



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2022 – 08:21 PM JST

PDB ID : 7X9S  
Title : Crystal structure of a complex between the antirepressor GmaR and the transcriptional repressor MogR  
Authors : Cho, S.Y.; Na, H.W.; Oh, H.B.; Kwak, Y.M.; Song, W.S.; Park, S.C.; Yoon, S.I.  
Deposited on : 2022-03-16  
Resolution : 3.11 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
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

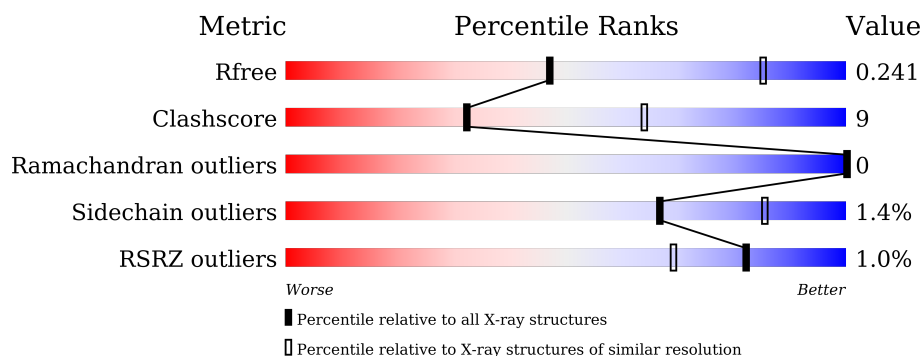
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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	413	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 21%, green 77%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>77%</span> <span>21%</span> <span>.</span> </div> </div>
1	C	413	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 77%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>77%</span> <span>18%</span> <span>.</span> </div> </div>
1	E	413	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 73%, yellow 22%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>73%</span> <span>22%</span> <span>.</span> </div> </div>
2	B	168	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 67%, yellow 14%, grey 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>67%</span> <span>14%</span> <span>20%</span> </div> </div>
2	D	168	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 10%, green 56%, grey 29%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>56%</span> <span>10%</span> <span>35%</span> </div> </div>
2	F	168	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 67%, grey 21%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>67%</span> <span>11%</span> <span>.</span> <span>21%</span> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12093 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 GmaR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3230	2088	517	613	12			
1	C	395	Total	C	N	O	S	0	0	0
			3130	2033	504	582	11			
1	E	395	Total	C	N	O	S	0	0	0
			3000	1947	480	563	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	GLY	-	expression tag	UNP A0A3A6YDN3
A	226	SER	-	expression tag	UNP A0A3A6YDN3
A	227	ALA	-	expression tag	UNP A0A3A6YDN3
A	228	LYS	-	expression tag	UNP A0A3A6YDN3
A	229	ASP	-	expression tag	UNP A0A3A6YDN3
A	230	PRO	-	expression tag	UNP A0A3A6YDN3
C	225	GLY	-	expression tag	UNP A0A3A6YDN3
C	226	SER	-	expression tag	UNP A0A3A6YDN3
C	227	ALA	-	expression tag	UNP A0A3A6YDN3
C	228	LYS	-	expression tag	UNP A0A3A6YDN3
C	229	ASP	-	expression tag	UNP A0A3A6YDN3
C	230	PRO	-	expression tag	UNP A0A3A6YDN3
E	225	GLY	-	expression tag	UNP A0A3A6YDN3
E	226	SER	-	expression tag	UNP A0A3A6YDN3
E	227	ALA	-	expression tag	UNP A0A3A6YDN3
E	228	LYS	-	expression tag	UNP A0A3A6YDN3
E	229	ASP	-	expression tag	UNP A0A3A6YDN3
E	230	PRO	-	expression tag	UNP A0A3A6YDN3

- Molecule 2 is a protein called Motility gene repressor MogR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	135	Total	C	N	O	S	0	0	0
			992	642	161	185	4			
2	D	110	Total	C	N	O	S	0	0	0
			768	499	126	139	4			
2	F	132	Total	C	N	O	S	0	0	0
			973	628	156	185	4			

