



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 12:47 PM EST

PDB ID : 3PWG  
Title : Crystal structure of the mutant S29G.P34A of D-Glucarate dehydratase from Escherichia coli complexed with product 5-keto-4-deoxy-D-Glucarate  
Authors : Fedorov, A.A.; Fedorov, E.V.; Lukk, T.; Gerlt, J.A.; Almo, S.C.  
Deposited on : 2010-12-08  
Resolution : 2.00 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

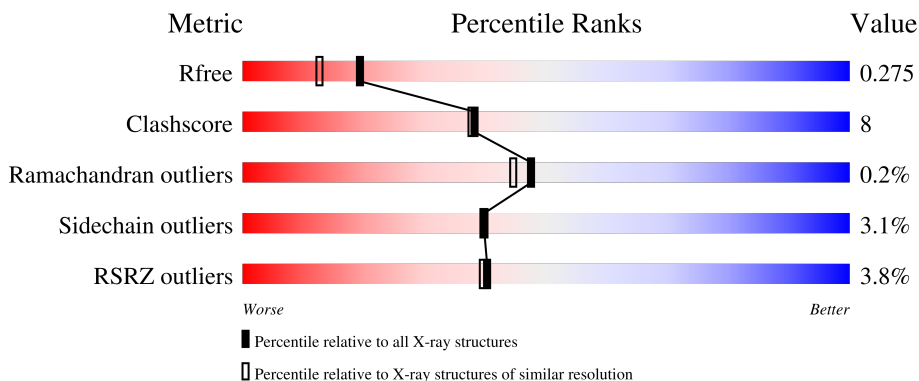
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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	446	 3% 84% 14% ..
1	B	446	 3% 87% 12% .
1	C	446	 5% 76% 20% ..
1	D	446	 4% 70% 24% ..

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13747 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 Glucarate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	Total 3421	C 2162	N 600	O 638	S 21	0	0	0
1	B	442	Total 3421	C 2162	N 600	O 638	S 21	0	0	0
1	C	433	Total 3359	C 2124	N 588	O 626	S 21	0	0	0
1	D	427	Total 3304	C 2093	N 575	O 615	S 21	0	0	0

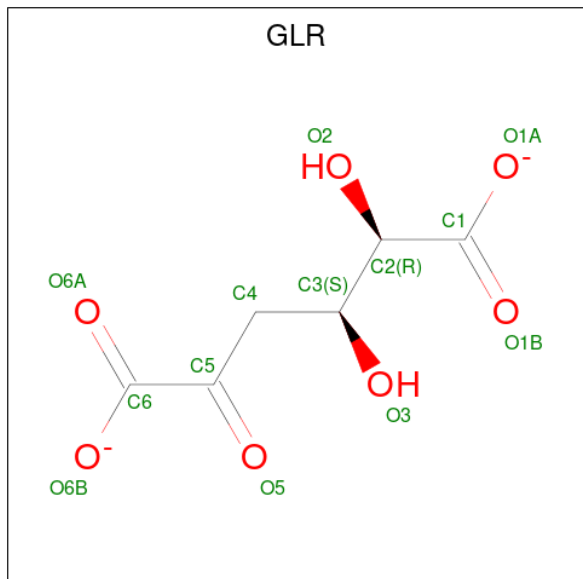
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	SER	engineered mutation	UNP E2KTD9
A	34	ALA	PRO	engineered mutation	UNP E2KTD9
B	29	GLY	SER	engineered mutation	UNP E2KTD9
B	34	ALA	PRO	engineered mutation	UNP E2KTD9
C	29	GLY	SER	engineered mutation	UNP E2KTD9
C	34	ALA	PRO	engineered mutation	UNP E2KTD9
D	29	GLY	SER	engineered mutation	UNP E2KTD9
D	34	ALA	PRO	engineered mutation	UNP E2KTD9

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

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

- Molecule 3 is 2,3-DIHYDROXY-5-OXO-HEXANEDIOATE (three-letter code: GLR) (formula:  $C_6H_6O_7$ ).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

