



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 10:15 AM EST

PDB ID : 6DDA  
Title : Nurr1 Covalently Modified by a Dopamine Metabolite  
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Deposited on : 2018-05-09  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

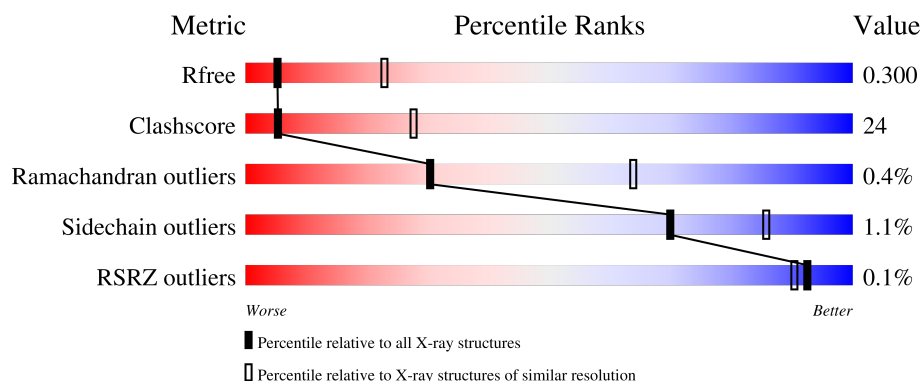
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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	B	272	
1	C	272	
2	A	272	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	G7J	C	605	-	-	X	-
5	BR	C	601	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5552 atoms, of which 27 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 Nuclear receptor subfamily 4 group A member 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	236	Total	C	H	N	O	S	0	0	0
			1884	1206	3	319	346	10			
1	C	225	Total	C	H	N	O	S	0	0	0
			1805	1160	3	305	328	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	327	SER	-	expression tag	UNP P43354
C	327	SER	-	expression tag	UNP P43354

- Molecule 2 is a protein called Nuclear receptor subfamily 4 group A member 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	224	Total	C	H	N	O	S	0	0	0
			1800	1156	3	303	329	9			

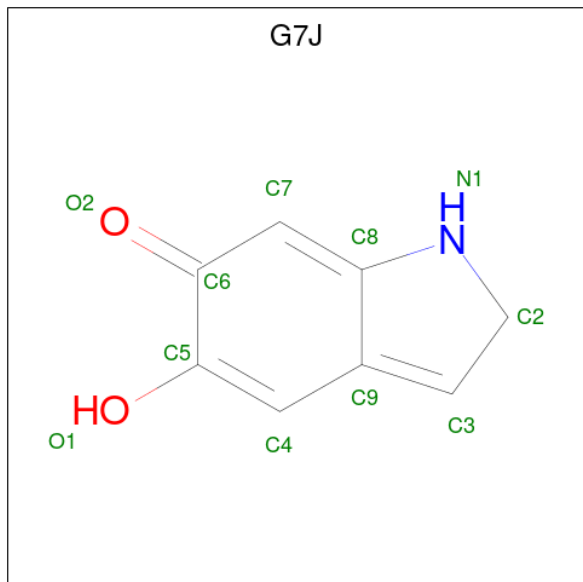
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	SER	-	expression tag	UNP P43354

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 4 is 5-hydroxy-1,2-dihydro-6H-indol-6-one (three-letter code: G7J) (formula:  $C_8H_7NO_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	0
			17	8	6	1	2		
4	A	1	Total	C	H	N	O	0	0
			17	8	6	1	2		
4	C	1	Total	C	H	N	O	0	0
			17	8	6	1	2		