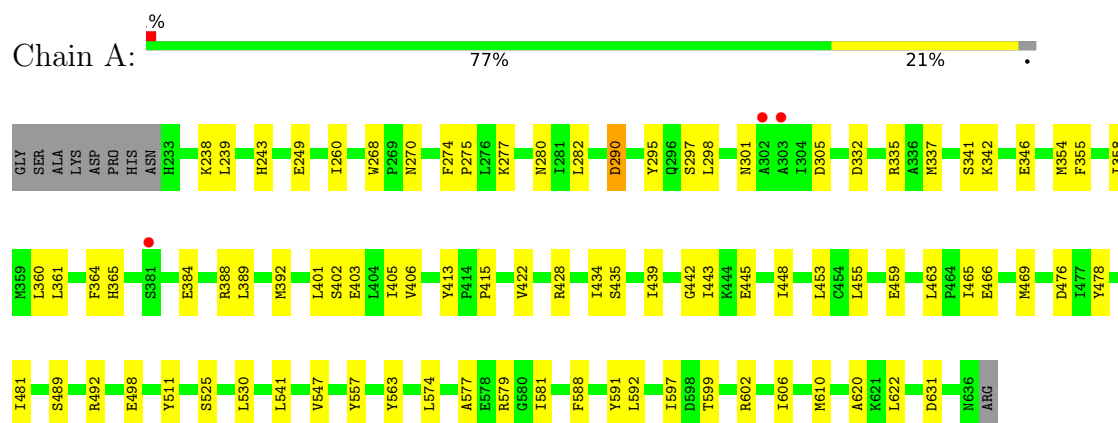
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP A0A3H0QY60
B	-4	SER	-	expression tag	UNP A0A3H0QY60
B	-3	ALA	-	expression tag	UNP A0A3H0QY60
B	-2	LYS	-	expression tag	UNP A0A3H0QY60
B	-1	ASP	-	expression tag	UNP A0A3H0QY60
B	0	PRO	-	expression tag	UNP A0A3H0QY60
D	-5	GLY	-	expression tag	UNP A0A3H0QY60
D	-4	SER	-	expression tag	UNP A0A3H0QY60
D	-3	ALA	-	expression tag	UNP A0A3H0QY60
D	-2	LYS	-	expression tag	UNP A0A3H0QY60
D	-1	ASP	-	expression tag	UNP A0A3H0QY60
D	0	PRO	-	expression tag	UNP A0A3H0QY60
F	-5	GLY	-	expression tag	UNP A0A3H0QY60
F	-4	SER	-	expression tag	UNP A0A3H0QY60
F	-3	ALA	-	expression tag	UNP A0A3H0QY60
F	-2	LYS	-	expression tag	UNP A0A3H0QY60
F	-1	ASP	-	expression tag	UNP A0A3H0QY60
F	0	PRO	-	expression tag	UNP A0A3H0QY60

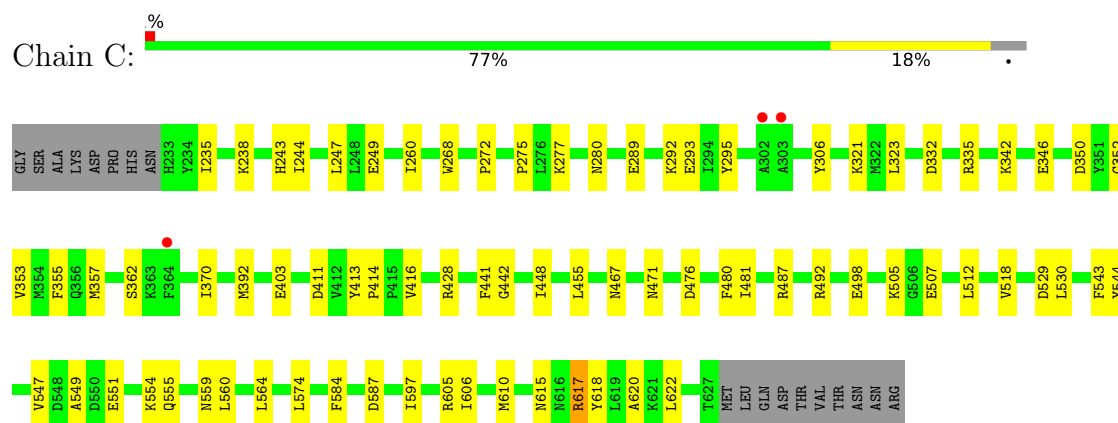
### 3 Residue-property plots

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.

