



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:34 AM UTC

PDB ID : 3P0W / pdb_00003p0w
Title : Crystal structure of D-Glucarate dehydratase from *Ralstonia solanacearum* complexed with Mg and D-glucarate
Authors : Fedorov, A.A.; Fedorov, E.V.; Gerlt, J.A.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2010-09-29
Resolution : 1.71 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

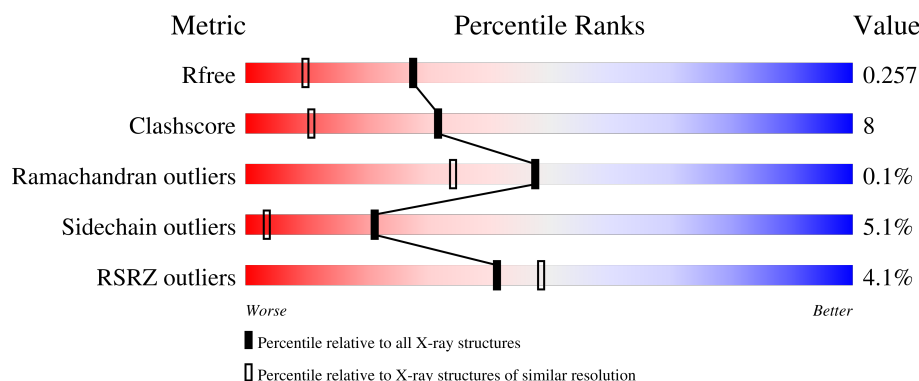
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

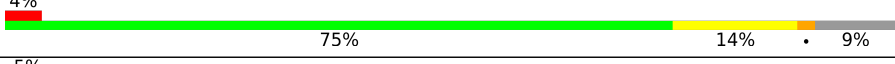
The reported resolution of this entry is 1.71 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	470	
1	B	470	
1	C	470	
1	D	470	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13261 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 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3237	2040	587	590	20			
1	B	428	Total	C	N	O	S	0	0	0
			3270	2061	592	597	20			
1	C	421	Total	C	N	O	S	0	0	0
			3220	2031	583	586	20			
1	D	425	Total	C	N	O	S	0	0	0
			3244	2044	588	592	20			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP B2UIZ1
A	2	SER	-	expression tag	UNP B2UIZ1
A	3	LEU	-	expression tag	UNP B2UIZ1
A	463	GLU	-	expression tag	UNP B2UIZ1
A	464	GLY	-	expression tag	UNP B2UIZ1
A	465	HIS	-	expression tag	UNP B2UIZ1
A	466	HIS	-	expression tag	UNP B2UIZ1
A	467	HIS	-	expression tag	UNP B2UIZ1
A	468	HIS	-	expression tag	UNP B2UIZ1
A	469	HIS	-	expression tag	UNP B2UIZ1
A	470	HIS	-	expression tag	UNP B2UIZ1
B	1	MET	-	expression tag	UNP B2UIZ1
B	2	SER	-	expression tag	UNP B2UIZ1
B	3	LEU	-	expression tag	UNP B2UIZ1
B	463	GLU	-	expression tag	UNP B2UIZ1
B	464	GLY	-	expression tag	UNP B2UIZ1
B	465	HIS	-	expression tag	UNP B2UIZ1
B	466	HIS	-	expression tag	UNP B2UIZ1
B	467	HIS	-	expression tag	UNP B2UIZ1
B	468	HIS	-	expression tag	UNP B2UIZ1
B	469	HIS	-	expression tag	UNP B2UIZ1

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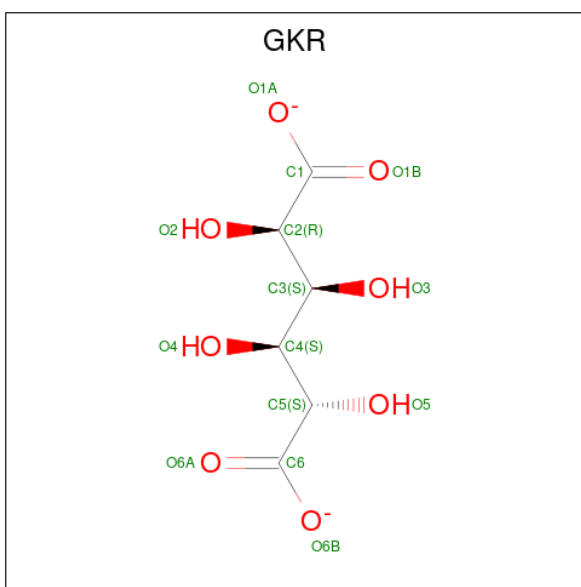
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Chain	Residue	Modelled	Actual	Comment	Reference
B	470	HIS	-	expression tag	UNP B2UIZ1
C	1	MET	-	expression tag	UNP B2UIZ1
C	2	SER	-	expression tag	UNP B2UIZ1
C	3	LEU	-	expression tag	UNP B2UIZ1
C	463	GLU	-	expression tag	UNP B2UIZ1
C	464	GLY	-	expression tag	UNP B2UIZ1
C	465	HIS	-	expression tag	UNP B2UIZ1
C	466	HIS	-	expression tag	UNP B2UIZ1
C	467	HIS	-	expression tag	UNP B2UIZ1
C	468	HIS	-	expression tag	UNP B2UIZ1
C	469	HIS	-	expression tag	UNP B2UIZ1
C	470	HIS	-	expression tag	UNP B2UIZ1
D	1	MET	-	expression tag	UNP B2UIZ1
D	2	SER	-	expression tag	UNP B2UIZ1
D	3	LEU	-	expression tag	UNP B2UIZ1
D	463	GLU	-	expression tag	UNP B2UIZ1
D	464	GLY	-	expression tag	UNP B2UIZ1
D	465	HIS	-	expression tag	UNP B2UIZ1
D	466	HIS	-	expression tag	UNP B2UIZ1
D	467	HIS	-	expression tag	UNP B2UIZ1
D	468	HIS	-	expression tag	UNP B2UIZ1
D	469	HIS	-	expression tag	UNP B2UIZ1
D	470	HIS	-	expression tag	UNP B2UIZ1

