WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 12:37 AM EDT

PDB ID	:	3P0W
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 (i) 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 (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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.
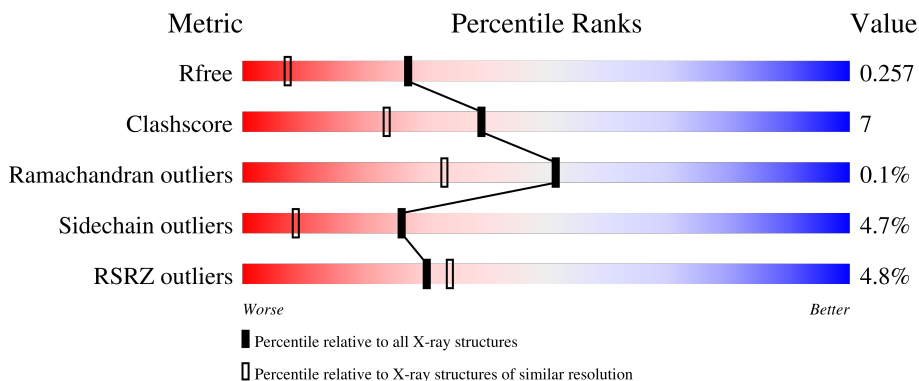
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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 <=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	2% 78% 11% · 10%
1	B	470	6% 77% 13% · 9%
1	C	470	4% 71% 17% · 10%
1	D	470	5% 72% 17% · 10%

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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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 (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 D-GLUCARATE (three-letter code: GKR) (formula: $C_6H_8O_8$).

GKR

O1A
O⁻

C1 ── O O1B

O2 HO ▶ C2(R)

C3(S) ◀ OH O3

O4 HO ▶ C4(S)

C5(S) ┈┈┈ OH O5

O6A O ═ C6

O⁻
O6B
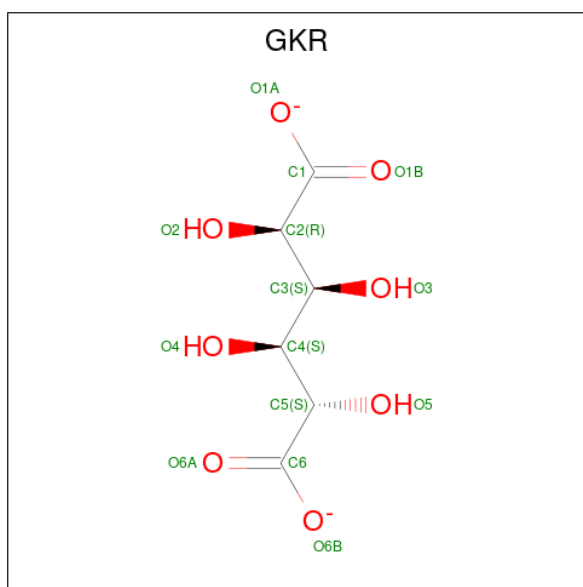
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 14	C 6	O 8	0	0
3	B	1	Total 14	C 6	O 8	0	0
3	C	1	Total 14	C 6	O 8	0	0
3	D	1	Total 14	C 6	O 8	0	0

- Molecule 4 is water.