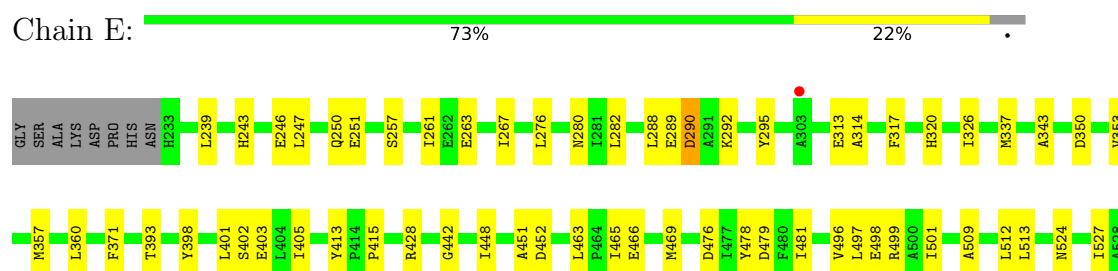
#### • Molecule 1: GmaR

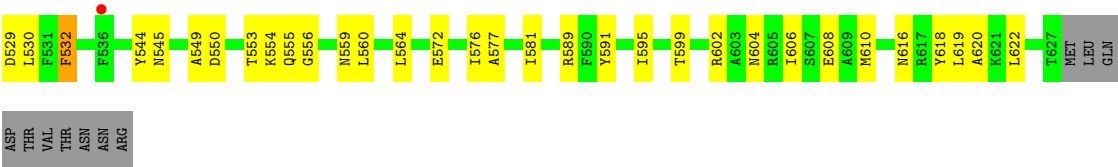


#### • Molecule 1: GmaR



#### • Molecule 1: GmaR

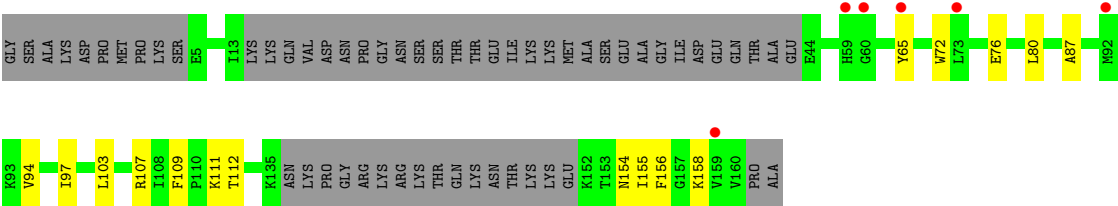




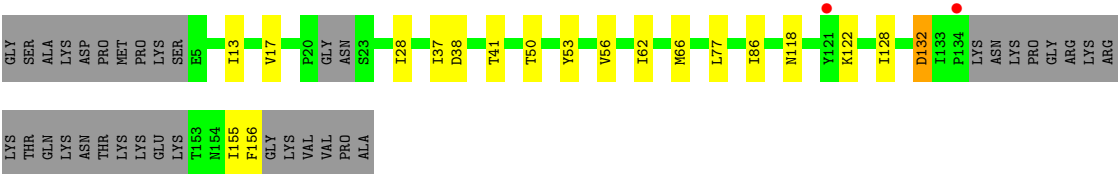
● Molecule 2: Motility gene repressor MogR



● Molecule 2: Motility gene repressor MogR



● Molecule 2: Motility gene repressor MogR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.87Å 91.99Å 268.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.49 – 3.11 29.49 – 3.08	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.49-3.11) 99.5 (29.49-3.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 3.05Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.195 , 0.241 0.195 , 0.241	Depositor DCC
$R_{free}$ test set	2192 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.9	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 72.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12093	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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

### 5.1 Standard geometry

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	0.43	0/3306	0.56	0/4503
1	C	0.40	0/3206	0.55	0/4368
1	E	0.34	0/3074	0.50	0/4205
2	B	0.34	0/1007	0.48	0/1371
2	D	0.33	0/779	0.47	0/1065
2	F	0.31	0/988	0.51	0/1350
All	All	0.38	0/12360	0.53	0/16862

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	3230	0	3075	63	0
1	C	3130	0	2979	54	0
1	E	3000	0	2698	61	0
2	B	992	0	911	14	0
2	D	768	0	666	13	0
2	F	973	0	885	14	0
All	All	12093	0	11214	206	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 9.