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is D-GLUCARATE (CCD ID: GKR) (formula: C₆H₈O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	6	8		
3	B	1	Total	C	O	0	0
			14	6	8		
3	C	1	Total	C	O	0	0
			14	6	8		
3	D	1	Total	C	O	0	0
			14	6	8		

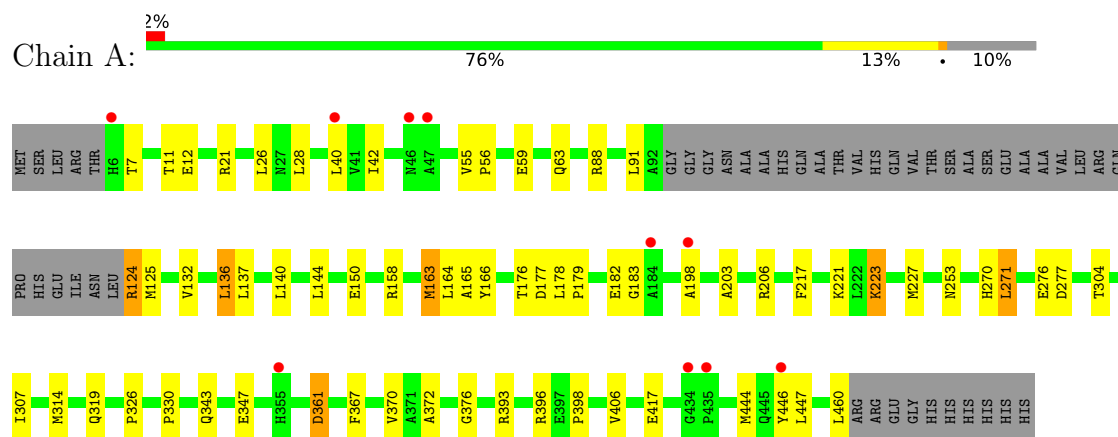
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	99	Total	O	0	0
			99	99		
4	C	42	Total	O	0	0
			42	42		
4	D	38	Total	O	0	0
			38	38		

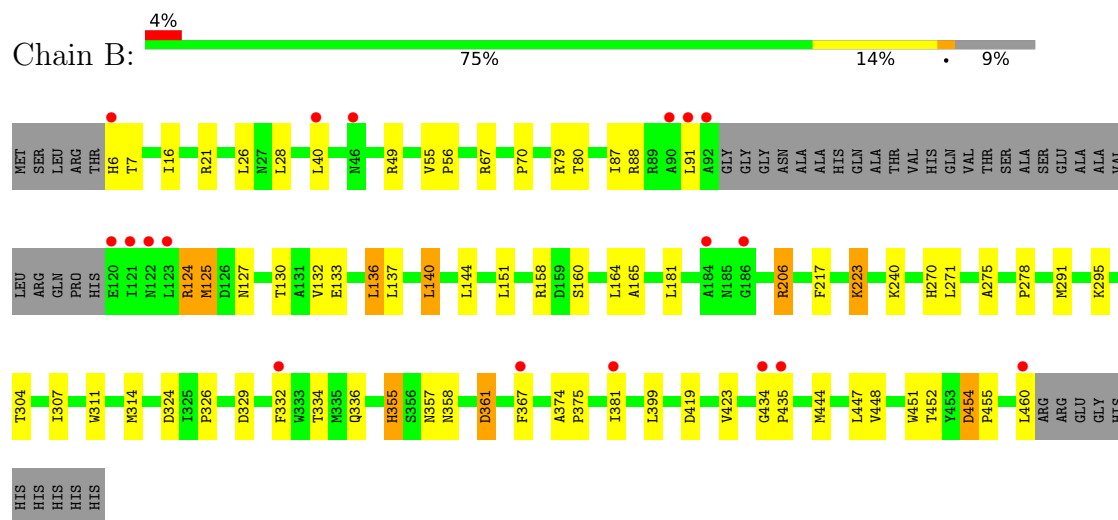
3 Residue-property plots

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.

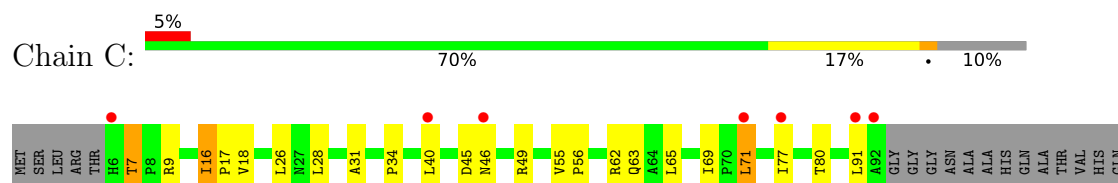
- Molecule 1: Mandelate racemase/muconate lactonizing protein