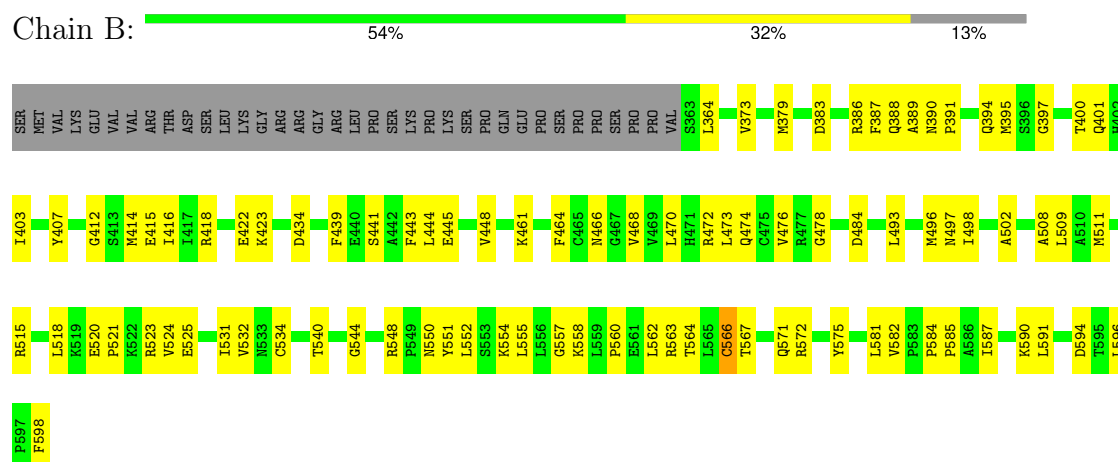
- Molecule 5 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Br	0	0
			4	4		
5	C	3	Total	Br	0	0
			3	3		

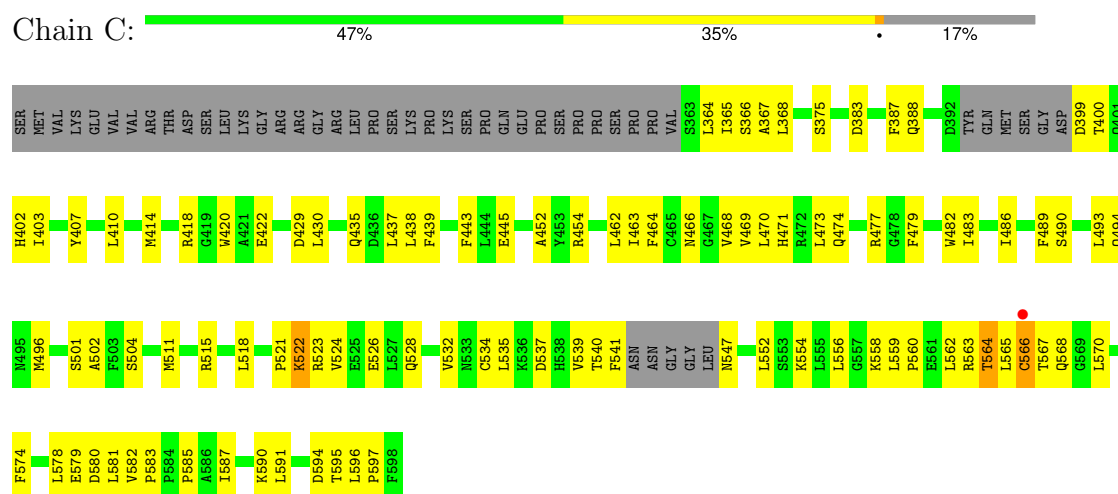
### 3 Residue-property plots

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: Nuclear receptor subfamily 4 group A member 2



- Molecule 1: Nuclear receptor subfamily 4 group A member 2



- Molecule 2: Nuclear receptor subfamily 4 group A member 2



E561	G478	GLN	SER
L562	F479	MET	MET
R563		SER	VAL
T564	V482	GLY	LVS
L565	I483	ASP	GLU
C566	T486	D399	VAL
T567		T400	VAL
Q568	F489	Q401	ARG
R572	S490	H402	THR
I573	S491		ASP
F574	V492	F406	SER
L575	L493	L409	LEU
L576	Q494	L410	LVS
K577	K495	T411	GLY
L578	M496	G412	ARG
		S413	GLY
L581	F503	M414	ARG
V582		E415	LEU
P583	I506	T416	PRO
P584		I417	SER
	L509	R418	LVS
I587	V510		PRO
L588	N511	G426	LVS
D589			SER
K590	L518	D436	PRO
	E520	F439	GLU
L593	P521	E440	PRO
F598	K522	F443	SER
	R523	L444	PRO
	V524	E445	SER
	E525	L446	PRO
	E526		PRO
	L527	L449	PRO
	Q528		VAL
		A452	S363
	N532	V453	L364
	C534	R454	I365
		S455	
	F541	V456	V369
ASN	ASN	P457	R370
ASN	GLY		
GLY	L462	K461	N376
LEU	I463	T463	P377
ASN	F464	F464	M379
	G465		T380
R548	P549	M466	S381
P549	N550	G467	L382
V551	V551	V468	D383
L552	L552	V469	Y384
		L470	S385
L555	L556		R386
	G557	L473	F387
K558		Q474	Q388
L559		C475	
D560		V476	P391
		P477	D392

