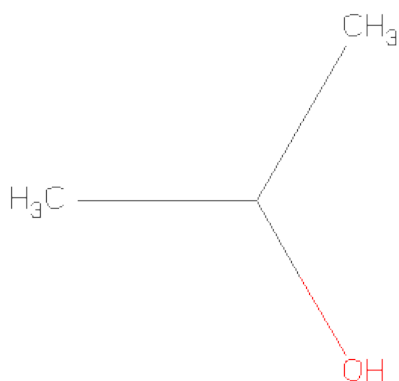
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2,3-DIHYDROXY-5-OXO-HEXANEDIOATE (three-letter code: GLR) (formula: C<sub>6</sub>H<sub>6</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 ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 3 1	0	0
4	D	1	Total C O 4 3 1	0	0
4	A	1	Total C O 4 3 1	0	0
4	B	1	Total C O 4 3 1	0	0
4	A	1	Total C O 4 3 1	0	0
4	B	1	Total C O 4 3 1	0	0
4	C	1	Total C O 4 3 1	0	0
4	D	1	Total C O 4 3 1	0	0

- Molecule 5 is water.

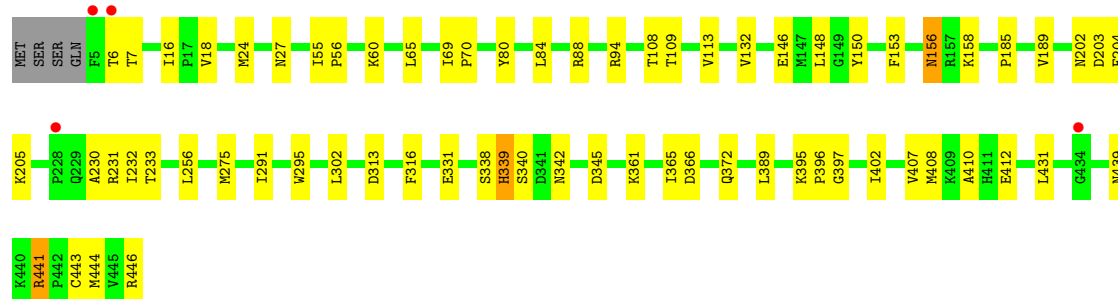
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	275	Total O 275 275	0	0
5	B	234	Total O 234 234	0	0
5	C	320	Total O 320 320	0	0
5	D	307	Total O 307 307	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

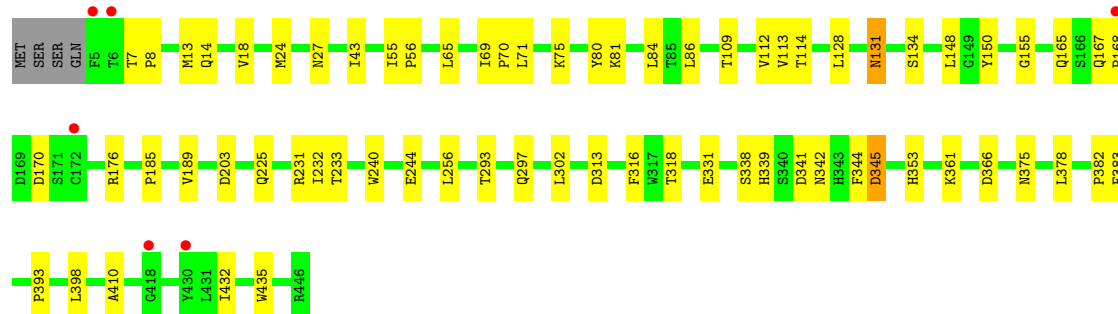
#### • Molecule 1: Glucarate Dehydratase

Chain A: 



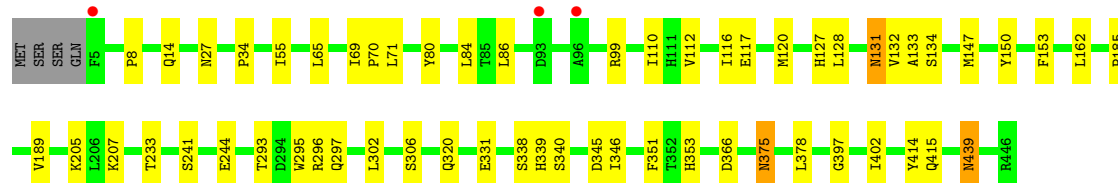
#### • Molecule 1: Glucarate Dehydratase

