



# Full wwPDB X-ray Structure Validation Report

May 30, 2014 – 01:40 AM EDT

PDB ID : 4C5R  
Title : Structural Investigations into the Stereochemistry and Activity of a Phenylalanine-2,3-Aminomutase from *Taxus chinensis*  
Authors : Wybenga, G.G.; Szymanski, W.; Wu, B.; Feringa, B.L.; Janssen, D.B.; Dijkstra, B.W.  
Deposited on : 2013-09-16  
Resolution : 2.14 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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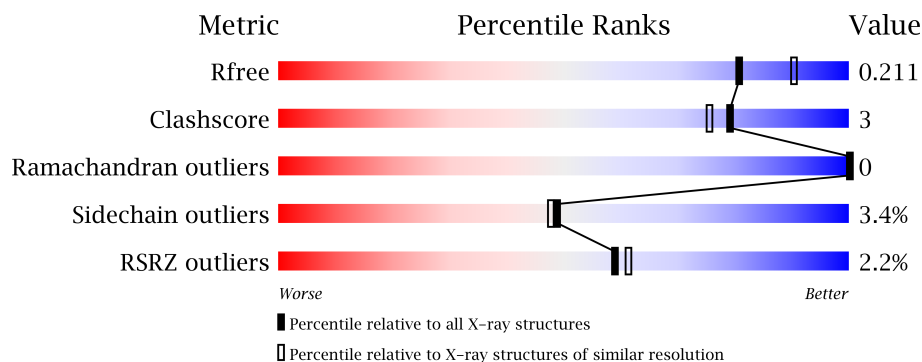
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23161  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23161

# 1 Overall quality at a glance

The reported resolution of this entry is 2.14 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1116 (2.16-2.12)
Clashscore	79885	1302 (2.16-2.12)
Ramachandran outliers	78287	1281 (2.16-2.12)
Sidechain outliers	78261	1281 (2.16-2.12)
RSRZ outliers	66119	1116 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	705	
1	B	705	
1	C	705	
1	D	705	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	A	1679	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20505 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

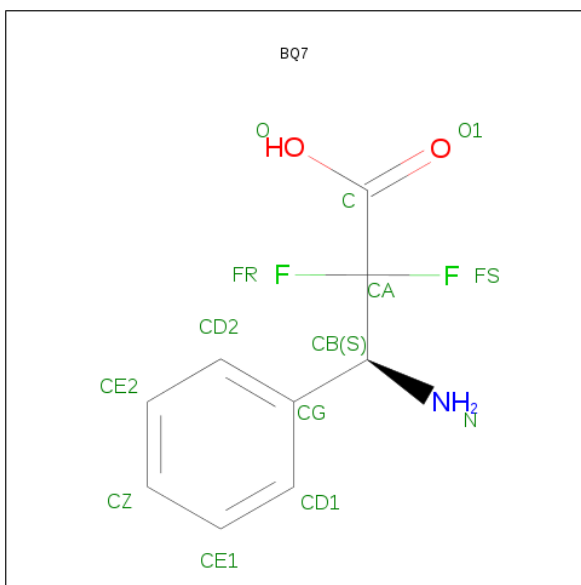
- Molecule 1 is a protein called PHENYLALANINE AMMONIA-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	635	Total	C	N	O	S	0	0	0
			4926	3129	847	927	23			
1	B	640	Total	C	N	O	S	0	0	0
			4967	3152	855	937	23			
1	C	640	Total	C	N	O	S	0	0	0
			4968	3153	855	937	23			
1	D	636	Total	C	N	O	S	0	0	0
			4935	3132	848	932	23			

There are 12 discrepancies between the modelled and reference sequences:

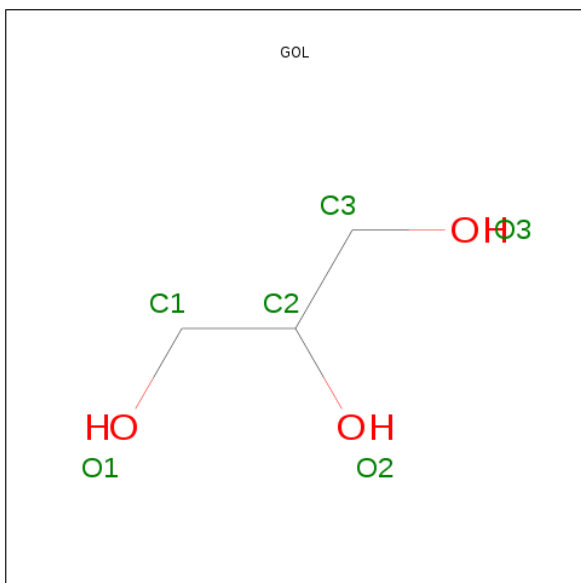
Chain	Residue	Modelled	Actual	Comment	Reference
A	175	MDO	ALA	CHROMOPHORE	UNP Q68G84
A	175	MDO	SER	CHROMOPHORE	UNP Q68G84
A	175	MDO	GLY	CHROMOPHORE	UNP Q68G84
B	175	MDO	ALA	CHROMOPHORE	UNP Q68G84
B	175	MDO	SER	CHROMOPHORE	UNP Q68G84
B	175	MDO	GLY	CHROMOPHORE	UNP Q68G84
C	175	MDO	ALA	CHROMOPHORE	UNP Q68G84
C	175	MDO	SER	CHROMOPHORE	UNP Q68G84
C	175	MDO	GLY	CHROMOPHORE	UNP Q68G84
D	175	MDO	ALA	CHROMOPHORE	UNP Q68G84
D	175	MDO	SER	CHROMOPHORE	UNP Q68G84
D	175	MDO	GLY	CHROMOPHORE	UNP Q68G84