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.59Å 80.59Å 225.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.29 – 3.20 40.29 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.29-3.20) 88.0 (40.29-3.20)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.49 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.250 , 0.294 0.252 , 0.300	Depositor DCC
$R_{free}$ test set	13255 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.7	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 96.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5552	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.0667e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

Bond lengths and bond angles in the following residue types are not validated in this section: K, G7J, OCS, BR

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	B	0.43	2/1921 (0.1%)	0.70	0/2601
1	C	0.43	3/1839 (0.2%)	0.61	0/2488
2	A	0.47	3/1824 (0.2%)	0.71	0/2466
All	All	0.44	8/5584 (0.1%)	0.67	0/7555

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	C	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	566	CYS	N-CA	-7.30	1.31	1.46
1	C	566	CYS	N-CA	-7.29	1.31	1.46
1	B	566	CYS	N-CA	-7.27	1.31	1.46
1	C	564	THR	C-N	6.18	1.48	1.34
1	C	566	CYS	CA-CB	-6.10	1.40	1.53
1	B	566	CYS	CA-CB	-6.08	1.40	1.53
2	A	566	CYS	CA-CB	-6.07	1.40	1.53
2	A	567	THR	C-N	5.99	1.47	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	564	THR	Mainchain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1881	3	1886	88	1
1	C	1802	3	1817	90	2
2	A	1797	3	1808	87	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	11	6	0	1	0
4	B	11	6	0	0	0
4	C	11	6	0	5	0
5	A	4	0	0	0	0
5	C	3	0	0	5	1
All	All	5525	27	5511	261	2

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 24.