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

3 Residue-property plots ⓘ

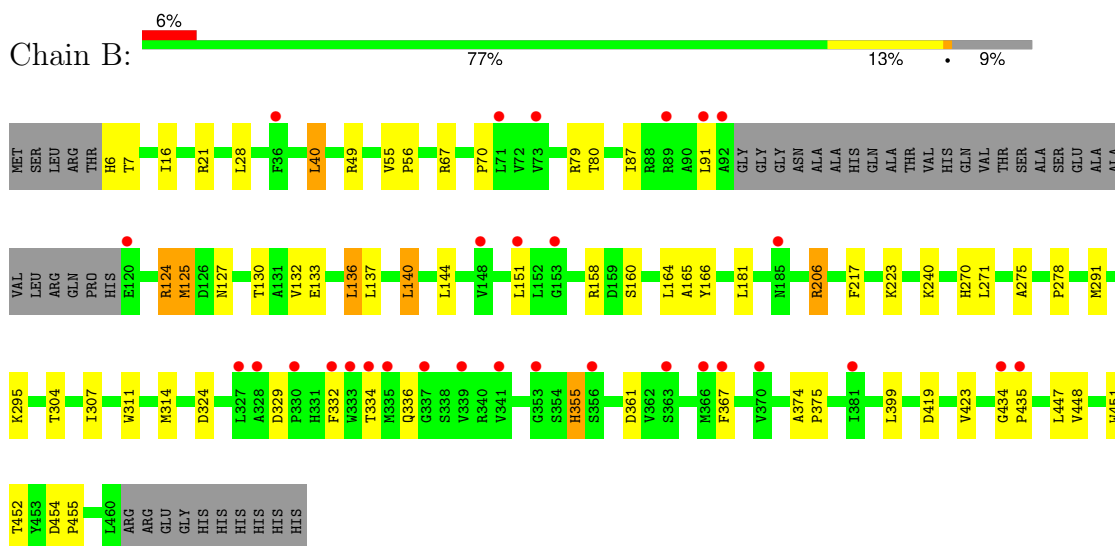These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.
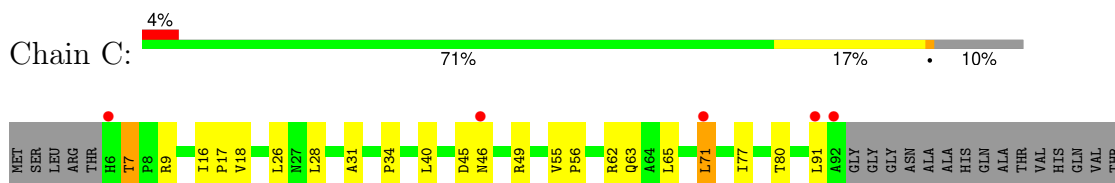
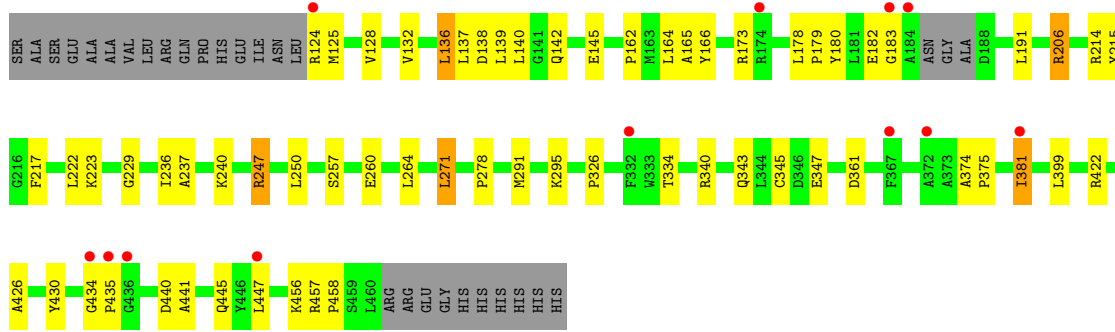- Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain A:

- Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain B:

- Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain C:

SER ALA SER GLU ALA ALA VAL LEU ARG GLN PRO HIS GLU ILE ASN LEU R124 M125 V128 V132 L136 L137 D138 L139 L140 G141 Q142 E145 P162 M163 L164 A165 Y166 R173 R174 L178 P179 Y180 L181 E182 G183 A184 ASN GLY ALA D188 L191 R206 R214 Y215

G216 F217 L222 K223 G229 I236 A237 K240 R247 L250 S257 E260 L264 L271 P278 M291 K295 P326 F332 W333 T334 R340 Q343 L344 C345 D346 E347 D361 F367 A372 A373 A374 P375 I381 L399 R422

A426 Y430 G434 P435 G436 D440 A441 Q445 Y446 L447 K456 R457 P458 S459 L460 ARG GLU GLY HIS HIS HIS HIS HIS HIS

• Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain D:

MET SER LEU ARG T5 H6 T7 T11 E12 P17 V18 M24 L25 L26 N27 L28 P34 F35 L40 K44 V52 G53 E54 V55 P56 R62 L71 Q75 S76 I77 S85 R89 A90 L91 A92 GLY GLY GLY ASN ALA ALA HIS GLN ALA THR VAL HIS GLN

VAL THR SER ALA SER GLU ALA ALA VAL LEU ARG GLN PRO HIS GLU ILE ASN LEU R124 M125 T130 E133 L136 L137 L140 G141 Q142 F143 L144 R158 D159 S160 A165 Y166 V170 T176 D177 L178 P179 A184 N185 G186 A187 D188 A198 A205 R206 E209