- Molecule 2 is (3S)-3-AMINO-2,2-DIFLUORO-3-PHENYLPROPANOICACID (three-letter code: BQ7) (formula: C<sub>9</sub>H<sub>9</sub>F<sub>2</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			14	9	2	1	2		
2	B	1	Total	C	F	N	O	0	0
			14	9	2	1	2		
2	C	1	Total	C	F	N	O	0	0
			14	9	2	1	2		
2	D	1	Total	C	F	N	O	0	0
			14	9	2	1	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 4 is water.

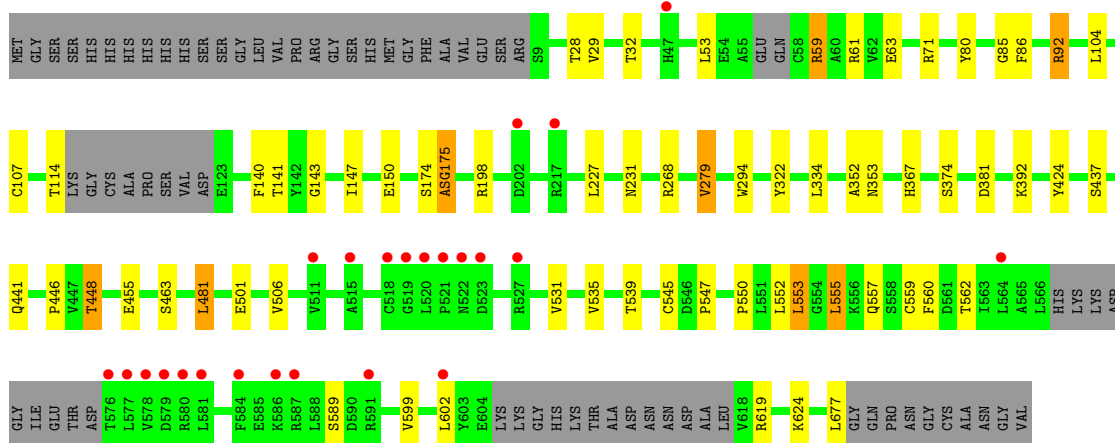
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	181	Total	O	0	0
			181	181		
4	B	154	Total	O	0	0
			154	154		
4	C	161	Total	O	0	0
			161	161		
4	D	145	Total	O	0	0
			145	145		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

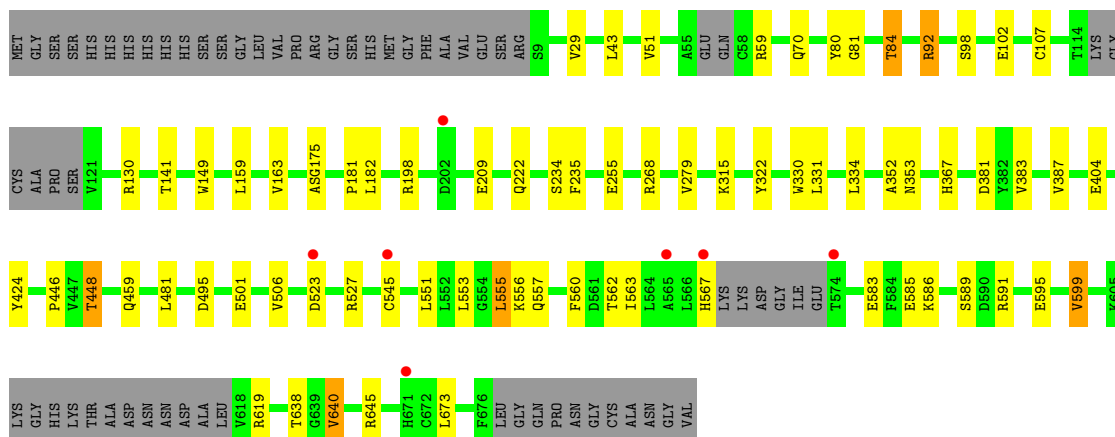
#### • Molecule 1: PHENYLALANINE AMMONIA-LYASE

Chain A: 



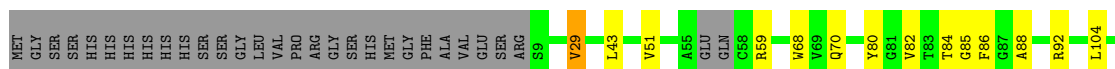
#### • Molecule 1: PHENYLALANINE AMMONIA-LYASE