All (261) 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:B:388:GLN:H	1:B:474:GLN:HE22	1.03	1.01
5:C:601:BR:BR	5:C:602:BR:BR	2.94	0.96
1:C:596:LEU:HD12	1:C:597:PRO:HD2	1.52	0.92
1:C:522:LYS:O	1:C:526:GLU:HG2	1.75	0.85
1:C:563:ARG:HD2	4:C:605:G7J:C7	2.06	0.85
1:C:563:ARG:CD	4:C:605:G7J:C7	2.55	0.84
1:B:445:GLU:O	1:B:562:LEU:HD11	1.77	0.84
1:C:439:PHE:HD1	1:C:511:MET:HE1	1.43	0.82
1:B:388:GLN:H	1:B:474:GLN:NE2	1.78	0.82
1:C:521:PRO:O	1:C:524:VAL:HG12	1.80	0.81
1:B:373:VAL:O	2:A:370:ARG:NH2	2.13	0.81
1:B:563:ARG:HH21	1:B:567:THR:HG21	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:GLN:O	1:B:474:GLN:NE2	2.14	0.81
1:B:445:GLU:HB3	1:B:562:LEU:HG	1.62	0.81
1:C:414:MET:HA	1:C:443:PHE:CE1	2.16	0.80
1:C:438:LEU:HD23	1:C:515:ARG:HG3	1.62	0.80
1:C:367:ALA:HA	5:C:601:BR:BR	2.39	0.77
1:B:418:ARG:HB2	1:B:439:PHE:CZ	2.22	0.75
1:B:390:ASN:O	1:B:394:GLN:HG3	1.86	0.75
1:B:387:PHE:CZ	1:B:461:LYS:HE2	2.22	0.74
1:C:596:LEU:HD12	1:C:597:PRO:CD	2.18	0.74
2:A:518:LEU:HD13	2:A:524:VAL:HG11	1.71	0.72
1:C:579:GLU:HG2	1:C:581:LEU:HB2	1.70	0.72
1:C:518:LEU:HD23	1:C:524:VAL:HG11	1.71	0.71
2:A:383:ASP:OD1	2:A:468:VAL:HA	1.91	0.70
1:C:468:VAL:HG12	1:C:470:LEU:HD23	1.74	0.69
1:B:389:ALA:HA	1:B:394:GLN:HE21	1.57	0.69
2:A:452:ALA:HB1	2:A:490:SER:HA	1.75	0.69
1:B:412:GLY:O	1:B:415:GLU:HG2	1.92	0.69
1:C:445:GLU:O	1:C:562:LEU:HD11	1.93	0.68
1:B:563:ARG:HG3	1:B:564:THR:N	2.09	0.68
1:C:581:LEU:CD1	1:C:582:VAL:HG23	2.24	0.68
2:A:563:ARG:HG3	4:A:608:G7J:C7	2.24	0.68
1:C:581:LEU:HD13	1:C:582:VAL:HG23	1.76	0.68
1:C:552:LEU:O	1:C:556:LEU:HD13	1.94	0.68
1:C:574:PHE:CE2	1:C:578:LEU:HD11	2.29	0.68
1:C:522:LYS:H	1:C:522:LYS:HD2	1.60	0.67
1:B:414:MET:HA	1:B:443:PHE:CE1	2.30	0.67
2:A:470:LEU:HD12	2:A:474:GLN:OE1	1.95	0.66
2:A:414:MET:HA	2:A:443:PHE:CE1	2.30	0.66
2:A:587:ILE:H	2:A:587:ILE:HD12	1.61	0.65
1:B:581:LEU:HD12	1:B:582:VAL:HG23	1.79	0.65
1:B:470:LEU:HD12	1:B:474:GLN:OE1	1.97	0.65
1:C:528:GLN:O	1:C:532:VAL:HG23	1.97	0.65
1:B:497:ASN:CB	2:A:541:PHE:HE2	2.11	0.64
1:B:581:LEU:CD1	1:B:582:VAL:HG23	2.28	0.63
1:C:402:HIS:CD2	1:C:477:ARG:HB3	2.33	0.62
1:B:557:GLY:O	1:B:560:PRO:HD2	2.00	0.62
1:B:383:ASP:OD1	1:B:468:VAL:HA	2.00	0.62
2:A:457:PRO:HB2	2:A:491:SER:OG	1.99	0.62
1:C:430:LEU:O	1:C:435:GLN:NE2	2.27	0.62
2:A:479:PHE:CD2	2:A:483:ILE:HD13	2.35	0.61
1:B:391:PRO:HA	1:B:394:GLN:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:GLY:O	1:B:416:ILE:HG12	1.99	0.61
2:A:572:ARG:NH2	2:A:576:LEU:HD21	2.16	0.61
1:C:595:THR:HG22	4:C:605:G7J:C3	2.31	0.61
1:B:478:GLY:O	1:B:572:ARG:NH2	2.33	0.61
2:A:479:PHE:CG	2:A:483:ILE:HD13	2.36	0.60
1:C:563:ARG:HD3	4:C:605:G7J:C7	2.31	0.60
1:B:554:LYS:HE2	1:B:558:LYS:NZ	2.15	0.60
2:A:454:ARG:O	2:A:463:ILE:HD12	2.00	0.60
1:C:367:ALA:CA	5:C:601:BR:BR	3.04	0.60