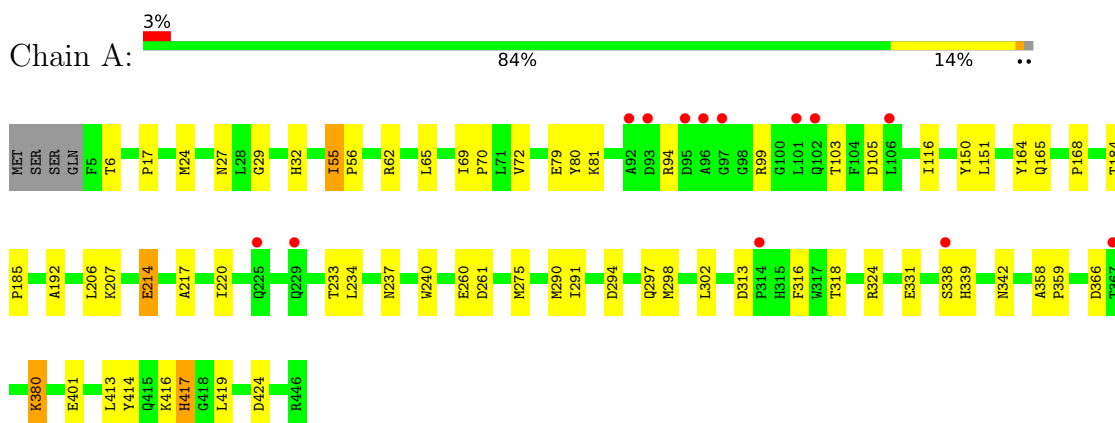
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	56	Total O 56 56	0	0
5	B	67	Total O 67 67	0	0
5	C	28	Total O 28 28	0	0
5	D	17	Total O 17 17	0	0

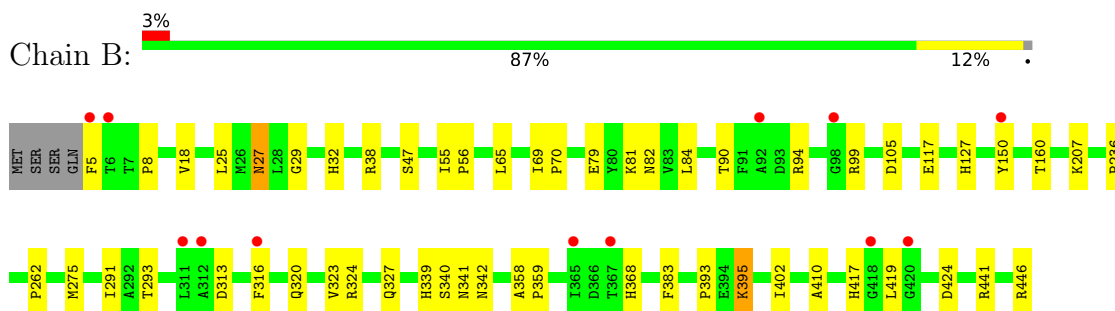
### 3 Residue-property plots [i](#)

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.