Chain B: 



#### • Molecule 1: Glucarate Dehydratase

Chain C: 



#### • Molecule 1: Glucarate Dehydratase

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.92Å 83.93Å 98.22Å 104.11° 93.75° 113.12°	Depositor
Resolution (Å)	20.00 – 2.00 19.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.00) 97.4 (19.84-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.198 , 0.233 0.193 , 0.225	Depositor DCC
$R_{free}$ test set	6561 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.4	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 130650 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14868	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLR, IPA, 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	0.32	0/3500	0.56	1/4743 (0.0%)
1	B	0.31	0/3475	0.56	0/4715
1	C	0.33	0/3496	0.58	1/4739 (0.0%)
1	D	0.33	0/3489	0.57	1/4730 (0.0%)
All	All	0.32	0/13960	0.57	3/18927 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	153	PHE	N-CA-C	-5.48	96.19	111.00
1	A	153	PHE	N-CA-C	-5.05	97.37	111.00
1	D	153	PHE	N-CA-C	-5.05	97.38	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3421	0	3353	41	0
1	B	3396	0	3305	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3417	0	3344	40	0
1	D	3410	0	3332	51	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	6	0	0
3	B	13	0	6	0	0
3	C	13	0	6	0	0
3	D	13	0	6	0	0
4	A	8	0	16	3	0
4	B	8	0	16	4	0
4	C	8	0	16	2	0
4	D	8	0	16	4	0
5	A	275	0	0	1	0
5	B	234	0	0	6	0
5	C	320	0	0	2	0
5	D	307	0	0	2	0
All	All	14868	0	13422	175	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (175) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:7:THR:HG21	1:C:128:LEU:HA	1.46	0.97
1:B:7:THR:HG21	1:D:128:LEU:HA	1.46	0.97
1:B:128:LEU:HA	1:D:7:THR:HG21	1.60	0.81
1:C:375:ASN:H	1:C:375:ASN:HD22	1.30	0.79
1:B:293:THR:H	1:B:297:GLN:HE21	1.32	0.78
1:D:275:MET:HG3	1:D:291:ILE:HD13	1.68	0.76
1:C:293:THR:H	1:C:297:GLN:HE21	1.35	0.74
1:B:293:THR:H	1:B:297:GLN:NE2	1.87	0.72
1:B:24:MET:HE2	1:B:155:GLY:C	2.09	0.72
1:D:156:ASN:HD21	1:D:158:LYS:HB2	1.56	0.71
1:C:293:THR:H	1:C:297:GLN:NE2	1.89	0.69
1:A:275:MET:HG3	1:A:291:ILE:HD13	1.75	0.67
1:A:302:LEU:HD22	4:C:3601:IPA:H32	1.77	0.66
1:C:55:ILE:HD11	1:C:65:LEU:HD11	1.78	0.66
1:D:13:MET:HG3	1:D:43:ILE:HG12	1.78	0.66
1:C:296:ARG:HH12	1:D:267:GLN:NE2	1.95	0.65
1:B:55:ILE:HD11	1:B:65:LEU:HD11	1.80	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:4603:HOH:O	4:D:3602:IPA:H33	1.99	0.63