F217 I236 A237 K240 V248 P252 L271 A275 E276 D277 P278 M291 I307 Q319 D329 P330 T334 R340 Q343 E347 G353 S354 H355 F367 I381 D382 E389 A390 R396 P409 E410 R411 P412 E417 I418 D419 V423

A426 H427 K431 T432 L433 G434 P435 G436 A437 M444 Q445 Y446 L447 G450 W451 T452 Y453 R457 L460 ARG ARG GLU GLY HIS HIS HIS HIS HIS HIS

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
$< I/\sigma(I) >$ [1]	0.83 (at 1.71Å)	Xtriage
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	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 35.6	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.40	0/3312	0.58	0/4504
1	B	0.42	0/3345	0.60	0/4549
1	C	0.39	0/3294	0.55	0/4478
1	D	0.40	0/3319	0.55	0/4514
All	All	0.41	0/13270	0.57	0/18045

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 ⓘ

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	35	1
1	B	3270	0	3230	49	0
1	C	3220	0	3181	53	0
1	D	3244	0	3203	63	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	192	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 7.

All (192) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:91:LEU:HD12	1:D:125:MET:HE1	1.81	0.61
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: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:B:164:LEU:C	1:B:164:LEU:HD12	2.24	0.58
1:D:206:ARG:HG3	1:D:206:ARG:NH1	2.18	0.58
1:A:91:LEU:HB2	1:A:125:MET:HE2	1.85	0.57
1:D:236:ILE:HG22	1:D:271:LEU:CD1	2.35	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:163:MET:HE2	1:A:381:ILE:HD11	1.88	0.55
1:C:173:ARG:HH22	1:C:182:GLU:CD	2.09	0.55
1:D:24:MET:HE1	1:D:447:LEU:HD11	1.89	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: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:295:LYS:HZ2	1:B:324:ASP:CG	2.11	0.53
1:A:40:LEU:C	1:A:40:LEU:HD12	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:444:MET:CE	1:D:460:LEU:HD21	2.42	0.50
1:B:124:ARG:HH11	1:B:124:ARG:CG	2.23	0.49
1:D:11:THR:C	1:D:12:GLU:HG2	2.32	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
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:A:304:THR:HG21	1:A:307:ILE:HG12	1.97	0.47
1:C:223:LYS:HD2	4:C:507:HOH:O	2.14	0.47
1:D:24:MET:HE1	1:D:447:LEU:CD1	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:B:419:ASP:O	1:B:423:VAL:HG23	2.17	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:MET:HE1	1:A:460:LEU:HD21	2.00	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: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:D:444:MET:HE1	1:D:460:LEU:HD21	2.00	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: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: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:B:314:MET:HB2	1:B:314:MET:HE2	1.88	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: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: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:D:188:ASP:OD1	1:D:188:ASP:C	2.60	0.40
1:B:21:ARG:HD3	1:B:181:LEU:HD11	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	47	30
1	D	421/470 (90%)	407 (97%)	14 (3%)	0	100	100
All	All	1680/1880 (89%)	1634 (97%)	45 (3%)	1 (0%)	51	33

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%)	34	14
1	B	329/361 (91%)	314 (95%)	15 (5%)	27	9
1	C	324/361 (90%)	306 (94%)	18 (6%)	21	6
1	D	326/361 (90%)	310 (95%)	16 (5%)	25	8
All	All	1304/1444 (90%)	1243 (95%)	61 (5%)	26	9

All (61) 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
1	A	140	LEU
1	A	158	ARG
1	A	166	TYR
1	A	223	LYS
1	A	271	LEU
1	A	361	ASP
1	A	447	LEU
1	B	6	HIS
1	B	28	LEU
1	B	40	LEU
1	B	124	ARG
1	B	125	MET
1	B	136	LEU
1	B	137	LEU
1	B	140	LEU
1	B	166	TYR
1	B	206	ARG
1	B	271	LEU
1	B	355	HIS
1	B	399	LEU
1	B	447	LEU
1	B	452	THR
1	C	7	THR
1	C	26	LEU
1	C	28	LEU