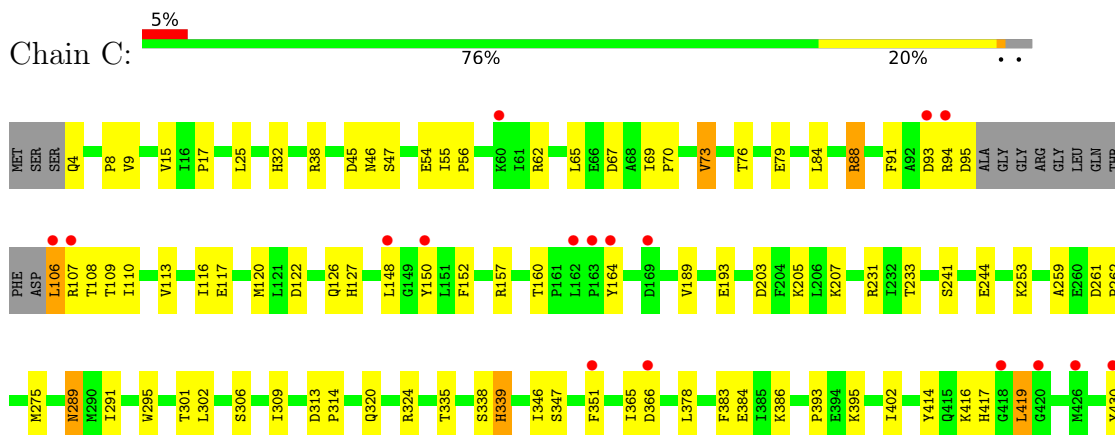
- Molecule 1: Glucarate dehydratase

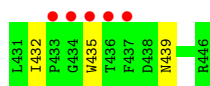


- Molecule 1: Glucarate dehydratase

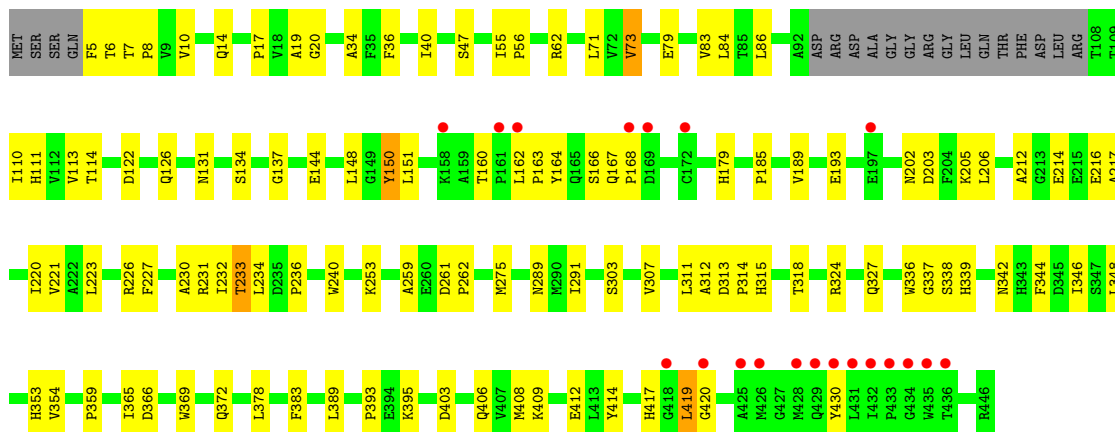


- Molecule 1: Glucarate dehydratase





- Molecule 1: Glucarate dehydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.12Å 130.66Å 158.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.87 – 2.00 39.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.7 (39.87-2.00) 92.8 (39.87-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 2.00Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.231 , 0.280 0.226 , 0.275	Depositor DCC
$R_{free}$ test set	6467 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.4	Xtrriage
Anisotropy	0.486	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 35.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13747	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.39% 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: GLR, GOL, 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	0.44	0/3499	0.57	0/4740
1	B	0.43	0/3499	0.57	0/4740
1	C	0.38	0/3435	0.54	0/4653
1	D	0.36	0/3380	0.51	0/4580
All	All	0.40	0/13813	0.55	0/18713

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	3421	0	3357	39	0
1	B	3421	0	3357	40	0
1	C	3359	0	3298	53	0
1	D	3304	0	3245	83	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	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	6	0	0
3	C	13	0	6	0	0
3	D	13	0	6	0	0
4	A	6	0	8	1	0
4	B	6	0	8	0	0
4	D	6	0	8	2	0
5	A	56	0	0	1	0
5	B	67	0	0	1	0
5	C	28	0	0	2	0
5	D	17	0	0	2	0
All	All	13747	0	13305	203	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 8.