1:C:375:ASN:H	1:C:375:ASN:ND2	1.97	0.62
1:D:81:LYS:HZ3	1:D:320:GLN:HE22	1.47	0.62
1:C:346:ILE:HD11	1:C:402:ILE:HD13	1.83	0.61
1:A:203:ASP:OD1	1:A:231:ARG:HB2	2.01	0.61
1:B:80:TYR:O	1:B:84:LEU:HG	2.01	0.61
4:B:3604:IPA:H11	5:B:4603:HOH:O	2.01	0.60
1:A:109:THR:O	1:A:113:VAL:HG23	2.02	0.59
1:A:402:ILE:HD11	1:A:407:VAL:HG21	1.86	0.58
1:D:417:HIS:HB2	1:D:419:LEU:HG	1.86	0.57
1:D:402:ILE:HD11	1:D:407:VAL:CG2	2.35	0.57
1:A:156:ASN:ND2	1:A:158:LYS:H	2.02	0.57
1:D:402:ILE:HD11	1:D:407:VAL:HG21	1.86	0.57
1:D:81:LYS:NZ	1:D:320:GLN:HE22	2.03	0.57
1:B:383:PHE:CZ	1:B:393:PRO:HG2	2.40	0.56
1:B:338:SER:O	1:B:366:ASP:HB2	2.04	0.56
1:B:302:LEU:HD22	4:D:3602:IPA:H2	1.88	0.56
1:B:233:THR:HA	1:B:256:LEU:HD22	1.88	0.55
1:A:55:ILE:HD11	1:A:65:LEU:HD11	1.86	0.55
1:C:340:SER:HB2	5:C:4649:HOH:O	2.06	0.54
1:D:262:PRO:HD2	1:D:275:MET:CE	2.37	0.54
1:A:156:ASN:HD21	1:A:158:LYS:HB2	1.71	0.54
1:D:344:PHE:CD2	1:D:378:LEU:HD13	2.43	0.54
1:B:168:PRO:O	1:B:176:ARG:HG3	2.08	0.54
1:C:296:ARG:HH12	1:D:267:GLN:HE22	1.55	0.54
1:B:75:LYS:HA	5:B:4524:HOH:O	2.09	0.53
1:D:156:ASN:ND2	1:D:158:LYS:H	2.05	0.53
1:C:69:ILE:HB	1:C:70:PRO:HD3	1.91	0.53
1:B:240:TRP:HB3	1:B:244:GLU:HG3	1.88	0.53
4:A:3603:IPA:H32	1:C:302:LEU:HD22	1.90	0.53
1:A:408:MET:O	1:A:412:GLU:HG3	2.08	0.53
1:D:76:THR:CG2	1:D:79:GLU:HG3	2.39	0.53
1:B:345:ASP:OD2	1:B:345:ASP:N	2.41	0.53
1:B:65:LEU:HD23	1:B:112:VAL:HG13	1.91	0.53
1:A:88:ARG:HG3	4:A:3605:IPA:H33	1.90	0.52
1:C:414:TYR:HD1	1:C:415:GLN:HE21	1.58	0.52
1:B:13:MET:HG3	1:B:43:ILE:HG12	1.90	0.52
1:A:148:LEU:HD12	1:A:148:LEU:C	2.31	0.51
1:B:81:LYS:HG2	5:B:4526:HOH:O	2.10	0.51
4:B:3604:IPA:H2	1:D:302:LEU:HD22	1.93	0.51
1:D:69:ILE:N	1:D:70:PRO:HD2	2.25	0.51
1:A:80:TYR:O	1:A:84:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:207:LYS:HA	1:D:207:LYS:HE3	1.93	0.51
1:C:375:ASN:HD22	1:C:375:ASN:N	1.97	0.50
1:A:338:SER:HB3	1:A:365:ILE:HG23	1.94	0.50
1:D:81:LYS:NZ	1:D:320:GLN:NE2	2.59	0.50
1:B:69:ILE:N	1:B:70:PRO:HD2	2.27	0.50
1:B:167:GLN:HB3	1:B:170:ASP:HB2	1.93	0.50
1:C:185:PRO:O	1:C:189:VAL:HG23	2.11	0.50
1:A:60:LYS:HE2	1:A:94:ARG:HD3	1.94	0.50
1:A:345:ASP:N	1:A:345:ASP:OD2	2.44	0.50
1:A:60:LYS:HG3	1:A:108:THR:HG21	1.93	0.50
1:C:131:ASN:HD22	1:C:131:ASN:C	2.15	0.50
1:A:146:GLU:HA	1:A:389:LEU:HD23	1.94	0.49
1:D:275:MET:HA	1:D:275:MET:HE2	1.94	0.49