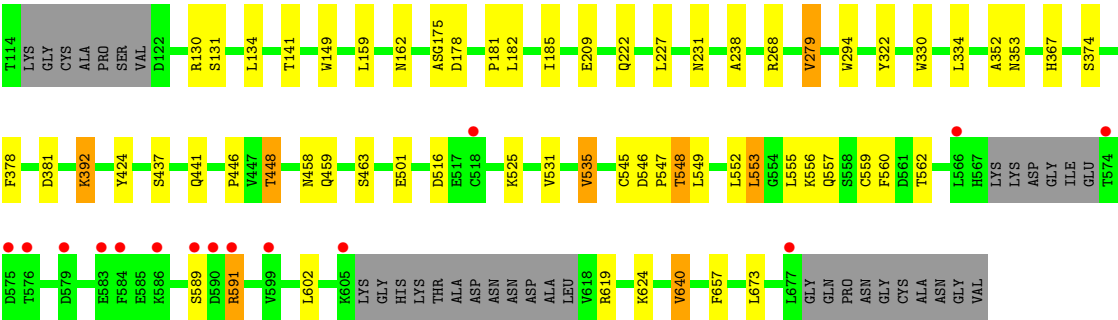
Chain B: 



#### • Molecule 1: PHENYLALANINE AMMONIA-LYASE

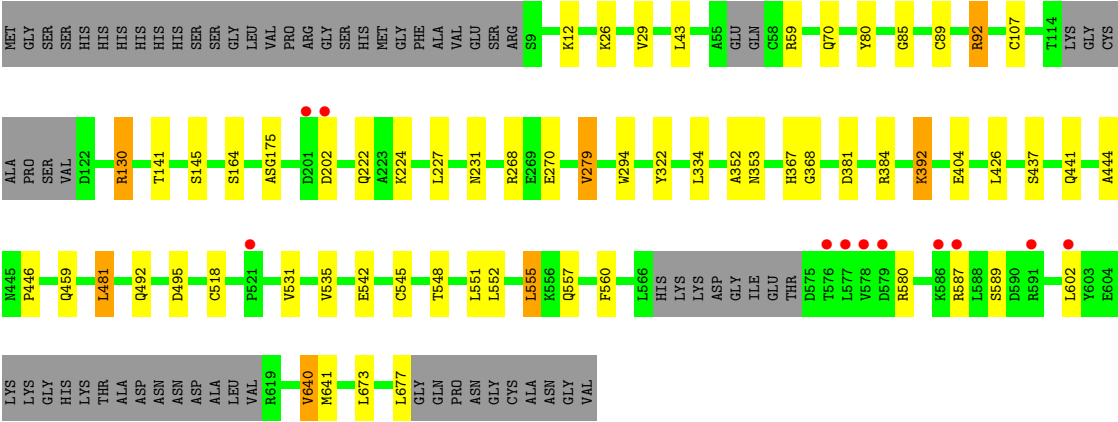
Chain C: 





● Molecule 1: PHENYLALANINE AMMONIA-LYASE

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.39Å 145.48Å 99.56Å 90.00° 99.54° 90.00°	Depositor
Resolution (Å)	49.09 – 2.14 49.09 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.09-2.14) 99.4 (49.09-2.15)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.172 , 0.210 0.174 , 0.211	Depositor DCC
$R_{free}$ test set	7602 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.0	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 31.8	EDS
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 151388 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	20505	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MDO, BQ7

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	0.53	2/4996 (0.0%)	0.61	2/6778 (0.0%)
1	B	0.53	2/5038 (0.0%)	0.61	0/6835
1	C	0.53	3/5039 (0.1%)	0.61	0/6836
1	D	0.53	2/5005 (0.0%)	0.63	3/6790 (0.0%)
All	All	0.53	9/20078 (0.0%)	0.62	5/27239 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	9

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	455	GLU	CD-OE2	-6.06	1.19	1.25
1	A	455	GLU	CD-OE1	-5.75	1.19	1.25
1	C	68	TRP	CD2-CE2	5.32	1.47	1.41
1	C	330	TRP	CD2-CE2	5.28	1.47	1.41
1	D	294	TRP	CD2-CE2	5.28	1.47	1.41
1	B	149	TRP	CD2-CE2	5.11	1.47	1.41
1	C	149	TRP	CD2-CE2	5.11	1.47	1.41
1	B	330	TRP	CD2-CE2	5.07	1.47	1.41
1	D	368	GLY	C-O	-5.01	1.15	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	130	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	71	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	481	LEU	CA-CB-CG	5.22	127.30	115.30
1	D	381	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	481	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	SER	Mainchain
1	A	175	MDO	Mainchain,Peptide
1	B	175	MDO	Mainchain,Peptide
1	C	175	MDO	Mainchain,Peptide
1	D	175	MDO	Mainchain,Peptide