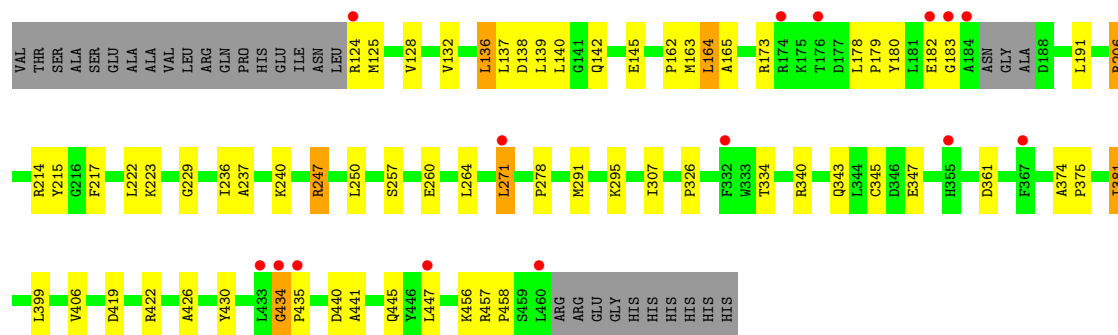


- Molecule 1: Mandelate racemase/muconate lactonizing protein

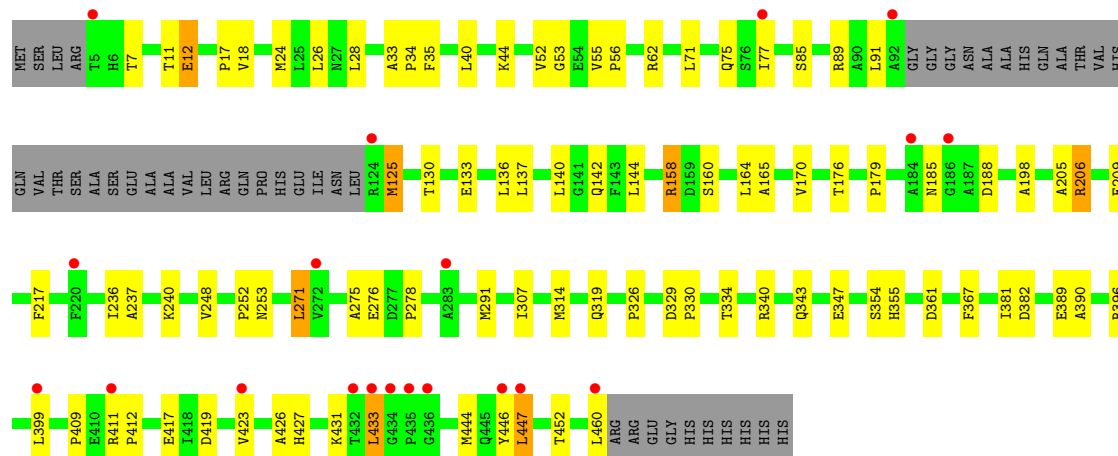


- Molecule 1: Mandelate racemase/muconate lactonizing protein





• Molecule 1: Mandelate racemase/muconate lactonizing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.96Å 128.82Å 178.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.01 – 1.71 39.01 – 1.71	Depositor EDS
% Data completeness (in resolution range)	76.7 (39.01-1.71) 76.8 (39.01-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 1.71Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.227 , 0.265 0.221 , 0.257	Depositor DCC
R_{free} test set	7649 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtrriage
Anisotropy	0.320	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 25.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13261	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GKR, 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	0.51	0/3312	0.84	2/4504 (0.0%)
1	B	0.53	0/3345	0.86	2/4549 (0.0%)
1	C	0.49	0/3294	0.85	3/4478 (0.1%)
1	D	0.52	0/3319	0.82	2/4514 (0.0%)
All	All	0.51	0/13270	0.84	9/18045 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	454	ASP	CA-C-N	5.59	125.20	119.56
1	B	454	ASP	C-N-CA	5.59	125.20	119.56
1	C	434	GLY	CA-C-N	5.23	126.38	119.84
1	C	434	GLY	C-N-CA	5.23	126.38	119.84
1	C	69	ILE	CB-CA-C	-5.22	108.74	113.70
1	D	33	ALA	CA-C-N	5.10	124.76	119.56
1	D	33	ALA	C-N-CA	5.10	124.76	119.56
1	A	227	MET	CA-C-N	-5.04	114.59	119.78
1	A	227	MET	C-N-CA	-5.04	114.59	119.78