All (203) 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:D:220:ILE:HD11	1:D:234:LEU:HD13	1.56	0.85
1:D:289:ASN:HD22	1:D:339:HIS:CD2	2.01	0.79
1:B:5:PHE:CD1	1:D:47:SER:HB3	2.18	0.78
1:C:205:LYS:HD2	5:C:464:HOH:O	1.84	0.77
1:C:205:LYS:HG3	1:C:233:THR:HG23	1.66	0.77
1:B:55:ILE:HD11	1:B:65:LEU:HD11	1.66	0.77
1:D:303:SER:OG	4:D:449:GOL:H32	1.85	0.76
1:C:9:VAL:HG22	1:C:76:THR:HG22	1.68	0.75
1:A:55:ILE:HD11	1:A:65:LEU:HD11	1.69	0.73
1:C:55:ILE:HD11	1:C:65:LEU:HD11	1.74	0.70
1:B:313:ASP:HB3	1:B:316:PHE:CE1	2.27	0.69
1:D:403:ASP:OD2	1:D:406:GLN:HG2	1.94	0.67
1:C:414:TYR:HA	1:C:419:LEU:HD12	1.77	0.67
1:D:344:PHE:CD2	1:D:378:LEU:HG	2.29	0.67
1:C:160:THR:HG22	1:C:430:TYR:HB2	1.74	0.67
1:C:259:ALA:HB1	1:C:262:PRO:HG3	1.79	0.65
1:A:103:THR:HG22	1:A:237:ASN:CG	2.18	0.63
1:D:417:HIS:HB2	1:D:419:LEU:HD11	1.81	0.62
1:C:241:SER:OG	1:C:244:GLU:HG3	1.99	0.62
1:B:275:MET:HG3	1:B:291:ILE:HD13	1.82	0.62
1:C:189:VAL:O	1:C:193:GLU:HG3	2.01	0.61
1:C:67:ASP:O	1:C:70:PRO:HD2	2.02	0.60
1:C:289:ASN:C	1:C:289:ASN:HD22	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:ALA:HB1	1:D:262:PRO:HG3	1.84	0.60
1:D:339:HIS:HA	1:D:366:ASP:HB2	1.83	0.59
1:B:5:PHE:CE1	1:D:47:SER:HB3	2.37	0.59
1:D:160:THR:HG22	1:D:430:TYR:HB2	1.85	0.59
1:C:94:ARG:HB3	1:C:108:THR:HB	1.85	0.59
1:D:148:LEU:HD11	1:D:366:ASP:HA	1.85	0.58
1:C:203:ASP:OD1	1:C:231:ARG:HB2	2.03	0.58
1:A:416:LYS:HE2	1:A:417:HIS:CE1	2.38	0.58
1:C:95:ASP:OD2	1:C:107:ARG:HG2	2.02	0.58
1:D:383:PHE:CZ	1:D:393:PRO:HG2	2.39	0.58
1:C:338:SER:HB3	1:C:365:ILE:HG23	1.86	0.58
1:B:99:ARG:HG3	1:B:105:ASP:OD2	2.04	0.57
1:D:203:ASP:OD1	1:D:231:ARG:HB2	2.04	0.57
1:D:144:GLU:CD	1:D:389:LEU:HD13	2.25	0.57
1:A:94:ARG:HH11	1:A:94:ARG:HG3	1.70	0.56
1:C:95:ASP:CG	1:C:107:ARG:HG2	2.24	0.56
1:D:122:ASP:O	1:D:126:GLN:HG3	2.05	0.56
1:B:69:ILE:HB	1:B:70:PRO:HD3	1.85	0.56
1:D:338:SER:HB3	1:D:365:ILE:HD12	1.87	0.56
1:D:342:ASN:HD22	1:D:372:GLN:HE22	1.53	0.56
1:A:55:ILE:HB	1:A:56:PRO:CD	2.35	0.56
1:C:275:MET:HG3	1:C:291:ILE:HD13	1.87	0.56
1:D:314:PRO:HG3	1:D:354:VAL:HG11	1.88	0.56
1:D:414:TYR:O	1:D:419:LEU:HD12	2.06	0.56
1:C:416:LYS:HD3	1:C:417:HIS:CE1	2.40	0.55
1:D:303:SER:HG	4:D:449:GOL:H32	1.70	0.55
1:D:275:MET:HG3	1:D:291:ILE:HD13	1.89	0.55
1:A:24:MET:HG3	1:A:164:TYR:CZ	2.42	0.55
1:D:17:PRO:HG3	1:D:62:ARG:CD	2.37	0.54
1:D:131:ASN:HB2	1:D:353:HIS:CE1	2.43	0.54
1:D:185:PRO:O	1:D:189:VAL:HG23	2.08	0.53
1:B:341:ASN:HA	1:B:368:HIS:CE1	2.44	0.53
1:D:144:GLU:OE1	1:D:389:LEU:HD13	2.07	0.53
4:A:449:GOL:H12	1:C:302:LEU:O	2.08	0.53
1:B:5:PHE:HD1	1:D:47:SER:HB3	1.70	0.53
1:D:261:ASP:HB2	5:D:463:HOH:O	2.09	0.52
1:A:80:TYR:OH	1:A:81:LYS:HE3	2.10	0.52
1:D:226:ARG:HG3	1:D:227:PHE:CE1	2.45	0.52
1:C:432:ILE:O	1:C:435:TRP:HB2	2.11	0.51
1:D:10:VAL:HG12	1:D:73:VAL:HA	1.92	0.51
1:D:131:ASN:HB2	1:D:353:HIS:HE1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:HD11	1:B:117:GLU:HG3	1.92	0.51
1:D:223:LEU:HB3	1:D:232:ILE:HD13	1.93	0.51
1:B:417:HIS:HB2	1:B:419:LEU:HG	1.91	0.51
1:C:417:HIS:HB2	1:C:419:LEU:HG	1.92	0.51
1:D:313:ASP:OD2	1:D:314:PRO:HD2	2.11	0.51