1:A:338:SER:O	1:A:366:ASP:HB2	2.13	0.48
1:D:8:PRO:HB3	1:D:45:ASP:HB2	1.95	0.48
1:B:81:LYS:HB2	5:D:4786:HOH:O	2.14	0.48
1:B:185:PRO:O	1:B:189:VAL:HG23	2.12	0.48
1:D:83:VAL:O	1:D:87:VAL:HG23	2.14	0.48
1:C:131:ASN:ND2	1:C:134:SER:H	2.11	0.47
1:D:338:SER:O	1:D:366:ASP:HB2	2.14	0.47
1:B:131:ASN:ND2	1:B:134:SER:H	2.12	0.47
1:C:338:SER:O	1:C:366:ASP:HB2	2.13	0.47
1:C:378:LEU:O	1:C:402:ILE:HD12	2.14	0.47
1:D:299:GLY:O	4:D:3602:IPA:H32	2.14	0.47
1:A:205:LYS:HG3	1:A:233:THR:HG23	1.96	0.47
1:A:202:ASN:O	1:A:230:ALA:CB	2.63	0.47
1:D:88:ARG:HG3	4:D:3608:IPA:H12	1.96	0.47
1:B:353:HIS:HE1	1:B:398:LEU:O	1.98	0.47
1:C:133:ALA:H	1:C:353:HIS:HD2	1.63	0.47
1:B:165:GLN:HE22	1:B:375:ASN:ND2	2.12	0.46
1:A:204:PHE:O	1:A:232:ILE:HA	2.15	0.46
1:B:148:LEU:HD12	1:B:148:LEU:C	2.35	0.46
1:A:24:MET:CE	1:A:431:LEU:HD11	2.46	0.46
1:C:207:LYS:HE3	1:C:207:LYS:HA	1.97	0.46
1:C:147:MET:CE	1:C:351:PHE:HE2	2.28	0.46
1:A:205:LYS:NZ	1:A:366:ASP:OD2	2.46	0.46
4:B:3604:IPA:H2	1:D:302:LEU:HB3	1.97	0.46
1:A:16:ILE:HD13	1:A:408:MET:CE	2.46	0.46
1:B:131:ASN:HD22	1:B:131:ASN:C	2.19	0.46
1:A:6:THR:HG22	1:A:7:THR:N	2.31	0.45
1:D:8:PRO:HA	1:D:46:ASN:OD1	2.16	0.45
1:D:109:THR:O	1:D:113:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:148:LEU:HD12	1:B:148:LEU:O	2.16	0.45
1:C:345:ASP:OD1	1:C:345:ASP:N	2.45	0.45
1:C:80:TYR:O	1:C:84:LEU:HG	2.17	0.45
1:C:241:SER:OG	1:C:244:GLU:HG3	2.16	0.45
1:A:361:LYS:C	1:A:361:LYS:HD3	2.37	0.45
1:A:339:HIS:CG	1:A:340:SER:N	2.85	0.45
1:D:262:PRO:HD2	1:D:275:MET:HE3	1.97	0.45
1:B:344:PHE:CD2	1:B:378:LEU:HG	2.51	0.45
1:B:7:THR:HA	1:B:8:PRO:HD3	1.79	0.45
1:A:295:TRP:HB3	1:C:331:GLU:HB3	1.99	0.44
1:C:65:LEU:HD23	1:C:112:VAL:HG13	1.98	0.44
1:D:13:MET:HB3	1:D:69:ILE:HG23	2.00	0.44
1:D:383:PHE:CZ	1:D:393:PRO:HG2	2.53	0.44
1:D:156:ASN:ND2	1:D:158:LYS:HB2	2.28	0.44
1:C:116:ILE:O	1:C:120:MET:HG2	2.18	0.44
1:A:331:GLU:HB3	1:C:295:TRP:HB3	2.00	0.44
1:B:313:ASP:HB2	1:B:339:HIS:HB3	2.00	0.44
1:A:443:CYS:SG	1:A:444:MET:HE3	2.58	0.44
1:D:148:LEU:HD12	1:D:148:LEU:O	2.17	0.43
1:B:109:THR:O	1:B:113:VAL:HG23	2.17	0.43
1:A:69:ILE:HB	1:A:70:PRO:HD3	2.00	0.43
1:A:132:VAL:HG23	1:A:397:GLY:C	2.39	0.43
1:A:55:ILE:HB	1:A:56:PRO:HD2	2.01	0.43
1:A:18:VAL:HB	1:A:410:ALA:HB1	1.99	0.43
1:B:432:ILE:O	1:B:435:TRP:HB2	2.19	0.43
1:C:34:PRO:HG2	1:C:162:LEU:HB3	2.01	0.43
1:B:341:ASP:O	1:B:342:ASN:C	2.57	0.43