All (206) 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:A:541:LEU:HD11	1:A:563:TYR:CE2	1.98	0.99
1:E:498:GLU:HG3	1:E:530:LEU:HD21	1.60	0.84
1:A:463:LEU:HB3	1:A:465:ILE:HD13	1.60	0.83
2:F:13:ILE:HG12	2:F:28:ILE:HD13	1.66	0.76
1:C:280:ASN:ND2	1:C:295:TYR:OH	2.21	0.73
1:A:525:SER:HB2	1:A:547:VAL:HG11	1.75	0.69
2:D:154:ASN:HB3	2:D:156:PHE:H	1.56	0.69
1:A:541:LEU:HD11	1:A:563:TYR:CZ	2.28	0.68
1:A:249:GLU:OE2	1:A:277:LYS:NZ	2.26	0.68
1:A:280:ASN:ND2	1:A:295:TYR:OH	2.26	0.68
1:C:442:GLY:HA3	1:C:448:ILE:HD12	1.76	0.68
1:E:313:GLU:HB3	1:E:317:PHE:HB3	1.75	0.68
1:A:355:PHE:HE1	1:A:389:LEU:HD23	1.58	0.68
1:E:463:LEU:HB3	1:E:465:ILE:HD13	1.77	0.66
1:C:249:GLU:OE2	1:C:277:LYS:NZ	2.23	0.65
1:C:293:GLU:OE2	1:C:617:ARG:NH2	2.32	0.63
2:D:103:LEU:HA	2:D:107:ARG:HG2	1.80	0.63
1:E:498:GLU:HG3	1:E:530:LEU:CD2	2.28	0.63
2:B:45:ILE:HD11	2:B:86:ILE:HG21	1.81	0.63
1:E:337:MET:HG2	1:E:360:LEU:HD11	1.81	0.62
2:F:53:TYR:O	2:F:56:VAL:HG12	1.99	0.62
2:D:154:ASN:HD22	2:D:156:PHE:HD2	1.48	0.61
1:C:467:ASN:O	1:C:471:ASN:ND2	2.35	0.59
1:E:549:ALA:HB2	2:F:155:ILE:HA	1.84	0.59
1:E:524:ASN:HA	1:E:527:ILE:HD12	1.83	0.59
1:A:297:SER:O	1:A:301:ASN:HB2	2.03	0.59
1:A:260:ILE:HD11	1:E:239:LEU:HD12	1.84	0.58
2:B:71:SER:HB2	2:B:135:LYS:HG2	1.84	0.58
1:A:239:LEU:HD12	1:C:260:ILE:HD11	1.84	0.58
1:A:384:GLU:OE2	1:A:388:ARG:NH1	2.36	0.58
1:A:442:GLY:HA3	1:A:448:ILE:HD12	1.86	0.58
1:E:292:LYS:HG3	1:E:326:ILE:HG21	1.86	0.58
1:E:451:ALA:HA	1:E:496:VAL:HG12	1.86	0.58
1:E:466:GLU:HB2	1:E:478:TYR:CZ	2.39	0.57
1:A:364:PHE:HB2	1:A:365:HIS:CD2	2.40	0.57
1:A:599:THR:HG22	1:A:602:ARG:NH2	2.19	0.57
1:C:321:LYS:HD2	1:C:353:VAL:HG13	1.86	0.57
1:A:606:ILE:HD13	1:A:622:LEU:HB3	1.85	0.57
2:F:17:VAL:HG13	2:F:50:THR:HG22	1.86	0.57
1:C:554:LYS:HE2	1:C:587:ASP:OD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:LEU:H	1:E:288:LEU:HD12	1.71	0.56
1:E:555:GLN:HG3	1:E:559:ASN:HD21	1.69	0.56
1:A:243:HIS:NE2	1:C:243:HIS:NE2	2.53	0.56
1:C:498:GLU:HG3	1:C:530:LEU:CD2	2.37	0.55
1:C:244:ILE:HG22	1:C:260:ILE:HD12	1.88	0.55
1:E:606:ILE:HD13	1:E:622:LEU:HB3	1.88	0.55
1:E:599:THR:HG22	1:E:602:ARG:HH11	1.71	0.55
2:F:62:ILE:O	2:F:66:MET:HG3	2.06	0.54
1:E:532:PHE:CD2	1:E:559:ASN:HB3	2.42	0.54
1:A:355:PHE:CE1	1:A:389:LEU:HD23	2.41	0.54
1:A:355:PHE:HA	1:A:392:MET:HE2	1.89	0.54
1:E:481:ILE:HD13	1:E:512:LEU:HD21	1.90	0.54
2:B:72:TRP:CZ3	2:B:80:LEU:HD12	2.42	0.53
1:C:342:LYS:O	1:C:346:GLU:HG2	2.07	0.53