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Mol	Chain	Res	Type
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	166	TYR
1	C	206	ARG
1	C	247	ARG
1	C	271	LEU
1	C	381	ILE
1	C	399	LEU
1	C	447	LEU
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	166	TYR
1	D	185	ASN
1	D	240	LYS
1	D	271	LEU
1	D	447	LEU
1	D	452	THR
1	D	457	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 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	A	472	2	13,13,13	1.92	3 (23%)	16,18,18	1.40	2 (12%)
3	GKR	B	472	2	13,13,13	2.09	3 (23%)	16,18,18	1.47	2 (12%)
3	GKR	C	472	2	13,13,13	2.00	3 (23%)	16,18,18	1.27	1 (6%)
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	A	472	2	-	8/20/20/20	-
3	GKR	B	472	2	-	11/20/20/20	-
3	GKR	C	472	2	-	9/20/20/20	-
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms
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 ⓘ

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, 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%)	0.07	11 (2%)	56	60	31, 39, 51, 68	0
1	B	428/470 (91%)	0.24	30 (7%)	16	19	28, 37, 50, 69	0
1	C	421/470 (89%)	0.24	17 (4%)	38	42	30, 41, 55, 73	0
1	D	425/470 (90%)	0.31	24 (5%)	24	27	31, 41, 58, 70	0
All	All	1698/1880 (90%)	0.22	82 (4%)	30	34	28, 39, 55, 73	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	92	ALA	6.5
1	B	434	GLY	6.3
1	D	435	PRO	6.2
1	D	434	GLY	5.1
1	C	435	PRO	5.1
1	C	434	GLY	4.8
1	D	186	GLY	4.8
1	D	433	LEU	4.7
1	B	435	PRO	4.3
1	D	436	GLY	4.2
1	D	185	ASN	4.0
1	D	411	ARG	4.0
1	B	92	ALA	3.7
1	C	447	LEU	3.6
1	D	184	ALA	3.5
1	B	367	PHE	3.4
1	C	184	ALA	3.4
1	B	366	MET	3.4
1	C	436	GLY	3.4
1	B	148	VAL	3.4
1	D	410	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	6	HIS	3.2
1	D	381	ILE	3.1
1	B	91	LEU	3.0
1	B	370	VAL	3.0
1	B	332	PHE	3.0
1	C	367	PHE	3.0
1	D	446	TYR	3.0
1	D	187	ALA	3.0
1	C	91	LEU	2.9
1	B	334	THR	2.9
1	B	341	VAL	2.8
1	B	335	MET	2.8
1	B	337	GLY	2.8
1	A	435	PRO	2.8
1	D	447	LEU	2.8
1	B	381	ILE	2.7
1	C	332	PHE	2.7
1	D	452	THR	2.7
1	B	363	SER	2.7
1	D	457	ARG	2.6
1	A	339	VAL	2.6
1	B	356	SER	2.6
1	C	174	ARG	2.6
1	B	333	TRP	2.5
1	A	450	GLY	2.5
1	B	339	VAL	2.5
1	B	328	ALA	2.4
1	A	186	GLY	2.4
1	B	120	GLU	2.4
1	B	71	LEU	2.4
1	D	177	ASP	2.4
1	D	353	GLY	2.4
1	D	178	LEU	2.3
1	B	353	GLY	2.3
1	C	124	ARG	2.3
1	A	449	PRO	2.3
1	B	330	PRO	2.3
1	D	432	THR	2.2
1	A	185	ASN	2.2
1	B	151	LEU	2.2
1	A	434	GLY	2.2
1	C	183	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	450	GLY	2.2
1	B	327	LEU	2.2
1	A	410	GLU	2.2
1	D	396	ARG	2.2
1	B	185	ASN	2.2
1	D	453	TYR	2.1
1	B	36	PHE	2.1
1	B	89	ARG	2.1
1	A	341	VAL	2.1
1	C	372	ALA	2.1
1	C	46	ASN	2.1
1	D	437	ALA	2.1
1	B	153	GLY	2.1
1	C	381	ILE	2.1
1	B	73	VAL	2.0
1	A	446	TYR	2.0
1	C	71	LEU	2.0
1	D	460	LEU	2.0
1	A	436	GLY	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 monosaccharides 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. 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(Å²)	Q<0.9
3	GKR	D	472	14/14	0.80	0.14	43,50,53,60	0
3	GKR	C	472	14/14	0.81	0.14	43,47,52,52	0
3	GKR	A	472	14/14	0.85	0.12	41,46,50,50	0
3	GKR	B	472	14/14	0.88	0.11	35,41,42,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	D	471	1/1	0.90	0.09	45,45,45,45	0
2	MG	A	471	1/1	0.93	0.12	40,40,40,40	0
2	MG	C	471	1/1	0.94	0.06	43,43,43,43	0
2	MG	B	471	1/1	0.95	0.15	38,38,38,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.