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	3237	0	3196	41	1
1	B	3270	0	3230	53	0
1	C	3220	0	3181	58	0
1	D	3244	0	3203	65	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	14	0	8	0	0
3	B	14	0	8	3	0
3	C	14	0	8	0	0
3	D	14	0	8	0	0
4	A	51	0	0	3	0
4	B	99	0	0	2	0
4	C	42	0	0	5	0
4	D	38	0	0	1	1
All	All	13261	0	12842	209	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 (209) 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:C:206:ARG:HH11	1:C:206:ARG:HG3	1.07	1.10
1:B:206:ARG:HG3	1:B:206:ARG:HH11	1.02	1.08
1:C:9:ARG:H	1:C:46:ASN:HB2	1.31	0.94
1:D:158:ARG:HH11	1:D:158:ARG:HG2	1.33	0.91
1:B:206:ARG:HG3	1:B:206:ARG:NH1	1.83	0.88
1:C:206:ARG:HG3	1:C:206:ARG:NH1	1.87	0.87
1:A:343:GLN:O	1:A:347:GLU:HG2	1.76	0.85
1:C:236:ILE:HG22	1:C:271:LEU:HD12	1.62	0.82
1:B:91:LEU:HD13	1:B:125:MET:HB2	1.61	0.81
1:C:16:ILE:HB	1:C:40:LEU:HD11	1.66	0.78
1:B:206:ARG:HH11	1:B:206:ARG:CG	1.93	0.77
1:B:355:HIS:CD2	3:B:472:GKR:H51	2.21	0.76
1:D:444:MET:HE1	1:D:460:LEU:HD21	1.69	0.75
1:D:158:ARG:HH11	1:D:158:ARG:CG	2.00	0.75
1:B:16:ILE:HB	1:B:40:LEU:CD1	2.17	0.74
1:A:166:TYR:CZ	1:A:221:LYS:HE2	2.23	0.73
1:A:166:TYR:CE1	1:A:221:LYS:HE2	2.24	0.72
1:D:319:GLN:NE2	4:D:503:HOH:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ARG:HH11	1:C:206:ARG:CG	1.96	0.70
1:B:16:ILE:HB	1:B:40:LEU:HD11	1.72	0.70
1:D:55:VAL:HB	1:D:56:PRO:HD2	1.73	0.69
1:B:124:ARG:HG2	1:B:124:ARG:HH11	1.56	0.69
1:B:275:ALA:HB1	1:B:278:PRO:HG3	1.75	0.68
1:B:158:ARG:NH1	1:B:374:ALA:O	2.25	0.68
1:D:206:ARG:HH11	1:D:206:ARG:HG3	1.57	0.68
1:D:343:GLN:O	1:D:347:GLU:HG2	1.94	0.66
1:D:165:ALA:HB2	1:D:217:PHE:CD2	2.31	0.66
1:C:16:ILE:HB	1:C:40:LEU:CD1	2.27	0.65
1:D:409:PRO:HB3	1:D:411:ARG:NH2	2.13	0.64
1:C:340:ARG:HG3	1:D:340:ARG:HD2	1.79	0.63
1:D:133:GLU:O	1:D:137:LEU:HD23	1.99	0.63
1:B:164:LEU:C	1:B:164:LEU:HD12	2.24	0.62
1:A:444:MET:HE1	1:A:460:LEU:HD21	1.82	0.60
1:B:124:ARG:HG2	1:B:124:ARG:NH1	2.13	0.60
1:A:21:ARG:HD2	4:A:520:HOH:O	2.02	0.60
1:C:278:PRO:HD2	1:C:291:MET:SD	2.42	0.60
1:A:132:VAL:HG12	1:A:136:LEU:HD22	1.84	0.60
1:C:173:ARG:HH22	1:C:182:GLU:CD	2.09	0.59
1:D:133:GLU:HG2	1:D:137:LEU:HD23	1.84	0.59
1:B:355:HIS:NE2	3:B:472:GKR:H51	2.16	0.59
1:A:91:LEU:HB2	1:A:125:MET:HE2	1.83	0.59
1:D:206:ARG:HG3	1:D:206:ARG:NH1	2.18	0.58
1:A:40:LEU:C	1:A:40:LEU:HD12	2.29	0.58
1:D:236:ILE:HG22	1:D:271:LEU:CD1	2.35	0.57
1:B:88:ARG:HG3	1:B:125:MET:HE1	1.87	0.57
1:C:17:PRO:HB2	1:C:430:TYR:CD2	2.40	0.57
1:D:278:PRO:HD2	1:D:291:MET:SD	2.44	0.57
1:B:132:VAL:HG12	1:B:136:LEU:HD22	1.87	0.57
1:A:150:GLU:HG3	1:B:79:ARG:NH1	2.20	0.56
1:C:457:ARG:HG2	1:C:458:PRO:O	2.05	0.56
1:C:326:PRO:HG2	1:C:345:CYS:SG	2.46	0.56
1:D:158:ARG:CG	1:D:158:ARG:NH1	2.66	0.56
1:B:448:VAL:O	1:B:451:TRP:HB2	2.06	0.56
1:B:367:PHE:HZ	4:B:557:HOH:O	1.90	0.55
1:D:236:ILE:HG22	1:D:271:LEU:HD12	1.87	0.55
1:A:270:HIS:CD2	1:A:271:LEU:HD13	2.42	0.54
1:C:237:ALA:HA	1:C:271:LEU:HD11	1.90	0.54
1:A:314:MET:HE1	1:A:326:PRO:HB3	1.88	0.54
1:D:11:THR:C	1:D:12:GLU:HG2	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ILE:HB	1:B:40:LEU:HD12	1.88	0.54
1:A:144:LEU:HA	1:B:7:THR:HG21	1.90	0.54
1:A:223:LYS:HE3	1:A:253:ASN:OD1	2.08	0.54
1:B:444:MET:HE1	1:B:460:LEU:HD21	1.89	0.53