1:E:442:GLY:HA3	1:E:448:ILE:HD12	1.88	0.53
1:E:393:THR:OG1	1:E:402:SER:HB3	2.08	0.53
1:A:401:LEU:O	1:A:405:ILE:HG13	2.08	0.53
1:A:466:GLU:HB2	1:A:478:TYR:CZ	2.44	0.53
2:B:62:ILE:O	2:B:66:MET:HG3	2.09	0.53
1:E:280:ASN:ND2	1:E:295:TYR:OH	2.42	0.52
1:E:604:ASN:O	1:E:608:GLU:HG3	2.09	0.52
1:E:616:ASN:OD1	1:E:619:LEU:HG	2.09	0.52
1:A:243:HIS:NE2	1:E:243:HIS:NE2	2.58	0.52
1:E:476:ASP:N	1:E:476:ASP:OD1	2.41	0.52
1:A:342:LYS:O	1:A:346:GLU:HG2	2.10	0.52
1:E:371:PHE:HE2	1:E:405:ILE:HA	1.74	0.52
1:A:481:ILE:O	1:A:511:TYR:OH	2.24	0.52
1:A:541:LEU:CD1	1:A:563:TYR:CZ	2.92	0.52
1:E:610:MET:HE2	1:E:620:ALA:HA	1.92	0.51
1:E:610:MET:CE	1:E:620:ALA:HA	2.39	0.51
1:C:610:MET:HE2	1:C:620:ALA:HA	1.92	0.51
1:E:257:SER:O	1:E:261:ILE:HG12	2.11	0.51
1:A:574:LEU:HB2	1:A:597:ILE:HG21	1.91	0.51
1:C:606:ILE:HD13	1:C:622:LEU:HB3	1.93	0.51
1:E:595:ILE:HD13	1:E:606:ILE:HG12	1.91	0.51
1:C:555:GLN:HG3	1:C:559:ASN:HD21	1.76	0.51
1:E:289:GLU:HG2	1:E:618:TYR:CD1	2.46	0.51
1:A:453:LEU:HD22	1:A:465:ILE:HG13	1.93	0.50
1:A:476:ASP:N	1:A:476:ASP:OD1	2.38	0.50
1:A:332:ASP:OD2	1:A:335:ARG:HD2	2.11	0.50
2:D:154:ASN:HB2	2:D:158:LYS:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:122:LYS:HB3	2:F:128:ILE:HG13	1.94	0.50
1:A:355:PHE:CD2	1:A:392:MET:HG3	2.46	0.50
1:E:581:ILE:HG23	1:E:591:TYR:CZ	2.47	0.50
1:E:337:MET:SD	1:E:360:LEU:HD21	2.52	0.49
2:B:16:GLN:HG3	2:B:28:ILE:HD11	1.93	0.49
1:C:549:ALA:HB2	2:D:154:ASN:O	2.13	0.49
1:E:413:TYR:CD2	1:E:415:PRO:HD2	2.47	0.49
1:C:554:LYS:HE3	1:C:584:PHE:HB3	1.94	0.49
1:A:498:GLU:HG3	1:A:530:LEU:HD21	1.95	0.49
1:C:487:ARG:NH1	1:C:518:VAL:O	2.46	0.49
1:A:337:MET:O	1:A:341:SER:OG	2.25	0.48
1:E:577:ALA:O	1:E:581:ILE:HG13	2.13	0.48
1:C:574:LEU:HB2	1:C:597:ILE:HG21	1.95	0.48
1:E:246:GLU:O	1:E:250:GLN:HG3	2.14	0.48
1:E:357:MET:HA	1:E:360:LEU:CD2	2.43	0.48
1:E:398:TYR:HB3	1:E:401:LEU:HB3	1.95	0.48
1:C:350:ASP:OD1	1:C:352:GLY:N	2.43	0.48
1:A:588:PHE:HE2	1:A:592:LEU:HD22	1.79	0.48
1:C:332:ASP:OD2	1:C:335:ARG:HD2	2.14	0.48
1:C:507:GLU:H	1:C:507:GLU:CD	2.17	0.48
1:A:489:SER:OG	1:A:492:ARG:HG3	2.14	0.47
1:A:455:LEU:O	1:A:459:GLU:HG3	2.14	0.47
1:C:323:LEU:HD23	1:C:323:LEU:HA	1.71	0.47
1:C:455:LEU:HD21	1:C:505:LYS:HE3	1.96	0.47
1:C:529:ASP:OD1	1:C:544:TYR:OH	2.28	0.47
2:D:87:ALA:HB1	2:D:97:ILE:HG12	1.96	0.47
1:C:498:GLU:HG3	1:C:530:LEU:HD21	1.96	0.46
1:C:549:ALA:HB2	2:D:155:ILE:HA	1.97	0.46
2:B:72:TRP:CH2	2:B:80:LEU:HD12	2.50	0.46
1:C:292:LYS:HG3	1:C:323:LEU:CD2	2.45	0.46