## 5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4926	0	4995	41	0
1	B	4967	0	5028	42	0
1	C	4968	0	5029	48	0
1	D	4935	0	4994	34	0
2	A	14	0	0	0	0
2	B	14	0	0	0	0
2	C	14	0	0	0	0
2	D	14	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	181	0	0	7	0
4	B	154	0	0	0	0
4	C	161	0	0	4	0
4	D	145	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20505	0	20062	139	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (139) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:506:VAL:HG21	1:B:599:VAL:HG11	1.45	0.96
1:A:352:ALA:HB3	1:B:279:VAL:CG1	2.03	0.87
1:C:381:ASP:OD2	1:C:448:THR:HB	1.74	0.86
1:A:279:VAL:HG13	1:B:352:ALA:HB3	1.57	0.84
1:C:279:VAL:HG13	1:D:352:ALA:HB3	1.60	0.83
1:A:381:ASP:OD2	1:A:448:THR:HB	1.79	0.82
1:D:145:SER:O	1:D:224:LYS:HE3	1.80	0.81
1:C:294:TRP:CH2	1:C:624:LYS:HE2	2.17	0.79
1:C:352:ALA:HB3	1:D:279:VAL:HG13	1.65	0.78
1:B:381:ASP:OD2	1:B:448:THR:HB	1.88	0.74
1:B:501:GLU:OE1	1:B:619:ARG:HD2	1.90	0.71
1:A:352:ALA:HB3	1:B:279:VAL:HG13	1.71	0.71
1:C:29:VAL:HG23	1:C:141:THR:HG21	1.74	0.68
1:A:29:VAL:HG22	1:A:141:THR:HG21	1.76	0.67
1:A:501:GLU:OE1	1:A:619:ARG:HD2	1.95	0.66
1:A:557:GLN:OE1	1:D:557:GLN:NE2	2.28	0.65
1:A:294:TRP:CH2	1:A:624:LYS:HE2	2.32	0.65
1:A:92:ARG:NH1	1:A:92:ARG:HB3	2.13	0.63
1:C:546:ASP:OD1	1:C:548:THR:HB	2.00	0.62
1:A:279:VAL:CG1	1:B:352:ALA:HB3	2.28	0.61
1:A:92:ARG:HB3	1:A:92:ARG:HH11	1.65	0.60
1:D:130:ARG:HD2	4:D:2037:HOH:O	2.01	0.60
4:A:2103:HOH:O	1:B:448:THR:HG23	2.01	0.58
1:C:446:PRO:HD3	1:D:446:PRO:HD3	1.85	0.58
1:C:501:GLU:OE1	1:C:619:ARG:HD2	2.04	0.58
1:C:279:VAL:CG1	1:D:352:ALA:HB3	2.33	0.57
1:A:446:PRO:HD3	1:B:446:PRO:HD3	1.87	0.56
1:C:84:THR:HG22	1:C:85:GLY:O	2.04	0.56
1:B:557:GLN:NE2	1:C:557:GLN:OE1	2.27	0.56
1:C:352:ALA:HB3	1:D:279:VAL:CG1	2.36	0.56
1:C:591:ARG:HB2	1:C:591:ARG:HH11	1.70	0.56
1:A:437:SER:O	1:A:441:GLN:HG2	2.06	0.55
1:C:516:ASP:OD1	1:C:525:LYS:HE3	2.06	0.55
1:C:131:SER:HB2	1:C:238:ALA:HB1	1.89	0.54
1:C:531:VAL:O	1:C:535:VAL:HG13	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:61:ARG:HG3	1:A:143:GLY:HA3	1.88	0.54
1:D:43:LEU:O	1:D:130:ARG:NH2	2.42	0.53
1:D:227:LEU:O	1:D:231:ASN:HB2	2.09	0.53
1:D:29:VAL:HG23	1:D:141:THR:HG21	1.91	0.52
1:B:181:PRO:HB2	1:B:235:PHE:CD2	2.44	0.52
1:C:70:GLN:OE1	1:C:222:GLN:HB3	2.10	0.52
1:D:437:SER:O	1:D:441:GLN:HG2	2.09	0.52
1:C:548:THR:HG22	1:C:549:LEU:HD23	1.92	0.52
1:A:545:CYS:HA	1:A:552:LEU:HD23	1.92	0.51
1:A:322:TYR:CZ	1:B:459:GLN:HG2	2.45	0.51
1:A:59:ARG:HD2	1:A:63:GLU:CD	2.31	0.51
1:C:43:LEU:HD22	1:C:134:LEU:HD22	1.93	0.50
1:C:459:GLN:HG2	1:D:322:TYR:CZ	2.45	0.50
1:B:424:TYR:OH	1:D:85:GLY:HA2	2.12	0.50
1:A:85:GLY:HA2	1:C:424:TYR:OH	2.12	0.50
1:C:546:ASP:HB3	1:C:549:LEU:HG	1.94	0.50
1:C:437:SER:O	1:C:441:GLN:HG2	2.13	0.49
1:B:545:CYS:SG	1:B:589:SER:HA	2.52	0.49
1:B:315:LYS:NZ	1:C:548:THR:HG21	2.28	0.49
1:A:506:VAL:HG21	1:A:599:VAL:HG11	1.94	0.49
1:A:150:GLU:HB2	4:A:2042:HOH:O	2.11	0.48
1:C:80:TYR:HB3	1:C:367:HIS:CD2	2.48	0.48
1:B:51:VAL:HG21	1:B:159:LEU:HD13	1.95	0.48
1:B:495:ASP:CB	1:B:640:VAL:HG13	2.44	0.48
1:C:374:SER:HA	1:C:463:SER:HB2	1.95	0.48
4:A:2103:HOH:O	1:B:448:THR:CG2	2.61	0.47
1:D:495:ASP:CB	1:D:640:VAL:HG13	2.44	0.47
1:B:551:LEU:HG	1:B:555:LEU:HD22	1.96	0.47
1:A:531:VAL:HG11	1:A:555:LEU:HD13	1.96	0.47
1:B:560:PHE:HB2	1:C:560:PHE:HB2	1.96	0.47
1:A:545:CYS:SG	1:A:589:SER:HA	2.54	0.47
1:C:178:ASP:HB3	1:C:181:PRO:HG2	1.95	0.47
1:B:506:VAL:HG21	1:B:599:VAL:CG1	2.31	0.46
1:B:556:LYS:HE2	1:B:585:GLU:OE2	2.15	0.46
1:D:392:LYS:HD3	1:D:392:LYS:HA	1.64	0.46