1:C:229:GLY:HA3	1:C:264:LEU:HD11	1.91	0.53
1:A:223:LYS:HD2	4:A:513:HOH:O	2.08	0.53
1:D:176:THR:HG22	1:D:446:TYR:CB	2.39	0.53
1:D:427:HIS:O	1:D:431:LYS:HG2	2.09	0.53
1:D:12:GLU:HG3	1:D:44:LYS:HB2	1.91	0.53
1:D:55:VAL:HB	1:D:56:PRO:CD	2.38	0.52
1:D:130:THR:OG1	1:D:334:THR:HA	2.09	0.52
1:C:178:LEU:HD12	1:C:180:TYR:HE1	1.74	0.52
1:C:257:SER:OG	1:C:260:GLU:HG3	2.09	0.52
1:B:223:LYS:HE3	1:B:223:LYS:HA	1.90	0.52
1:C:91:LEU:HD11	1:C:128:VAL:HG11	1.90	0.52
1:A:330:PRO:HD2	1:A:367:PHE:HE1	1.75	0.51
1:C:49:ARG:HD2	4:C:501:HOH:O	2.09	0.51
1:A:55:VAL:HB	1:A:56:PRO:HD2	1.92	0.51
1:C:138:ASP:O	1:C:142:GLN:HG3	2.10	0.51
1:C:240:LYS:HG3	1:C:271:LEU:HD13	1.93	0.51
1:D:236:ILE:HD12	1:D:248:VAL:HG12	1.92	0.51
1:C:456:LYS:HD3	4:C:506:HOH:O	2.11	0.51
1:B:133:GLU:OE2	1:B:336:GLN:HG2	2.10	0.51
1:D:125:MET:HE3	1:D:125:MET:HA	1.93	0.50
1:B:87:ILE:O	1:B:91:LEU:HG	2.11	0.50
1:B:361:ASP:OD1	1:B:361:ASP:N	2.44	0.50
1:C:162:PRO:O	1:C:381:ILE:HG23	2.11	0.50
1:A:7:THR:HG21	1:B:144:LEU:HA	1.93	0.50
1:B:124:ARG:HH11	1:B:124:ARG:CG	2.23	0.49
1:D:91:LEU:HD12	1:D:125:MET:HE1	1.94	0.49
1:D:133:GLU:O	1:D:137:LEU:CD2	2.60	0.48
1:A:198:ALA:HB1	1:A:203:ALA:HB1	1.95	0.48
1:D:17:PRO:HG3	1:D:62:ARG:HD3	1.95	0.48
1:C:206:ARG:HD2	4:C:510:HOH:O	2.13	0.48
1:C:222:LEU:O	1:C:250:LEU:HD12	2.13	0.48
1:D:355:HIS:HA	1:D:382:ASP:HB2	1.96	0.48
1:C:45:ASP:HB3	1:C:139:LEU:HD13	1.95	0.48
1:D:35:PHE:CB	1:D:433:LEU:HD11	2.42	0.48
1:D:176:THR:HG22	1:D:446:TYR:HB3	1.96	0.48
1:D:396:ARG:HD3	1:D:417:GLU:OE2	2.14	0.48
1:D:419:ASP:O	1:D:423:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:MET:HE3	1:A:406:VAL:CG2	2.44	0.48
1:A:176:THR:HA	1:A:446:TYR:CD1	2.49	0.48
1:B:329:ASP:HB3	1:B:332:PHE:CE1	2.49	0.48
1:D:35:PHE:CD2	1:D:433:LEU:HD21	2.49	0.48
1:B:314:MET:HE1	1:B:326:PRO:HB3	1.94	0.47
1:A:304:THR:HG21	1:A:307:ILE:HG12	1.97	0.47
1:D:444:MET:CE	1:D:460:LEU:HD21	2.42	0.47
1:C:223:LYS:HD2	4:C:507:HOH:O	2.14	0.47
1:A:178:LEU:HA	1:A:179:PRO:HD3	1.74	0.47
1:C:55:VAL:HB	1:C:56:PRO:HD2	1.97	0.47
1:C:361:ASP:OD1	1:C:361:ASP:N	2.36	0.47
1:D:176:THR:HG22	1:D:446:TYR:CG	2.50	0.46
1:A:40:LEU:HD13	1:A:42:ILE:HG13	1.96	0.46
1:D:291:MET:HG3	1:D:307:ILE:HD13	1.97	0.46
1:B:80:THR:HG23	1:B:136:LEU:HD23	1.96	0.46
1:D:330:PRO:HD2	1:D:367:PHE:HE1	1.79	0.46
1:B:49:ARG:HD2	4:B:559:HOH:O	2.14	0.46
1:C:163:MET:HE3	1:C:406:VAL:HG21	1.98	0.46
1:D:34:PRO:HG2	1:D:179:PRO:HD2	1.96	0.46
1:A:330:PRO:HG3	1:A:370:VAL:HG11	1.96	0.46
1:C:247:ARG:NH1	4:C:499:HOH:O	2.48	0.46
1:B:278:PRO:HD2	1:B:291:MET:SD	2.56	0.46
1:D:133:GLU:HG2	1:D:137:LEU:CD2	2.45	0.46
1:A:88:ARG:CZ	4:A:519:HOH:O	2.64	0.45
1:C:62:ARG:NH2	1:C:63:GLN:HG2	2.32	0.45
1:D:18:VAL:HB	1:D:426:ALA:HB1	1.98	0.45
1:A:124:ARG:HA	1:A:124:ARG:HD3	1.83	0.45
1:D:205:ALA:O	1:D:209:GLU:HG3	2.15	0.45
1:C:18:VAL:HB	1:C:426:ALA:HB1	1.99	0.45
1:B:434:GLY:HA3	1:B:435:PRO:HD3	1.66	0.45
1:C:65:LEU:HD23	1:C:128:VAL:HG13	1.98	0.45
1:A:150:GLU:HG3	1:B:79:ARG:HH11	1.80	0.45
1:D:188:ASP:OD1	1:D:188:ASP:C	2.60	0.45
1:D:275:ALA:HB1	1:D:278:PRO:HG3	1.99	0.45
1:C:215:TYR:HB2	1:C:217:PHE:CE2	2.51	0.45
1:D:237:ALA:HA	1:D:271:LEU:HD11	1.98	0.45
1:A:361:ASP:OD1	1:A:361:ASP:N	2.40	0.45