1:D:34:PRO:HG2	1:D:162:LEU:HB3	2.00	0.43
1:C:205:LYS:HG3	1:C:233:THR:HG23	2.00	0.43
1:C:375:ASN:ND2	1:C:375:ASN:N	2.60	0.43
1:D:262:PRO:HG2	1:D:275:MET:HE3	2.01	0.43
1:D:346:ILE:HD11	1:D:402:ILE:HD13	2.00	0.43
1:C:133:ALA:H	1:C:353:HIS:CD2	2.37	0.43
1:B:165:GLN:HE22	1:B:375:ASN:HD21	1.67	0.42
1:D:345:ASP:OD2	1:D:345:ASP:N	2.45	0.42
1:D:8:PRO:HD3	1:D:127:HIS:CE1	2.54	0.42
1:B:71:LEU:HD22	1:B:86:LEU:HD21	2.02	0.42
1:C:132:VAL:HG23	1:C:397:GLY:C	2.40	0.42
1:B:114:THR:OG1	1:B:318:THR:HA	2.20	0.42
4:B:3604:IPA:H32	5:B:4602:HOH:O	2.19	0.42
1:C:71:LEU:HD22	1:C:86:LEU:HD21	2.02	0.42
1:D:7:THR:HA	1:D:8:PRO:HD3	1.87	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:361:LYS:HD3	1:B:361:LYS:C	2.40	0.42
1:D:131:ASN:HD22	1:D:131:ASN:C	2.23	0.41
1:A:313:ASP:HB3	1:A:316:PHE:CE1	2.55	0.41
1:A:441:ARG:HG2	1:A:446:ARG:NH1	2.34	0.41
1:C:99:ARG:HD2	1:C:293:THR:HG21	2.02	0.41
1:D:156:ASN:HD22	1:D:156:ASN:C	2.22	0.41
1:C:8:PRO:HD3	1:C:127:HIS:CE1	2.55	0.41
1:B:18:VAL:HB	1:B:410:ALA:HB1	2.03	0.41
1:D:313:ASP:HB3	1:D:316:PHE:CE1	2.56	0.41
1:B:232:ILE:HG22	1:B:233:THR:N	2.34	0.41
1:B:313:ASP:HB3	1:B:316:PHE:CE1	2.56	0.41
1:C:110:ILE:HA	1:C:110:ILE:HD12	1.89	0.41
1:C:117:GLU:OE1	1:C:320:GLN:HG3	2.20	0.41
4:A:3603:IPA:H33	5:C:4505:HOH:O	2.21	0.41
1:C:439:ASN:HD22	1:C:439:ASN:N	2.18	0.41
1:D:262:PRO:CD	1:D:275:MET:HE3	2.51	0.41
1:D:148:LEU:HD12	1:D:148:LEU:C	2.41	0.41
1:D:55:ILE:HB	1:D:56:PRO:HD2	2.02	0.41
1:A:395:LYS:HA	1:A:396:PRO:HD3	1.92	0.41
1:B:128:LEU:HD23	1:D:7:THR:HG21	2.03	0.41
1:D:184:THR:HA	5:D:4606:HOH:O	2.21	0.41
1:A:185:PRO:O	1:A:189:VAL:HG23	2.20	0.40
1:D:156:ASN:ND2	1:D:156:ASN:C	2.75	0.40
1:B:55:ILE:HB	1:B:56:PRO:HD2	2.02	0.40
1:A:233:THR:HA	1:A:256:LEU:HD22	2.03	0.40
1:A:342:ASN:HD22	1:A:372:GLN:HE22	1.69	0.40
5:A:4775:HOH:O	4:C:3601:IPA:H33	2.21	0.40
1:B:75:LYS:HD3	5:B:4524:HOH:O	2.20	0.40
1:D:429:GLN:NE2	1:D:434:GLY:H	2.18	0.40
1:B:345:ASP:OD1	1:B:382:PRO:HG3	2.22	0.40
1:B:203:ASP:CG	1:B:231:ARG:HB2	2.41	0.40
1:B:331:GLU:HB3	1:D:295:TRP:HB3	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	440/446 (99%)	427 (97%)	13 (3%)	0	100	100
1	B	440/446 (99%)	427 (97%)	13 (3%)	0	100	100
1	C	440/446 (99%)	426 (97%)	14 (3%)	0	100	100
1	D	440/446 (99%)	428 (97%)	11 (2%)	1 (0%)	56	51
All	All	1760/1784 (99%)	1708 (97%)	51 (3%)	1 (0%)	59	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	46	ASN