1:D:492:GLN:HB2	1:D:641:MET:HE3	1.98	0.46
1:A:227:LEU:O	1:A:231:ASN:HB2	2.15	0.46
1:A:352:ALA:CB	1:B:279:VAL:HG13	2.45	0.46
1:C:51:VAL:HG21	1:C:159:LEU:HD13	1.98	0.45
1:A:560:PHE:HB2	1:D:560:PHE:HB2	1.97	0.45
1:B:495:ASP:HB3	1:B:640:VAL:HG13	1.97	0.45
1:D:518:CYS:O	1:D:580:ARG:HD3	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:80:TYR:HB3	1:A:367:HIS:CD2	2.51	0.45
1:B:98:SER:O	1:B:102:GLU:HG2	2.16	0.45
1:A:448:THR:HG23	4:A:2139:HOH:O	2.17	0.45
1:B:70:GLN:OE1	1:B:222:GLN:HB3	2.17	0.45
1:C:322:TYR:CZ	1:D:459:GLN:HG2	2.52	0.44
1:B:81:GLY:H	1:B:84:THR:HG22	1.82	0.44
1:D:531:VAL:O	1:D:535:VAL:HG12	2.16	0.44
1:B:29:VAL:HG12	1:B:141:THR:HG21	1.99	0.44
1:A:392:LYS:HE3	4:A:2105:HOH:O	2.17	0.44
1:A:424:TYR:OH	1:C:85:GLY:HA2	2.18	0.44
1:D:641:MET:HE2	4:D:2121:HOH:O	2.18	0.44
1:B:583:GLU:HA	1:B:586:LYS:HE3	1.99	0.44
1:B:595:GLU:O	1:B:599:VAL:HG13	2.18	0.44
1:A:374:SER:HA	1:A:463:SER:HB2	2.00	0.43
1:B:523:ASP:O	1:B:527:ARG:HG3	2.18	0.43
1:D:426:LEU:HD21	1:D:641:MET:HE1	1.99	0.43
1:C:545:CYS:SG	1:C:589:SER:HA	2.58	0.43
1:C:547:PRO:O	1:C:553:LEU:HD13	2.16	0.43
1:D:70:GLN:OE1	1:D:222:GLN:HB3	2.18	0.43
1:B:255:GLU:HG2	1:B:331:LEU:HD13	2.01	0.43
1:B:80:TYR:HB3	1:B:367:HIS:CD2	2.53	0.43
1:A:392:LYS:HA	1:A:392:LYS:HD3	1.77	0.43
1:A:392:LYS:CE	4:A:2105:HOH:O	2.66	0.43
1:B:557:GLN:HG3	1:C:557:GLN:HG3	2.01	0.42
1:A:539:THR:HB	1:A:550:PRO:HG2	2.01	0.42
1:C:392:LYS:HE2	4:C:2105:HOH:O	2.18	0.42
1:C:559:CYS:O	1:C:562:THR:HG22	2.19	0.42
1:B:563:ILE:O	1:B:567:HIS:HB2	2.19	0.42
1:C:227:LEU:O	1:C:231:ASN:HB2	2.18	0.42
1:D:545:CYS:HA	1:D:552:LEU:HD13	2.02	0.42
1:D:89:CYS:O	1:D:92:ARG:HG3	2.18	0.42
1:C:43:LEU:O	1:C:130:ARG:NH2	2.52	0.42
1:C:86:PHE:CE2	1:C:104:LEU:HB2	2.55	0.42
1:A:114:THR:HG22	1:C:657:PHE:CZ	2.55	0.42
1:C:640:VAL:HG23	4:C:2153:HOH:O	2.19	0.41
1:B:182:LEU:HD21	1:B:234:SER:HB2	2.02	0.41
1:D:80:TYR:HB3	1:D:367:HIS:CD2	2.55	0.41
1:D:92:ARG:HB3	1:D:92:ARG:NH1	2.35	0.41
1:C:182:LEU:HD23	1:C:185:ILE:HD12	2.02	0.41
1:C:448:THR:CG2	4:C:2126:HOH:O	2.67	0.41
1:D:12:LYS:HE3	1:D:677:LEU:HB3	2.03	0.41
1:B:43:LEU:O	1:B:130:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:92:ARG:HB3	1:D:92:ARG:HH11	1.84	0.41
1:A:86:PHE:CE2	1:A:104:LEU:HB2	2.55	0.41
1:D:270:GLU:HB2	4:D:2059:HOH:O	2.21	0.41
1:C:88:ALA:HB2	1:C:458:ASN:HB2	2.01	0.41
1:D:384:ARG:HG2	1:D:444:ALA:HA	2.02	0.41
1:A:29:VAL:HG13	1:A:53:LEU:HA	2.02	0.41
1:C:392:LYS:CE	4:C:2105:HOH:O	2.68	0.41
1:B:92:ARG:HH22	1:D:542:GLU:CD	2.24	0.41
1:A:559:CYS:O	1:A:562:THR:HG22	2.21	0.41
1:B:638:THR:HA	1:B:645:ARG:HH22	1.86	0.41
1:A:198:ARG:NH2	4:A:2031:HOH:O	2.55	0.40
1:A:175:MDO:HB1	1:B:322:TYR:HE2	1.86	0.40
1:C:392:LYS:HA	1:C:392:LYS:HD3	1.75	0.40
1:D:551:LEU:HG	1:D:555:LEU:HD22	2.03	0.40
1:C:378:PHE:CE2	1:C:448:THR:HG21	2.56	0.40
1:C:552:LEU:O	1:C:556:LYS:HG3	2.21	0.40
1:A:140:PHE:CG	1:A:147:ILE:HG21	2.56	0.40
1:B:163:VAL:HA	1:B:198:ARG:O	2.21	0.40
1:A:547:PRO:O	1:A:553:LEU:HD13	2.21	0.40
1:B:383:VAL:O	1:B:387:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	624/705 (88%)	615 (99%)	9 (1%)	0	100	100
1	B	629/705 (89%)	617 (98%)	12 (2%)	0	100	100
1	C	629/705 (89%)	618 (98%)	11 (2%)	0	100	100
1	D	625/705 (89%)	612 (98%)	13 (2%)	0	100	100
All	All	2507/2820 (89%)	2462 (98%)	45 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	537/592 (91%)	521 (97%)	16 (3%)	53	53
1	B	542/592 (92%)	524 (97%)	18 (3%)	50	49
1	C	542/592 (92%)	522 (96%)	20 (4%)	45	44
1	D	538/592 (91%)	518 (96%)	20 (4%)	45	44
All	All	2159/2368 (91%)	2085 (97%)	74 (3%)	49	48