1:C:34:PRO:HG2	1:C:179:PRO:HD2	1.99	0.45
1:D:158:ARG:HD3	1:D:160:SER:O	2.17	0.45
1:D:165:ALA:HB2	1:D:217:PHE:CG	2.51	0.45
1:C:132:VAL:HG12	1:C:136:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLU:O	1:A:277:ASP:C	2.60	0.44
1:B:419:ASP:O	1:B:423:VAL:HG23	2.17	0.44
1:D:24:MET:HE1	1:D:447:LEU:HD11	1.97	0.44
1:D:314:MET:HE1	1:D:326:PRO:HB3	1.99	0.44
1:A:11:THR:C	1:A:12:GLU:HG3	2.43	0.44
1:B:355:HIS:HE2	3:B:472:GKR:H51	1.79	0.44
1:A:59:GLU:HG3	1:A:63:GLN:NE2	2.32	0.44
1:A:158:ARG:NH2	1:A:376:GLY:O	2.50	0.44
1:A:396:ARG:HD3	1:A:417:GLU:OE1	2.17	0.44
1:C:164:LEU:C	1:C:164:LEU:HD12	2.42	0.44
1:D:170:VAL:H	1:D:198:ALA:HB3	1.83	0.44
1:B:67:ARG:O	1:B:70:PRO:HD2	2.17	0.43
1:B:130:THR:OG1	1:B:334:THR:HA	2.17	0.43
1:A:164:LEU:HD12	1:A:164:LEU:C	2.43	0.43
1:D:71:LEU:O	1:D:75:GLN:HG3	2.18	0.43
1:D:252:PRO:HG2	1:D:278:PRO:HA	2.01	0.43
1:B:55:VAL:HB	1:B:56:PRO:HD2	2.00	0.43
1:C:178:LEU:HD12	1:C:180:TYR:CE1	2.53	0.43
1:D:142:GLN:HA	1:D:412:PRO:HB2	1.99	0.43
1:C:295:LYS:HB3	1:C:295:LYS:HE2	1.52	0.43
1:B:295:LYS:HE2	1:B:295:LYS:HB3	1.76	0.43
1:C:182:GLU:HG3	1:C:183:GLY:N	2.33	0.43
1:C:145:GLU:OE1	1:D:7:THR:HG23	2.19	0.43
1:C:419:ASP:CG	1:C:422:ARG:HG2	2.43	0.43
1:A:158:ARG:HG2	1:A:372:ALA:HA	2.00	0.43
1:A:393:ARG:HG3	1:A:398:PRO:HG3	2.01	0.43
1:D:330:PRO:HD2	1:D:367:PHE:CE1	2.53	0.43
1:A:165:ALA:HB2	1:A:217:PHE:CD2	2.54	0.42
1:C:441:ALA:O	1:C:445:GLN:HG2	2.19	0.42
1:B:165:ALA:HB2	1:B:217:PHE:CD2	2.54	0.42
1:B:374:ALA:HA	1:B:375:PRO:HD3	1.68	0.42
1:C:434:GLY:HA3	1:C:435:PRO:HD3	1.71	0.42
1:D:411:ARG:HA	1:D:412:PRO:HD3	1.86	0.42
1:B:295:LYS:HZ1	1:B:324:ASP:CG	2.28	0.42
1:D:52:VAL:HG12	1:D:53:GLY:N	2.34	0.42
1:D:354:SER:HB3	1:D:381:ILE:HB	2.00	0.42
1:B:55:VAL:HG11	1:B:127:ASN:O	2.20	0.42
1:C:71:LEU:HD23	1:C:71:LEU:O	2.20	0.42
1:C:165:ALA:HB2	1:C:217:PHE:CD2	2.55	0.42
1:C:80:THR:HG23	1:C:136:LEU:HD23	2.01	0.42
1:C:419:ASP:OD1	1:C:419:ASP:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:THR:HG21	1:B:307:ILE:HG13	2.01	0.41
1:A:182:GLU:HG3	1:A:183:GLY:N	2.35	0.41
1:C:31:ALA:N	1:C:440:ASP:HB3	2.35	0.41
1:D:329:ASP:HB2	1:D:355:HIS:CE1	2.55	0.41
1:D:35:PHE:HB2	1:D:433:LEU:HD11	2.01	0.41
1:C:343:GLN:O	1:C:347:GLU:HG2	2.21	0.41
1:C:191:LEU:HD11	1:C:214:ARG:CZ	2.51	0.41
1:A:177:ASP:OD1	1:A:177:ASP:C	2.63	0.41
1:D:164:LEU:C	1:D:164:LEU:HD12	2.46	0.41
1:A:163:MET:HE3	1:A:406:VAL:HG21	2.02	0.41
1:C:422:ARG:HE	1:C:422:ARG:HB3	1.56	0.41
1:D:85:SER:O	1:D:89:ARG:HG3	2.21	0.41
1:D:252:PRO:HD2	1:D:276:GLU:O	2.21	0.41
1:D:389:GLU:O	1:D:390:ALA:HB3	2.19	0.41
1:C:236:ILE:CG2	1:C:271:LEU:HD12	2.44	0.41
1:B:164:LEU:C	1:B:164:LEU:CD1	2.93	0.40
1:A:347:GLU:HB3	1:B:311:TRP:HB3	2.02	0.40
1:B:140:LEU:HD13	1:B:151:LEU:HD13	2.03	0.40
1:C:291:MET:HE2	1:C:307:ILE:HD13	2.03	0.40
1:B:21:ARG:HD3	1:B:181:LEU:HD11	2.03	0.40
1:B:357:ASN:O	1:B:358:ASN:C	2.64	0.40
1:B:454:ASP:HA	1:B:455:PRO:HD3	1.83	0.40
1:B:240:LYS:HE2	1:B:270:HIS:O	2.21	0.40
1:C:374:ALA:HA	1:C:375:PRO:HD3	1.88	0.40
1:B:158:ARG:HD3	1:B:160:SER:O	2.22	0.40
1:C:7:THR:HG21	1:D:144:LEU:HA	2.04	0.40
1:C:191:LEU:HD23	1:C:191:LEU:HA	1.87	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:A:319:GLN:NE2	4:D:503:HOH:O[2_564]	2.18	0.02