1:C:261:ASP:HB2	5:C:474:HOH:O	2.09	0.51
1:D:17:PRO:HB2	1:D:414:TYR:CD1	2.46	0.51
1:C:339:HIS:HA	1:C:366:ASP:HB2	1.93	0.50
1:D:193:GLU:HG2	1:D:226:ARG:HH21	1.75	0.50
1:D:79:GLU:O	1:D:83:VAL:HG23	2.10	0.50
1:D:40:ILE:HD12	1:D:346:ILE:HD12	1.93	0.50
1:A:298:MET:O	1:A:302:LEU:HG	2.12	0.49
1:D:327:GLN:HA	1:D:359:PRO:HG2	1.94	0.49
1:C:313:ASP:HB2	1:C:339:HIS:ND1	2.28	0.49
1:D:223:LEU:HB3	1:D:232:ILE:CD1	2.43	0.49
1:B:5:PHE:HD1	1:D:47:SER:CB	2.26	0.49
1:A:184:THR:HB	1:A:185:PRO:HD2	1.94	0.48
1:A:234:LEU:HD23	1:A:240:TRP:HH2	1.78	0.48
1:B:340:SER:O	1:B:368:HIS:HE1	1.96	0.48
1:B:117:GLU:OE1	1:B:320:GLN:HG3	2.13	0.48
1:D:193:GLU:HG2	1:D:226:ARG:NH2	2.28	0.48
1:D:205:LYS:HA	1:D:233:THR:HG23	1.96	0.48
1:D:217:ALA:O	1:D:221:VAL:HG23	2.13	0.48
1:A:17:PRO:HB2	1:A:414:TYR:CD1	2.48	0.48
1:B:18:VAL:HB	1:B:410:ALA:HB1	1.95	0.48
1:C:313:ASP:OD2	1:C:314:PRO:HD2	2.14	0.48
1:B:47:SER:HB2	1:D:5:PHE:CD1	2.49	0.48
1:C:384:GLU:HB3	1:C:386:LYS:HE3	1.95	0.47
1:D:148:LEU:HD12	1:D:148:LEU:O	2.14	0.47
1:A:29:GLY:O	1:A:424:ASP:HB2	2.14	0.47
1:B:383:PHE:CZ	1:B:393:PRO:HG2	2.49	0.47
1:B:395:LYS:H	1:B:395:LYS:HG2	1.39	0.47
1:C:301:THR:HG23	1:C:306:SER:HB2	1.96	0.47
1:D:150:TYR:OH	1:D:205:LYS:HE2	2.14	0.47
1:B:441:ARG:HG2	1:B:446:ARG:NH1	2.29	0.47
1:C:157:ARG:HB2	1:C:164:TYR:HB2	1.96	0.47
1:D:110:ILE:CD1	1:D:318:THR:HG23	2.45	0.46
1:B:324:ARG:HD3	1:D:324:ARG:HG2	1.97	0.46
1:D:408:MET:O	1:D:412:GLU:HG3	2.15	0.46
1:D:212:ALA:O	1:D:216:GLU:HG3	2.15	0.46
1:A:151:LEU:HD11	1:A:192:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:SER:O	1:A:366:ASP:HB2	2.15	0.46
1:B:323:VAL:O	1:B:327:GLN:HG3	2.16	0.46
1:D:34:ALA:HA	1:D:164:TYR:CE2	2.50	0.46
1:D:166:SER:O	1:D:167:GLN:HG3	2.15	0.46
1:B:207:LYS:HD2	5:B:450:HOH:O	2.16	0.46
1:B:29:GLY:O	1:B:424:ASP:HB2	2.16	0.46
1:B:55:ILE:HB	1:B:56:PRO:HD2	1.97	0.46
1:D:110:ILE:HD11	1:D:318:THR:HG23	1.98	0.46
1:C:148:LEU:HD21	1:C:366:ASP:OD1	2.16	0.45
1:A:55:ILE:HB	1:A:56:PRO:HD2	1.97	0.45
1:A:324:ARG:HG2	1:C:324:ARG:HD3	1.98	0.45
1:C:84:LEU:HD22	1:C:113:VAL:HG13	1.97	0.45
1:A:275:MET:HG3	1:A:291:ILE:HD13	1.99	0.45
1:C:69:ILE:O	1:C:73:VAL:HG13	2.16	0.45
1:D:84:LEU:HD22	1:D:113:VAL:HG13	1.97	0.45
1:D:55:ILE:HB	1:D:56:PRO:HD2	1.99	0.45
1:D:20:GLY:HA3	1:D:36:PHE:CE1	2.52	0.45
1:A:17:PRO:HG3	1:A:62:ARG:CD	2.47	0.45
1:C:17:PRO:HG3	1:C:62:ARG:HD3	1.98	0.45
1:C:116:ILE:O	1:C:120:MET:HG2	2.17	0.45
1:B:5:PHE:CD1	1:D:47:SER:CB	2.94	0.44
1:B:5:PHE:CD2	1:D:6:THR:HB	2.53	0.44
1:B:236:PRO:HG2	1:B:262:PRO:HA	2.00	0.44
1:D:111:HIS:HD2	1:D:315:HIS:O	2.01	0.44
1:D:311:LEU:HD23	1:D:337:GLY:HA3	2.00	0.44
1:A:313:ASP:HB3	1:A:316:PHE:CE2	2.52	0.44
1:C:55:ILE:HB	1:C:56:PRO:HD2	2.00	0.44
1:D:259:ALA:CB	1:D:262:PRO:HG3	2.48	0.44
1:A:99:ARG:NH2	1:A:290:MET:HG2	2.33	0.43
1:C:38:ARG:NE	1:C:54:GLU:OE2	2.46	0.43
1:A:214:GLU:O	1:A:217:ALA:HB3	2.17	0.43
1:A:331:GLU:HB3	1:C:295:TRP:HB3	2.00	0.43
1:D:162:LEU:HA	1:D:163:PRO:HD3	1.69	0.43
1:D:202:ASN:O	1:D:230:ALA:HA	2.18	0.43
1:B:8:PRO:HD3	1:B:127:HIS:CE1	2.53	0.43
1:C:88:ARG:NH2	1:C:110:ILE:HD11	2.34	0.43