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	32	THR
1	A	59	ARG
1	A	92	ARG
1	A	107	CYS
1	A	268	ARG
1	A	279	VAL
1	A	334	LEU
1	A	353	ASN
1	A	448	THR
1	A	481	LEU
1	A	535	VAL
1	A	553	LEU
1	A	555	LEU
1	A	602	LEU
1	A	677	LEU
1	B	59	ARG
1	B	84	THR
1	B	92	ARG
1	B	107	CYS
1	B	209	GLU
1	B	268	ARG
1	B	334	LEU
1	B	353	ASN
1	B	404	GLU
1	B	448	THR

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Mol	Chain	Res	Type
1	B	481	LEU
1	B	553	LEU
1	B	555	LEU
1	B	562	THR
1	B	591	ARG
1	B	599	VAL
1	B	640	VAL
1	B	673	LEU
1	C	29	VAL
1	C	59	ARG
1	C	82	VAL
1	C	92	ARG
1	C	162	ASN
1	C	209	GLU
1	C	268	ARG
1	C	279	VAL
1	C	334	LEU
1	C	353	ASN
1	C	392	LYS
1	C	448	THR
1	C	535	VAL
1	C	548	THR
1	C	553	LEU
1	C	555	LEU
1	C	591	ARG
1	C	602	LEU
1	C	640	VAL
1	C	673	LEU
1	D	26	LYS
1	D	59	ARG
1	D	92	ARG
1	D	107	CYS
1	D	164	SER
1	D	202	ASP
1	D	268	ARG
1	D	279	VAL
1	D	334	LEU
1	D	353	ASN
1	D	392	LYS
1	D	404	GLU
1	D	481	LEU
1	D	548	THR