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	420/470 (89%)	410 (98%)	10 (2%)	0	100	100
1	B	424/470 (90%)	413 (97%)	11 (3%)	0	100	100
1	C	415/470 (88%)	404 (97%)	10 (2%)	1 (0%)	43	31
1	D	421/470 (90%)	407 (97%)	14 (3%)	0	100	100
All	All	1680/1880 (89%)	1634 (97%)	45 (3%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	334	THR

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	325/361 (90%)	313 (96%)	12 (4%)	30	8
1	B	329/361 (91%)	312 (95%)	17 (5%)	21	3
1	C	324/361 (90%)	306 (94%)	18 (6%)	19	3
1	D	326/361 (90%)	307 (94%)	19 (6%)	18	3
All	All	1304/1444 (90%)	1238 (95%)	66 (5%)	21	3

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	28	LEU
1	A	124	ARG
1	A	136	LEU
1	A	137	LEU

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Mol	Chain	Res	Type
1	A	140	LEU
1	A	163	MET
1	A	206	ARG
1	A	223	LYS
1	A	271	LEU
1	A	361	ASP
1	A	447	LEU
1	B	6	HIS
1	B	26	LEU
1	B	28	LEU
1	B	124	ARG
1	B	125	MET
1	B	136	LEU
1	B	137	LEU
1	B	140	LEU
1	B	206	ARG
1	B	223	LYS
1	B	271	LEU
1	B	355	HIS
1	B	361	ASP
1	B	381	ILE
1	B	399	LEU
1	B	447	LEU
1	B	452	THR
1	C	7	THR
1	C	16	ILE
1	C	26	LEU
1	C	28	LEU
1	C	71	LEU
1	C	77	ILE
1	C	124	ARG
1	C	125	MET
1	C	136	LEU
1	C	137	LEU
1	C	140	LEU
1	C	164	LEU
1	C	206	ARG
1	C	247	ARG
1	C	271	LEU
1	C	381	ILE
1	C	399	LEU
1	C	447	LEU

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Mol	Chain	Res	Type
1	D	12	GLU
1	D	26	LEU
1	D	28	LEU
1	D	40	LEU
1	D	77	ILE
1	D	125	MET
1	D	136	LEU
1	D	140	LEU
1	D	158	ARG
1	D	185	ASN
1	D	206	ARG
1	D	240	LYS
1	D	253	ASN
1	D	271	LEU
1	D	361	ASP
1	D	399	LEU
1	D	433	LEU
1	D	447	LEU
1	D	452	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	270	HIS
1	A	319	GLN
1	A	336	GLN
1	A	355	HIS
1	B	142	GLN
1	B	268	GLN
1	B	319	GLN
1	C	127	ASN
1	D	14	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 oligosaccharides 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	GKR	C	472	2	13,13,13	2.00	3 (23%)	16,18,18	1.27	1 (6%)
3	GKR	B	472	2	13,13,13	2.09	3 (23%)	16,18,18	1.47	2 (12%)
3	GKR	A	472	2	13,13,13	1.92	3 (23%)	16,18,18	1.40	2 (12%)
3	GKR	D	472	2	13,13,13	2.08	5 (38%)	16,18,18	1.37	2 (12%)

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	GKR	C	472	2	-	9/20/20/20	-
3	GKR	B	472	2	-	11/20/20/20	-
3	GKR	A	472	2	-	8/20/20/20	-
3	GKR	D	472	2	-	12/20/20/20	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	472	GKR	O2-C2	5.62	1.53	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	472	GKR	O2-C2	5.36	1.52	1.42
3	A	472	GKR	O2-C2	5.17	1.52	1.42
3	D	472	GKR	O2-C2	5.07	1.52	1.42
3	D	472	GKR	O6A-C6	2.71	1.30	1.22
3	B	472	GKR	C2-C1	-2.49	1.49	1.52
3	D	472	GKR	C4-C3	2.46	1.57	1.53
3	B	472	GKR	O6A-C6	2.44	1.29	1.22
3	A	472	GKR	C4-C3	2.37	1.57	1.53
3	A	472	GKR	O6A-C6	2.37	1.29	1.22
3	C	472	GKR	O6A-C6	2.37	1.29	1.22
3	D	472	GKR	C2-C1	-2.32	1.49	1.52
3	C	472	GKR	C4-C3	2.26	1.57	1.53
3	D	472	GKR	O5-C5	2.26	1.46	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	472	GKR	O4-C4-C3	3.23	117.00	109.46
3	C	472	GKR	O5-C5-C4	3.16	117.23	110.38
3	D	472	GKR	O5-C5-C4	2.99	116.87	110.38
3	A	472	GKR	O5-C5-C4	2.99	116.86	110.38
3	B	472	GKR	O5-C5-C4	2.94	116.75	110.38
3	D	472	GKR	O4-C4-C3	2.12	114.41	109.46
3	A	472	GKR	O1A-C1-C2	2.09	119.13	113.31