1:A:588:PHE:CE2	1:A:592:LEU:HD22	2.50	0.46
1:A:355:PHE:CG	1:A:392:MET:HG3	2.50	0.46
1:C:350:ASP:HB3	1:C:353:VAL:HG22	1.98	0.46
1:C:615:ASN:HD22	2:D:112:THR:HG21	1.80	0.46
1:E:247:LEU:O	1:E:251:GLU:HG3	2.14	0.46
1:A:422:VAL:HG21	1:A:434:ILE:HB	1.97	0.46
1:E:353:VAL:O	1:E:357:MET:HG3	2.16	0.46
1:E:555:GLN:HG3	1:E:559:ASN:ND2	2.31	0.46
1:A:280:ASN:N	1:A:280:ASN:HD22	2.13	0.46
1:A:610:MET:HE2	1:A:620:ALA:HA	1.98	0.46
1:E:350:ASP:HB3	1:E:353:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:GLU:HG2	1:C:618:TYR:CD1	2.51	0.46
1:E:497:LEU:O	1:E:501:ILE:HG13	2.16	0.45
1:E:572:GLU:O	1:E:576:ILE:HG13	2.16	0.45
2:F:118:ASN:O	2:F:122:LYS:HG3	2.17	0.45
1:C:481:ILE:HD13	1:C:512:LEU:HD21	1.98	0.45
1:A:402:SER:O	1:A:406:VAL:HG12	2.17	0.45
1:A:581:ILE:HG23	1:A:591:TYR:CZ	2.52	0.45
2:B:32:ALA:HB1	2:B:37:ILE:HB	1.98	0.45
1:E:290:ASP:OD1	1:E:616:ASN:ND2	2.50	0.45
1:E:452:ASP:OD1	1:E:499:ARG:NH1	2.50	0.45
1:A:465:ILE:HG23	1:A:469:MET:HG3	1.98	0.45
1:E:529:ASP:OD2	1:E:553:THR:OG1	2.24	0.45
2:B:154:ASN:HB2	2:B:157:GLY:H	1.82	0.45
1:E:509:ALA:O	1:E:513:LEU:HG	2.16	0.45
1:A:403:GLU:OE1	1:A:428:ARG:NH1	2.32	0.44
1:C:480:PHE:CD1	1:C:487:ARG:HA	2.52	0.44
1:A:243:HIS:CE1	1:C:247:LEU:HD11	2.52	0.44
1:A:610:MET:CE	1:A:620:ALA:HA	2.46	0.44
1:C:555:GLN:HG3	1:C:559:ASN:ND2	2.32	0.44
1:A:498:GLU:HG3	1:A:530:LEU:CD2	2.48	0.44
1:C:413:TYR:CD1	1:C:414:PRO:HD2	2.52	0.44
1:C:610:MET:CE	1:C:620:ALA:HA	2.47	0.44
2:F:37:ILE:HG23	2:F:86:ILE:HD11	1.99	0.44
1:A:274:PHE:HB2	1:A:275:PRO:HD3	2.00	0.44
1:E:402:SER:HA	1:E:405:ILE:HD12	1.98	0.44
1:C:530:LEU:HD23	1:C:530:LEU:HA	1.51	0.44
1:E:554:LYS:HE3	1:E:589:ARG:NH2	2.33	0.44
2:B:66:MET:O	2:B:135:LYS:NZ	2.49	0.44
1:A:355:PHE:HA	1:A:392:MET:CE	2.48	0.43
2:B:154:ASN:HB3	2:B:156:PHE:H	1.83	0.43
1:E:357:MET:O	1:E:360:LEU:HD23	2.19	0.43
2:D:80:LEU:HB2	2:D:109:PHE:CE2	2.53	0.43
1:A:298:LEU:HA	1:A:298:LEU:HD23	1.83	0.43
1:C:272:PRO:O	1:C:275:PRO:HD2	2.18	0.43
1:A:557:TYR:HE2	1:A:579:ARG:HG2	1.84	0.43
1:C:498:GLU:HG3	1:C:530:LEU:HD22	2.01	0.43
2:F:155:ILE:HG23	2:F:156:PHE:CD1	2.53	0.43
1:E:282:LEU:HD23	1:E:282:LEU:HA	1.80	0.43
1:A:238:LYS:HE2	1:A:268:TRP:CD1	2.54	0.43
1:A:238:LYS:HG2	1:A:268:TRP:CE2	2.54	0.42
1:C:272:PRO:HB3	1:C:306:TYR:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:HIS:NE2	1:E:243:HIS:NE2	2.67	0.42
1:A:530:LEU:HA	1:A:530:LEU:HD23	1.68	0.42
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.85	0.42