1:A:207:LYS:HE3	3:A:448:GLR:H21	2.01	0.43
1:C:122:ASP:O	1:C:126:GLN:HG3	2.18	0.43
1:A:207:LYS:HD2	5:A:462:HOH:O	2.17	0.43
1:A:99:ARG:HG3	1:A:105:ASP:HA	2.01	0.43
1:B:340:SER:O	1:B:368:HIS:CE1	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:VAL:HG21	1:A:116:ILE:HD13	2.00	0.43
1:A:220:ILE:HD11	1:A:234:LEU:HB2	2.01	0.43
1:C:45:ASP:C	1:C:47:SER:H	2.21	0.43
1:A:69:ILE:N	1:A:70:PRO:CD	2.81	0.42
1:B:341:ASN:O	1:B:342:ASN:C	2.57	0.42
1:C:378:LEU:O	1:C:402:ILE:HD12	2.19	0.42
1:D:289:ASN:ND2	1:D:339:HIS:CD2	2.81	0.42
1:D:151:LEU:O	1:D:206:LEU:HD12	2.19	0.42
1:B:82:ASN:HD21	1:D:134:SER:HB3	1.84	0.42
1:B:90:THR:HG22	1:B:90:THR:O	2.20	0.42
1:C:346:ILE:HD11	1:C:402:ILE:HD13	2.00	0.42
1:A:99:ARG:HG3	1:A:105:ASP:CG	2.40	0.42
1:C:25:LEU:HB2	1:C:32:HIS:CG	2.55	0.42
1:D:7:THR:HA	1:D:8:PRO:HD3	1.86	0.42
1:B:358:ALA:HA	1:B:359:PRO:HD3	1.86	0.42
1:C:69:ILE:HB	1:C:70:PRO:HD3	2.00	0.42
1:C:402:ILE:HD12	1:C:402:ILE:HA	1.86	0.42
1:B:38:ARG:HD3	1:B:342:ASN:O	2.20	0.42
1:D:372:GLN:NE2	5:D:466:HOH:O	2.35	0.42
1:A:32:HIS:CE1	1:A:342:ASN:OD1	2.72	0.42
1:A:358:ALA:HA	1:A:359:PRO:HD3	1.85	0.42
1:D:312:ALA:HB3	1:D:336:TRP:HE1	1.85	0.42
1:B:25:LEU:HB2	1:B:32:HIS:CG	2.55	0.42
1:C:106:LEU:HD23	1:C:106:LEU:N	2.35	0.42
1:D:148:LEU:HD12	1:D:148:LEU:C	2.40	0.42
1:D:71:LEU:HD22	1:D:86:LEU:HD21	2.01	0.41
1:D:289:ASN:HB2	1:D:339:HIS:CE1	2.55	0.41
1:B:27:ASN:N	1:B:27:ASN:HD22	2.18	0.41
1:B:99:ARG:HD2	1:B:293:THR:HG21	2.03	0.41
1:C:309:ILE:HA	1:C:335:THR:O	2.20	0.41
1:D:167:GLN:OE1	1:D:179:HIS:NE2	2.47	0.41
1:D:409:LYS:HE3	1:D:409:LYS:HB2	1.71	0.41
1:D:348:LEU:HD22	1:D:369:TRP:CD1	2.56	0.41
1:A:294:ASP:OD1	1:A:297:GLN:HG3	2.21	0.41
1:A:416:LYS:HE2	1:A:417:HIS:HE1	1.85	0.41
1:C:205:LYS:CG	1:C:233:THR:HG23	2.44	0.41
1:C:8:PRO:HD3	1:C:127:HIS:CE1	2.56	0.41
1:D:253:LYS:O	1:D:253:LYS:HD3	2.21	0.41
1:A:413:LEU:HD12	1:A:417:HIS:NE2	2.35	0.41
1:C:91:PHE:O	1:C:109:THR:OG1	2.31	0.41
1:D:19:ALA:HA	1:D:36:PHE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:LEU:CD2	1:D:337:GLY:HA3	2.50	0.41
1:A:206:LEU:HD23	1:A:234:LEU:HD13	2.03	0.41
1:C:152:PHE:CE1	1:C:207:LYS:HG2	2.55	0.41
1:B:99:ARG:HG3	1:B:105:ASP:CG	2.42	0.40
1:D:342:ASN:HD22	1:D:372:GLN:NE2	2.15	0.40
1:A:380:LYS:HG3	1:A:401:GLU:HB2	2.03	0.40
1:C:117:GLU:OE1	1:C:320:GLN:HG3	2.20	0.40
1:D:236:PRO:HG3	1:D:240:TRP:CZ2	2.56	0.40
1:B:81:LYS:HD3	1:D:137:GLY:O	2.21	0.40
1:C:383:PHE:CZ	1:C:393:PRO:HG2	2.57	0.40
1:A:165:GLN:HA	1:A:165:GLN:NE2	2.36	0.40
1:A:207:LYS:HE3	3:A:448:GLR:C2	2.52	0.40
1:A:260:GLU:O	1:A:261:ASP:C	2.58	0.40
1:B:55:ILE:HB	1:B:56:PRO:CD	2.51	0.40
1:D:114:THR:OG1	1:D:318:THR:HA	2.22	0.40
1:D:167:GLN:N	1:D:168:PRO:HD3	2.37	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	440/446 (99%)	423 (96%)	17 (4%)	0	100	100
1	B	440/446 (99%)	425 (97%)	15 (3%)	0	100	100
1	C	429/446 (96%)	408 (95%)	19 (4%)	2 (0%)	29	23
1	D	423/446 (95%)	397 (94%)	25 (6%)	1 (0%)	47	44
All	All	1732/1784 (97%)	1653 (95%)	76 (4%)	3 (0%)	47	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	419	LEU
1	C	46	ASN
1	D	420	GLY