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	472	GKR	C3-C4-C5-O5
3	A	472	GKR	C3-C4-C5-C6
3	A	472	GKR	O4-C4-C5-O5
3	A	472	GKR	O4-C4-C5-C6
3	B	472	GKR	C2-C3-C4-O4
3	B	472	GKR	O3-C3-C4-C5
3	B	472	GKR	C3-C4-C5-O5
3	B	472	GKR	C3-C4-C5-C6
3	B	472	GKR	O4-C4-C5-O5
3	B	472	GKR	O4-C4-C5-C6
3	C	472	GKR	C3-C4-C5-O5
3	C	472	GKR	C3-C4-C5-C6
3	C	472	GKR	O4-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
3	C	472	GKR	O4-C4-C5-C6
3	C	472	GKR	C4-C5-C6-O6B
3	D	472	GKR	C3-C4-C5-O5
3	D	472	GKR	C3-C4-C5-C6
3	D	472	GKR	O4-C4-C5-O5
3	D	472	GKR	O4-C4-C5-C6
3	D	472	GKR	C4-C5-C6-O6B
3	D	472	GKR	O5-C5-C6-O6A
3	D	472	GKR	O5-C5-C6-O6B
3	A	472	GKR	C4-C5-C6-O6A
3	A	472	GKR	C4-C5-C6-O6B
3	B	472	GKR	C4-C5-C6-O6B
3	C	472	GKR	C4-C5-C6-O6A
3	D	472	GKR	C4-C5-C6-O6A
3	A	472	GKR	O5-C5-C6-O6A
3	A	472	GKR	O5-C5-C6-O6B
3	C	472	GKR	O5-C5-C6-O6A
3	C	472	GKR	O5-C5-C6-O6B
3	B	472	GKR	C2-C3-C4-C5
3	B	472	GKR	O3-C3-C4-O4
3	B	472	GKR	C4-C5-C6-O6A
3	B	472	GKR	O5-C5-C6-O6B
3	D	472	GKR	C2-C3-C4-O4
3	D	472	GKR	O3-C3-C4-C5
3	D	472	GKR	O3-C3-C4-O4
3	D	472	GKR	C2-C3-C4-C5
3	C	472	GKR	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	472	GKR	3	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	424/470 (90%)	0.47	10 (2%) 59 67	31, 39, 51, 68	0
1	B	428/470 (91%)	0.37	18 (4%) 40 48	28, 37, 50, 69	0
1	C	421/470 (89%)	0.66	22 (5%) 33 38	30, 41, 55, 73	0
1	D	425/470 (90%)	0.68	20 (4%) 36 42	31, 41, 58, 70	0
All	All	1698/1880 (90%)	0.54	70 (4%) 41 49	28, 39, 55, 73	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	435	PRO	5.0
1	C	184	ALA	5.0
1	D	460	LEU	4.7
1	B	435	PRO	4.0
1	C	92	ALA	3.7
1	B	434	GLY	3.7
1	B	92	ALA	3.6
1	C	434	GLY	3.4
1	C	367	PHE	3.3
1	D	434	GLY	3.3
1	C	332	PHE	3.3
1	B	123	LEU	3.2
1	D	5	THR	3.2
1	A	435	PRO	3.2
1	C	435	PRO	3.2
1	B	367	PHE	3.2
1	B	120	GLU	3.2
1	D	436	GLY	3.1
1	C	6	HIS	3.1
1	B	121	ILE	3.1
1	C	183	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	432	THR	3.0
1	B	91	LEU	2.8
1	D	220	PHE	2.7
1	A	40	LEU	2.7
1	C	40	LEU	2.7
1	A	47	ALA	2.7
1	A	6	HIS	2.6
1	A	434	GLY	2.6
1	D	77	ILE	2.6
1	D	92	ALA	2.6
1	A	46	ASN	2.6
1	B	6	HIS	2.6
1	A	184	ALA	2.6
1	B	90	ALA	2.6
1	C	174	ARG	2.6
1	C	182	GLU	2.6
1	C	124	ARG	2.5
1	D	446	TYR	2.5
1	B	186	GLY	2.5
1	B	122	ASN	2.5
1	D	433	LEU	2.4
1	D	411	ARG	2.4
1	B	40	LEU	2.4
1	C	71	LEU	2.4
1	C	271	LEU	2.4
1	A	446	TYR	2.4
1	B	381	ILE	2.4
1	B	46	ASN	2.4
1	C	447	LEU	2.4
1	B	184	ALA	2.4
1	D	184	ALA	2.4
1	D	283	ALA	2.4
1	B	332	PHE	2.4
1	D	423	VAL	2.3
1	C	433	LEU	2.3
1	D	447	LEU	2.3
1	C	355	HIS	2.3
1	C	77	ILE	2.2
1	A	198	ALA	2.2
1	B	460	LEU	2.2
1	C	460	LEU	2.2
1	D	186	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	46	ASN	2.2
1	D	124	ARG	2.1
1	D	272	VAL	2.1
1	C	91	LEU	2.0
1	D	399	LEU	2.0
1	A	355	HIS	2.0
1	C	176	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GKR	D	472	14/14	0.78	0.13	43,50,53,60	0
3	GKR	C	472	14/14	0.80	0.12	43,47,52,52	0
3	GKR	A	472	14/14	0.80	0.11	41,46,50,50	0
3	GKR	B	472	14/14	0.85	0.10	35,41,42,44	0
2	MG	C	471	1/1	0.96	0.05	43,43,43,43	0
2	MG	D	471	1/1	0.96	0.06	45,45,45,45	0
2	MG	A	471	1/1	0.97	0.05	40,40,40,40	0
2	MG	B	471	1/1	0.97	0.05	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.