### 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	357/362 (99%)	351 (98%)	6 (2%)	73	75
1	B	351/362 (97%)	345 (98%)	6 (2%)	73	75
1	C	356/362 (98%)	348 (98%)	8 (2%)	64	65
1	D	353/362 (98%)	344 (98%)	9 (2%)	60	59
All	All	1417/1448 (98%)	1388 (98%)	29 (2%)	68	69

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	150	TYR
1	A	156	ASN
1	A	339	HIS
1	A	439	ASN
1	A	441	ARG
1	B	14	GLN
1	B	27	ASN

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Mol	Chain	Res	Type
1	B	131	ASN
1	B	150	TYR
1	B	225	GLN
1	B	345	ASP
1	C	14	GLN
1	C	27	ASN
1	C	131	ASN
1	C	150	TYR
1	C	306	SER
1	C	339	HIS
1	C	375	ASN
1	C	439	ASN
1	D	27	ASN
1	D	131	ASN
1	D	150	TYR
1	D	156	ASN
1	D	176	ARG
1	D	275	MET
1	D	339	HIS
1	D	340	SER
1	D	439	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	102	GLN
1	A	141	GLN
1	A	156	ASN
1	A	353	HIS
1	A	372	GLN
1	A	439	ASN
1	B	14	GLN
1	B	102	GLN
1	B	131	ASN
1	B	140	GLN
1	B	165	GLN
1	B	243	ASN
1	B	297	GLN
1	B	353	HIS
1	C	14	GLN
1	C	39	ASN