### 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	356/360 (99%)	343 (96%)	13 (4%)	34 32
1	B	356/360 (99%)	348 (98%)	8 (2%)	52 55
1	C	351/360 (98%)	336 (96%)	15 (4%)	29 26
1	D	345/360 (96%)	337 (98%)	8 (2%)	50 53
All	All	1408/1440 (98%)	1364 (97%)	44 (3%)	40 40

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	27	ASN
1	A	55	ILE
1	A	79	GLU
1	A	150	TYR
1	A	168	PRO
1	A	214	GLU
1	A	233	THR
1	A	318	THR
1	A	339	HIS
1	A	380	LYS
1	A	417	HIS
1	A	419	LEU
1	B	27	ASN
1	B	79	GLU
1	B	94	ARG
1	B	150	TYR
1	B	160	THR
1	B	339	HIS

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Mol	Chain	Res	Type
1	B	395	LYS
1	B	402	ILE
1	C	4	GLN
1	C	15	VAL
1	C	73	VAL
1	C	79	GLU
1	C	88	ARG
1	C	93	ASP
1	C	106	LEU
1	C	150	TYR
1	C	253	LYS
1	C	289	ASN
1	C	339	HIS
1	C	347	SER
1	C	351	PHE
1	C	395	LYS
1	C	439	ASN
1	D	14	GLN
1	D	73	VAL
1	D	150	TYR
1	D	214	GLU
1	D	233	THR
1	D	307	VAL
1	D	395	LYS
1	D	419	LEU

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

Mol	Chain	Res	Type
1	C	179	HIS
1	D	229	GLN
1	D	339	HIS
1	D	372	GLN

### 5.3.3 RNA

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 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	D	448	2	11,12,12	1.68	3 (27%)	10,16,16	2.18	4 (40%)
3	GLR	C	448	2	11,12,12	1.62	2 (18%)	10,16,16	1.75	4 (40%)
3	GLR	B	448	2	11,12,12	1.69	3 (27%)	10,16,16	1.40	2 (20%)
4	GOL	D	449	-	5,5,5	0.23	0	5,5,5	0.52	0
4	GOL	B	449	-	5,5,5	0.28	0	5,5,5	0.54	0
3	GLR	A	448	2	11,12,12	1.67	4 (36%)	10,16,16	1.41	2 (20%)
4	GOL	A	449	-	5,5,5	0.38	0	5,5,5	0.42	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLR	D	448	2	-	1/16/16/16	-
3	GLR	C	448	2	-	0/16/16/16	-
3	GLR	B	448	2	-	1/16/16/16	-
4	GOL	D	449	-	-	2/4/4/4	-
4	GOL	B	449	-	-	4/4/4/4	-
3	GLR	A	448	2	-	1/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	449	-	-	2/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	448	GLR	O5-C5	2.58	1.28	1.23
3	C	448	GLR	O5-C5	2.57	1.28	1.23
3	B	448	GLR	O5-C5	2.51	1.28	1.23
3	A	448	GLR	O5-C5	2.46	1.28	1.23
3	C	448	GLR	O2-C2	2.43	1.47	1.42
3	B	448	GLR	C5-C6	-2.38	1.50	1.53
3	D	448	GLR	C4-C5	2.28	1.55	1.51
3	A	448	GLR	O6A-C6	2.24	1.28	1.22
3	A	448	GLR	C4-C5	2.17	1.55	1.51
3	D	448	GLR	O2-C2	2.14	1.46	1.42
3	B	448	GLR	O6A-C6	2.12	1.28	1.22
3	A	448	GLR	C5-C6	-2.00	1.50	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	448	GLR	O5-C5-C6	3.73	124.83	119.43
3	D	448	GLR	O6A-C6-C5	-3.65	116.84	121.72
3	D	448	GLR	O6B-C6-C5	3.64	123.93	113.97
3	C	448	GLR	O6B-C6-C5	3.00	122.17	113.97
3	C	448	GLR	O5-C5-C6	2.97	123.73	119.43
3	B	448	GLR	O5-C5-C6	2.65	123.27	119.43
3	A	448	GLR	O6A-C6-C5	-2.50	118.38	121.72
3	C	448	GLR	O6A-C6-C5	-2.15	118.85	121.72
3	C	448	GLR	O6B-C6-O6A	-2.09	118.83	123.61
3	B	448	GLR	O6A-C6-C5	-2.07	118.96	121.72
3	D	448	GLR	O6B-C6-O6A	-2.02	118.97	123.61
3	A	448	GLR	O6B-C6-C5	2.02	119.49	113.97