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Mol	Chain	Res	Type
1	D	555	LEU
1	D	587	ARG
1	D	589	SER
1	D	602	LEU
1	D	640	VAL
1	D	673	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	360	HIS
1	B	362	ASN
1	D	47	HIS
1	D	162	ASN
1	D	671	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	MDO	A	175	1,2	13,13,14	13.15	6 (46%)	16,18,20	2.34	4 (25%)
1	MDO	B	175	1,2	13,13,14	13.66	8 (61%)	16,18,20	2.44	4 (25%)
1	MDO	C	175	1,2	13,13,14	12.80	8 (61%)	16,18,20	2.34	2 (12%)
1	MDO	D	175	1,2	13,13,14	12.54	7 (53%)	16,18,20	2.12	4 (25%)

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
1	MDO	A	175	1,2	-	0/4/23/24	0/1/1/1
1	MDO	B	175	1,2	-	0/4/23/24	0/1/1/1
1	MDO	C	175	1,2	-	0/4/23/24	0/1/1/1
1	MDO	D	175	1,2	-	0/4/23/24	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	MDO	O-C	48.15	1.44	1.11
1	A	175	MDO	O-C	46.24	1.43	1.11
1	C	175	MDO	O-C	45.00	1.42	1.11
1	D	175	MDO	O-C	44.02	1.42	1.11
1	D	175	MDO	O2-C2	6.30	1.36	1.23
1	A	175	MDO	O2-C2	6.24	1.36	1.23
1	B	175	MDO	O2-C2	5.82	1.35	1.23
1	C	175	MDO	O2-C2	5.29	1.34	1.23
1	B	175	MDO	CB2-CA2	4.68	1.53	1.34
1	C	175	MDO	CB2-CA2	4.58	1.52	1.34
1	A	175	MDO	CB2-CA2	4.51	1.52	1.34
1	D	175	MDO	CB2-CA2	4.36	1.51	1.34
1	B	175	MDO	CA3-C	4.31	1.54	1.48
1	C	175	MDO	CA3-C	3.95	1.54	1.48
1	C	175	MDO	C2-N3	-3.95	1.31	1.39
1	A	175	MDO	CA3-C	3.84	1.53	1.48
1	D	175	MDO	CA3-C	3.60	1.53	1.48
1	A	175	MDO	C2-N3	-3.41	1.32	1.39
1	B	175	MDO	C2-N3	-3.33	1.32	1.39
1	A	175	MDO	CA-C1	3.32	1.55	1.51
1	D	175	MDO	C2-N3	-3.22	1.32	1.39
1	D	175	MDO	CA-C1	3.13	1.55	1.51
1	C	175	MDO	C1-N2	2.57	1.36	1.32
1	C	175	MDO	CA-C1	2.39	1.54	1.51
1	B	175	MDO	CA2-N2	-2.36	1.33	1.39
1	D	175	MDO	CA2-N2	-2.33	1.33	1.39
1	B	175	MDO	CA-C1	2.25	1.54	1.51
1	B	175	MDO	CA2-C2	-2.09	1.39	1.43
1	C	175	MDO	CA2-N2	-2.03	1.34	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	MDO	CA2-C2-N3	7.98	107.90	103.18
1	B	175	MDO	CA2-C2-N3	6.91	107.27	103.18
1	A	175	MDO	CA2-C2-N3	6.23	106.87	103.18
1	D	175	MDO	CA2-C2-N3	5.71	106.56	103.18
1	B	175	MDO	O2-C2-CA2	-5.16	128.04	130.93
1	A	175	MDO	O2-C2-CA2	-4.87	128.21	130.93
1	D	175	MDO	O2-C2-CA2	-3.97	128.71	130.93
1	C	175	MDO	O2-C2-CA2	-3.33	129.07	130.93
1	D	175	MDO	N3-C1-N2	-2.78	109.48	111.47
1	A	175	MDO	N3-C1-N2	-2.74	109.51	111.47
1	D	175	MDO	CB2-CA2-N2	-2.59	124.43	128.04
1	B	175	MDO	N3-C1-N2	-2.27	109.84	111.47
1	A	175	MDO	CB-CA-C1	2.22	113.65	110.45
1	B	175	MDO	CB2-CA2-N2	-2.05	125.18	128.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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	$\# Z  > 2$
2	BQ7	A	1678	1	14,14,14	1.54	2 (14%)	20,20,20	1.16	3 (15%)
3	GOL	A	1679	-	5,5,5	0.15	0	5,5,5	0.35	0
2	BQ7	B	1678	1	14,14,14	1.44	1 (7%)	20,20,20	1.09	3 (15%)
3	GOL	B	1679	-	5,5,5	0.30	0	5,5,5	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BQ7	C	1678	1	14,14,14	1.51	2 (14%)	20,20,20	1.04	1 (5%)
2	BQ7	D	1678	1	14,14,14	1.49	2 (14%)	20,20,20	1.54	3 (15%)