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Mol	Chain	Res	Type
1	C	102	GLN
1	C	131	ASN
1	C	140	GLN
1	C	165	GLN
1	C	225	GLN
1	C	229	GLN
1	C	243	ASN
1	C	297	GLN
1	C	353	HIS
1	C	372	GLN
1	C	375	ASN
1	C	415	GLN
1	C	439	ASN
1	D	14	GLN
1	D	39	ASN
1	D	102	GLN
1	D	131	ASN
1	D	140	GLN
1	D	141	GLN
1	D	156	ASN
1	D	225	GLN
1	D	243	ASN
1	D	267	GLN
1	D	305	GLN
1	D	320	GLN
1	D	415	GLN
1	D	429	GLN
1	D	439	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	GLR	A	2510	2	6,12,12	2.20	2 (33%)	9,16,16	1.43	1 (11%)
4	IPA	A	3603	-	3,3,3	0.69	0	3,3,3	0.34	0
4	IPA	A	3605	-	3,3,3	0.71	0	3,3,3	0.29	0
3	GLR	B	2511	2	6,12,12	2.16	2 (33%)	9,16,16	1.48	2 (22%)
4	IPA	B	3604	-	3,3,3	0.59	0	3,3,3	0.35	0
4	IPA	B	3606	-	3,3,3	0.64	0	3,3,3	0.35	0
3	GLR	C	2512	2	6,12,12	2.22	2 (33%)	9,16,16	1.45	2 (22%)
4	IPA	C	3601	-	3,3,3	0.67	0	3,3,3	0.31	0
4	IPA	C	3607	-	3,3,3	0.71	0	3,3,3	0.31	0
3	GLR	D	2513	2	6,12,12	2.34	2 (33%)	9,16,16	1.43	2 (22%)
4	IPA	D	3602	-	3,3,3	0.68	0	3,3,3	0.32	0
4	IPA	D	3608	-	3,3,3	0.71	0	3,3,3	0.35	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	GLR	A	2510	2	-	0/8/16/16	0/0/0/0
4	IPA	A	3603	-	-	0/0/0/0	0/0/0/0
4	IPA	A	3605	-	-	0/0/0/0	0/0/0/0
3	GLR	B	2511	2	-	0/8/16/16	0/0/0/0
4	IPA	B	3604	-	-	0/0/0/0	0/0/0/0
4	IPA	B	3606	-	-	0/0/0/0	0/0/0/0
3	GLR	C	2512	2	-	0/8/16/16	0/0/0/0
4	IPA	C	3601	-	-	0/0/0/0	0/0/0/0
4	IPA	C	3607	-	-	0/0/0/0	0/0/0/0
3	GLR	D	2513	2	-	0/8/16/16	0/0/0/0
4	IPA	D	3602	-	-	0/0/0/0	0/0/0/0
4	IPA	D	3608	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2513	GLR	O2-C2	4.97	1.52	1.42
3	A	2510	GLR	O2-C2	4.92	1.52	1.42
3	C	2512	GLR	O2-C2	4.82	1.52	1.42
3	B	2511	GLR	O2-C2	4.69	1.52	1.42
3	D	2513	GLR	C4-C5	2.73	1.54	1.51
3	C	2512	GLR	C4-C5	2.30	1.53	1.51
3	B	2511	GLR	C4-C5	2.19	1.53	1.51
3	A	2510	GLR	C4-C5	2.02	1.53	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2510	GLR	O3-C3-C2	3.54	113.20	109.29
3	B	2511	GLR	O3-C3-C2	3.39	113.03	109.29
3	C	2512	GLR	O3-C3-C2	3.01	112.61	109.29
3	D	2513	GLR	O3-C3-C2	2.85	112.43	109.29
3	C	2512	GLR	O5-C5-C4	2.34	123.32	120.78
3	D	2513	GLR	O5-C5-C4	2.30	123.28	120.78
3	B	2511	GLR	O5-C5-C4	2.22	123.18	120.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	442/446 (99%)	-0.22	4 (0%) 81 82	21, 35, 46, 56	0
1	B	442/446 (99%)	-0.13	6 (1%) 72 72	20, 38, 56, 70	0
1	C	442/446 (99%)	-0.39	3 (0%) 84 85	18, 31, 42, 60	0
1	D	442/446 (99%)	-0.23	7 (1%) 68 69	20, 33, 50, 66	0
All	All	1768/1784 (99%)	-0.24	20 (1%) 77 78	18, 34, 50, 70	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	PHE	6.8
1	B	168	PRO	5.2
1	B	6	THR	4.3
1	D	5	PHE	3.9
1	A	5	PHE	3.8
1	C	93	ASP	3.2
1	C	5	PHE	3.1
1	D	48	GLY	2.8
1	D	418	GLY	2.8
1	D	433	PRO	2.8
1	D	93	ASP	2.8
1	B	172	CYS	2.6
1	A	228	PRO	2.5
1	D	96	ALA	2.4
1	A	434	GLY	2.3
1	C	96	ALA	2.3
1	D	97	GLY	2.3
1	A	6	THR	2.2
1	B	418	GLY	2.2
1	B	430	TYR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	IPA	B	3604	4/4	0.21	9.58	36,38,40,40	0
4	IPA	A	3603	4/4	0.17	9.53	35,38,39,40	0
4	IPA	D	3602	4/4	0.17	7.79	28,35,35,37	0
4	IPA	C	3601	4/4	0.14	6.61	38,39,39,39	0
4	IPA	D	3608	4/4	0.25	2.49	50,50,52,52	0
4	IPA	C	3607	4/4	0.24	2.42	49,49,49,49	0
4	IPA	B	3606	4/4	0.19	1.81	46,49,49,50	0
3	GLR	A	2510	13/13	0.13	1.77	30,40,47,47	0
4	IPA	A	3605	4/4	0.16	1.68	47,47,49,49	0
3	GLR	D	2513	13/13	0.12	1.33	26,37,43,44	0
3	GLR	C	2512	13/13	0.11	1.30	29,37,42,42	0
3	GLR	B	2511	13/13	0.11	0.91	34,37,43,43	0
2	MG	B	4501	1/1	0.07	-0.81	33,33,33,33	0
2	MG	A	4500	1/1	0.08	-0.97	32,32,32,32	0
2	MG	C	4502	1/1	0.06	-2.11	30,30,30,30	0
2	MG	D	4503	1/1	0.04	-2.32	26,26,26,26	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.