1:A:355:PHE:CZ	1:A:392:MET:HB2	2.55	0.42
1:C:362:SER:HA	1:C:370:ILE:HD11	2.00	0.42
2:D:65:TYR:OH	2:D:76:GLU:OE1	2.37	0.42
1:A:361:LEU:HD23	1:A:361:LEU:HA	1.72	0.42
2:B:38:ASP:HB3	2:B:41:THR:OG1	2.20	0.42
1:C:235:ILE:HG22	1:E:263:GLU:OE1	2.20	0.42
1:C:476:ASP:OD1	1:C:476:ASP:N	2.53	0.42
1:C:615:ASN:ND2	2:D:112:THR:HG21	2.34	0.42
1:C:416:VAL:HG23	1:C:441:PHE:CD1	2.55	0.42
1:E:544:TYR:OH	1:E:556:GLY:HA2	2.19	0.42
1:C:476:ASP:OD2	1:C:492:ARG:NH1	2.52	0.42
1:C:238:LYS:HE2	1:C:268:TRP:CD1	2.55	0.42
1:A:337:MET:HG2	1:A:360:LEU:CD2	2.51	0.41
1:E:560:LEU:O	1:E:564:LEU:HG	2.20	0.41
1:E:465:ILE:HG23	1:E:469:MET:HG3	2.01	0.41
1:C:353:VAL:O	1:C:357:MET:HG3	2.19	0.41
1:A:439:ILE:O	1:A:443:ILE:HG13	2.20	0.41
1:C:403:GLU:CD	1:C:428:ARG:HH12	2.24	0.41
1:E:320:HIS:HB3	1:E:343:ALA:HB2	2.03	0.41
1:E:549:ALA:CB	2:F:155:ILE:HA	2.50	0.41
2:D:94:VAL:HA	2:D:97:ILE:HD12	2.01	0.41
1:E:403:GLU:OE1	1:E:428:ARG:NH2	2.34	0.41
1:A:364:PHE:HB2	1:A:365:HIS:HD2	1.85	0.41
1:A:413:TYR:CD2	1:A:415:PRO:HD2	2.56	0.41
1:C:560:LEU:O	1:C:564:LEU:HG	2.21	0.41
1:E:276:LEU:HD22	1:E:314:ALA:HA	2.03	0.41
2:B:77:LEU:HD22	2:B:123:LEU:HD11	2.02	0.41
1:E:263:GLU:O	1:E:267:ILE:HG13	2.21	0.41
2:F:77:LEU:HD23	2:F:77:LEU:HA	1.78	0.41
1:A:282:LEU:HD13	1:A:290:ASP:HB3	2.03	0.40
2:F:38:ASP:HB3	2:F:41:THR:OG1	2.20	0.40
1:C:543:PHE:O	1:C:547:VAL:HG23	2.20	0.40
2:D:72:TRP:CH2	2:D:111:LYS:HG3	2.56	0.40
2:F:132:ASP:N	2:F:132:ASP:OD1	2.54	0.40
1:A:577:ALA:O	1:A:581:ILE:HG13	2.22	0.40
2:B:118:ASN:O	2:B:122:LYS:HG3	2.22	0.40
2:F:128:ILE:O	2:F:128:ILE:HD12	2.22	0.40
1:A:354:MET:O	1:A:358:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:GLN:O	2:B:89:LEU:HG	2.21	0.40
1:C:355:PHE:CZ	1:C:392:MET:HB2	2.56	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	402/413 (97%)	392 (98%)	10 (2%)	0	100	100
1	C	393/413 (95%)	384 (98%)	9 (2%)	0	100	100
1	E	393/413 (95%)	381 (97%)	12 (3%)	0	100	100
2	B	129/168 (77%)	127 (98%)	2 (2%)	0	100	100
2	D	104/168 (62%)	96 (92%)	8 (8%)	0	100	100
2	F	126/168 (75%)	123 (98%)	3 (2%)	0	100	100
All	All	1547/1743 (89%)	1503 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	335/363 (92%)	329 (98%)	6 (2%)	59	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	318/363 (88%)	314 (99%)	4 (1%)	69	86
1	E	278/363 (77%)	273 (98%)	5 (2%)	59	82
2	B	92/153 (60%)	92 (100%)	0	100	100
2	D	64/153 (42%)	64 (100%)	0	100	100
2	F	92/153 (60%)	91 (99%)	1 (1%)	73	88
All	All	1179/1548 (76%)	1163 (99%)	16 (1%)	67	85