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	448	GLR	C4-C5-C6-O6B
3	D	448	GLR	C4-C5-C6-O6B
4	A	449	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	B	449	GOL	C1-C2-C3-O3
4	D	449	GOL	O1-C1-C2-C3
4	A	449	GOL	O1-C1-C2-O2
4	B	449	GOL	O1-C1-C2-C3
4	D	449	GOL	O1-C1-C2-O2
3	A	448	GLR	O1B-C1-C2-C3
4	B	449	GOL	O1-C1-C2-O2
4	B	449	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	449	GOL	2	0
3	A	448	GLR	2	0
4	A	449	GOL	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

### 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%)	0.13	13 (2%) 51 50	32, 44, 61, 79	0
1	B	442/446 (99%)	0.12	12 (2%) 54 53	32, 44, 62, 76	0
1	C	433/446 (97%)	0.25	22 (5%) 28 27	35, 52, 71, 86	0
1	D	427/446 (95%)	0.26	20 (4%) 31 30	38, 57, 77, 88	0
All	All	1744/1784 (97%)	0.19	67 (3%) 40 39	32, 49, 70, 88	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	430	TYR	6.8
1	C	430	TYR	6.8
1	C	106	LEU	5.2
1	C	420	GLY	5.0
1	A	101	LEU	4.9
1	D	418	GLY	4.7
1	B	420	GLY	4.6
1	A	96	ALA	4.3
1	C	93	ASP	4.1
1	D	429	GLN	3.9
1	D	168	PRO	3.7
1	C	107	ARG	3.5
1	C	163	PRO	3.4
1	D	433	PRO	3.4
1	D	435	TRP	3.3
1	C	436	THR	3.3
1	D	436	THR	3.3
1	D	432	ILE	3.3
1	C	426	MET	3.2
1	D	162	LEU	3.2
1	B	418	GLY	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	93	ASP	3.2
1	C	94	ARG	3.2
1	D	420	GLY	3.2
1	C	162	LEU	3.2
1	D	426	MET	3.2
1	C	433	PRO	3.1
1	D	431	LEU	2.9
1	D	434	GLY	2.9
1	C	435	TRP	2.9
1	A	102	GLN	2.9
1	B	311	LEU	2.9
1	D	169	ASP	2.9
1	A	92	ALA	2.8
1	B	150	TYR	2.8
1	A	338	SER	2.8
1	D	425	ALA	2.8
1	C	148	LEU	2.8
1	D	161	PRO	2.8
1	C	437	PHE	2.8
1	B	98	GLY	2.7
1	B	367	THR	2.7
1	A	367	THR	2.6
1	A	97	GLY	2.5
1	D	428	MET	2.5
1	A	106	LEU	2.5
1	C	351	PHE	2.5
1	B	92	ALA	2.4
1	A	314	PRO	2.3
1	C	164	TYR	2.3
1	C	150	TYR	2.3
1	D	197	GLU	2.3
1	B	316	PHE	2.3
1	C	418	GLY	2.2
1	C	434	GLY	2.2
1	B	312	ALA	2.2
1	C	169	ASP	2.2
1	A	229	GLN	2.1
1	B	6	THR	2.1
1	D	158	LYS	2.1
1	B	5	PHE	2.1
1	A	95	ASP	2.1
1	A	225	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	172	CYS	2.1
1	B	365	ILE	2.0
1	C	60	LYS	2.0
1	C	366	ASP	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(Å <sup>2</sup> )	Q<0.9
3	GLR	D	448	13/13	0.66	0.24	57,65,67,67	0
2	MG	D	447	1/1	0.77	0.18	56,56,56,56	0
3	GLR	C	448	13/13	0.80	0.18	51,57,63,64	0
2	MG	C	447	1/1	0.83	0.18	57,57,57,57	0
2	MG	A	447	1/1	0.88	0.18	49,49,49,49	0
4	GOL	B	449	6/6	0.89	0.15	34,37,45,51	0
3	GLR	A	448	13/13	0.91	0.17	38,48,52,52	0
4	GOL	A	449	6/6	0.92	0.11	34,43,45,45	0
3	GLR	B	448	13/13	0.94	0.18	38,46,49,51	0
4	GOL	D	449	6/6	0.94	0.11	37,42,48,50	0
2	MG	B	447	1/1	0.95	0.25	46,46,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.