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
2	BQ7	A	1678	1	-	1/14/16/16	0/1/1/1
3	GOL	A	1679	-	-	0/4/4/4	0/0/0/0
2	BQ7	B	1678	1	-	1/14/16/16	0/1/1/1
3	GOL	B	1679	-	-	0/4/4/4	0/0/0/0
2	BQ7	C	1678	1	-	1/14/16/16	0/1/1/1
2	BQ7	D	1678	1	-	1/14/16/16	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1678	BQ7	CG-CB	3.98	1.56	1.52
2	B	1678	BQ7	CG-CB	3.91	1.56	1.52
2	A	1678	BQ7	CG-CB	3.36	1.55	1.52
2	C	1678	BQ7	CG-CB	3.21	1.55	1.52
2	A	1678	BQ7	CA-CB	3.10	1.57	1.53
2	C	1678	BQ7	CA-CB	2.84	1.56	1.53
2	D	1678	BQ7	CA-CB	2.63	1.56	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1678	BQ7	FS-CA-CB	3.70	113.44	108.49
2	D	1678	BQ7	O-C-CA	3.17	118.32	112.49
2	A	1678	BQ7	FS-CA-CB	3.14	112.69	108.49
2	D	1678	BQ7	CA-CB-CG	3.12	117.97	112.02
2	C	1678	BQ7	O-C-CA	2.88	117.80	112.49
2	B	1678	BQ7	O-C-CA	2.62	117.32	112.49
2	B	1678	BQ7	FS-CA-CB	2.11	111.31	108.49
2	A	1678	BQ7	CA-CB-CG	2.10	116.03	112.02
2	A	1678	BQ7	O-C-CA	2.02	116.21	112.49
2	B	1678	BQ7	CA-CB-CG	2.01	115.85	112.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1678	BQ7	CG-CB-CA-C
2	B	1678	BQ7	CG-CB-CA-C
2	A	1678	BQ7	CG-CB-CA-C
2	C	1678	BQ7	CG-CB-CA-C

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	635/705 (90%)	0.01	24 (3%)	38 41	11, 24, 49, 60	0
1	B	640/705 (90%)	-0.05	7 (1%)	77 81	12, 24, 40, 54	0
1	C	640/705 (90%)	-0.06	15 (2%)	57 60	12, 22, 42, 54	0
1	D	636/705 (90%)	-0.07	11 (1%)	67 72	11, 22, 45, 57	0
All	All	2551/2820 (90%)	-0.04	57 (2%)	59 61	11, 23, 44, 60	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	576	THR	4.1
1	C	591	ARG	3.6
1	A	522	ASN	3.6
1	A	586	LYS	3.5
1	A	515	ALA	3.4
1	A	580	ARG	3.4
1	A	576	THR	3.4
1	B	202	ASP	3.1
1	A	602	LEU	3.0
1	B	523	ASP	2.9
1	C	605	LYS	2.9
1	A	577	LEU	2.9
1	C	599	VAL	2.8
1	C	586	LYS	2.8
1	D	586	LYS	2.8
1	C	584	PHE	2.7
1	D	602	LEU	2.7
1	D	591	ARG	2.7
1	A	564	LEU	2.7
1	A	47	HIS	2.6
1	C	576	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	520	LEU	2.6
1	A	581	LEU	2.6
1	C	589	SER	2.6
1	C	590	ASP	2.5
1	B	567	HIS	2.5
1	D	578	VAL	2.5
1	A	518	CYS	2.5
1	B	545	CYS	2.5
1	B	565	ALA	2.4
1	A	579	ASP	2.4
1	C	566	LEU	2.4
1	D	201	ASP	2.4
1	A	217	ARG	2.4
1	D	579	ASP	2.4
1	A	587	ARG	2.4
1	D	577	LEU	2.4
1	A	202	ASP	2.4
1	A	578	VAL	2.3
1	A	521	PRO	2.3
1	C	677	LEU	2.3
1	A	591	ARG	2.2
1	B	574	THR	2.2
1	D	587	ARG	2.2
1	A	584	PHE	2.2
1	C	583	GLU	2.2
1	C	574	THR	2.2
1	A	527	ARG	2.2
1	A	523	ASP	2.2
1	C	579	ASP	2.2
1	D	202	ASP	2.2
1	D	521	PRO	2.2
1	C	575	ASP	2.1
1	A	519	GLY	2.1
1	A	511	VAL	2.0
1	B	671	HIS	2.0
1	C	518	CYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	MDO	C	175	13/14	0.11	-0.15	15,16,18,19	0
1	MDO	D	175	13/14	0.11	-0.38	16,18,19,21	0
1	MDO	B	175	13/14	0.10	-0.63	18,21,23,25	0
1	MDO	A	175	13/14	0.09	-1.14	18,19,20,22	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	A	1679	6/6	0.18	2.32	28,30,32,36	0
2	BQ7	A	1678	14/14	0.15	1.98	26,28,36,37	0
3	GOL	B	1679	6/6	0.13	1.18	28,32,32,35	0
2	BQ7	B	1678	14/14	0.12	0.56	27,31,37,40	0
2	BQ7	C	1678	14/14	0.12	0.16	24,25,30,31	0
2	BQ7	D	1678	14/14	0.10	-0.17	27,29,34,34	0

### 6.5 Other polymers

There are no such residues in this entry.