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
1	A	290	ASP
1	A	305	ASP
1	A	435	SER
1	A	445	GLU
1	A	631	ASP
1	C	411	ASP
1	C	551	GLU
1	C	605	ARG
1	C	617	ARG
1	E	290	ASP
1	E	479	ASP
1	E	532	PHE
1	E	545	ASN
1	E	550	ASP
2	F	132	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	ASN
1	A	296	GLN
1	A	316	ASN
1	A	365	HIS
1	A	583	ASN
1	C	280	ASN
1	C	555	GLN
1	C	559	ASN
1	C	583	ASN

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Mol	Chain	Res	Type
1	C	601	ASN
1	C	615	ASN
2	D	154	ASN
1	E	280	ASN
1	E	559	ASN
1	E	583	ASN
1	E	604	ASN

### 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 ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	404/413 (97%)	-0.34	3 (0%) 87 77	42, 66, 104, 141	0
1	C	395/413 (95%)	-0.35	3 (0%) 86 74	38, 71, 106, 140	0
1	E	395/413 (95%)	-0.14	2 (0%) 91 82	44, 114, 149, 170	0
2	B	135/168 (80%)	-0.13	0 100 100	58, 106, 157, 176	0
2	D	110/168 (65%)	0.20	6 (5%) 25 11	69, 107, 142, 161	0
2	F	132/168 (78%)	-0.07	2 (1%) 73 56	64, 93, 138, 154	0
All	All	1571/1743 (90%)	-0.21	16 (1%) 82 69	38, 84, 140, 176	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	302	ALA	4.0
2	D	59	HIS	3.7
1	C	303	ALA	3.2
2	D	60	GLY	3.2
1	A	302	ALA	3.0
2	D	65	TYR	3.0
1	E	303	ALA	3.0
1	E	536	PHE	2.7
1	A	303	ALA	2.6
2	D	92	MET	2.5
2	F	134	PRO	2.4
1	A	381	SER	2.3
2	D	73	LEU	2.3
2	F	121	TYR	2.2
2	D	159	VAL	2.1
1	C	364	PHE	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.