2:A:382:LEU:HB2	2:A:384:TYR:CE1	2.37	0.60
2:A:521:PRO:O	2:A:524:VAL:HG12	2.02	0.60
1:B:403:ILE:HG21	1:B:582:VAL:HB	1.84	0.59
2:A:440:GLU:OE2	2:A:590:LYS:NZ	2.35	0.59
1:C:537:ASP:O	1:C:541:PHE:HD2	1.86	0.59
2:A:557:GLY:O	2:A:560:PRO:HD2	2.02	0.59
2:A:468:VAL:HG12	2:A:470:LEU:HD22	1.85	0.59
1:C:403:ILE:HG21	1:C:582:VAL:HB	1.85	0.59
2:A:449:LEU:HB2	2:A:562:LEU:HD11	1.85	0.58
1:B:508:ALA:HB1	1:B:531:ILE:HD13	1.85	0.58
2:A:564:THR:O	2:A:568:GLN:HG3	2.03	0.58
1:C:407:TYR:CD2	1:C:585:PRO:HD3	2.38	0.58
1:B:509:LEU:HD21	1:B:532:VAL:HG23	1.86	0.57
1:C:590:LYS:HG2	1:C:594:ASP:OD2	2.04	0.57
1:B:386:ARG:HH21	1:B:468:VAL:HG11	1.69	0.57
1:B:441:SER:HB3	1:B:515:ARG:HE	1.70	0.56
1:B:497:ASN:HB3	2:A:541:PHE:HE2	1.69	0.56
1:B:521:PRO:O	1:B:524:VAL:HG12	2.05	0.56
2:A:388:GLN:HB3	2:A:474:GLN:HE21	1.71	0.56
1:B:548:ARG:HG3	1:B:551:TYR:H	1.70	0.56
2:A:399:ASP:OD1	2:A:400:THR:N	2.39	0.56
1:C:452:ALA:HB1	1:C:490:SER:HA	1.87	0.56
1:C:559:LEU:HB2	1:C:560:PRO:HD3	1.87	0.56
1:C:540:THR:HG23	1:C:547:ASN:HB3	1.88	0.56
2:A:382:LEU:HB2	2:A:384:TYR:HE1	1.68	0.56
1:B:518:LEU:CD2	1:B:524:VAL:HG11	2.37	0.55
1:C:489:PHE:CG	1:C:565:LEU:HD11	2.41	0.55
1:C:375:SER:CB	1:C:420:TRP:HB2	2.36	0.55
1:B:496:MET:HE1	1:B:555:LEU:HD12	1.88	0.54
1:B:518:LEU:HD21	1:B:524:VAL:HG11	1.89	0.54
1:B:551:TYR:O	1:B:555:LEU:HD13	2.08	0.54
1:B:468:VAL:HG12	1:B:470:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ARG:O	1:B:422:GLU:HG3	2.07	0.54
1:C:482:TRP:CE2	1:C:486:ILE:HD11	2.43	0.54
1:B:554:LYS:HE2	1:B:558:LYS:HZ3	1.73	0.53
2:A:399:ASP:HA	2:A:477:ARG:HH11	1.72	0.53
2:A:528:GLN:O	2:A:532:VAL:HG23	2.09	0.53
1:B:400:THR:HG23	1:B:401:GLN:N	2.24	0.52
2:A:520:GLU:OE1	2:A:523:ARG:HD2	2.09	0.52
1:C:574:PHE:CZ	1:C:578:LEU:HD11	2.44	0.52
2:A:388:GLN:N	2:A:474:GLN:NE2	2.58	0.52
2:A:399:ASP:CB	2:A:477:ARG:HD2	2.40	0.52
1:C:563:ARG:O	1:C:567:THR:HG23	2.10	0.52
1:C:567:THR:O	1:C:570:LEU:HB2	2.10	0.52
1:B:548:ARG:HG3	1:B:551:TYR:HB3	1.92	0.52
1:C:579:GLU:CG	1:C:581:LEU:HB2	2.39	0.52
1:B:439:PHE:HA	1:B:511:MET:HE1	1.92	0.52
1:B:551:TYR:CZ	1:B:555:LEU:HD11	2.45	0.52
2:A:552:LEU:HD13	2:A:552:LEU:C	2.30	0.52
1:C:387:PHE:CE1	1:C:471:HIS:HB2	2.45	0.52
2:A:378:ALA:C	2:A:380:THR:H	2.13	0.51
1:B:548:ARG:HG3	1:B:551:TYR:CB	2.40	0.51
1:C:595:THR:CG2	4:C:605:G7J:C3	2.89	0.51
1:B:496:MET:CE	1:B:555:LEU:HD12	2.41	0.51
1:B:391:PRO:HA	1:B:394:GLN:OE1	2.11	0.51
1:C:367:ALA:HB2	5:C:601:BR:BR	2.65	0.51
1:C:559:LEU:O	1:C:562:LEU:HB3	2.11	0.51
1:C:522:LYS:HD2	1:C:522:LYS:N	2.26	0.51
2:A:564:THR:HG22	2:A:568:GLN:HE21	1.76	0.50
1:C:418:ARG:HB2	1:C:439:PHE:CZ	2.46	0.50
1:C:445:GLU:HB3	1:C:562:LEU:HD21	1.92	0.50
1:B:575:TYR:CD1	1:B:575:TYR:C	2.84	0.50
1:C:522:LYS:HG2	1:C:523:ARG:N	2.26	0.50
1:C:587:ILE:N	1:C:587:ILE:HD12	2.26	0.50
1:B:472:ARG:HD2	1:B:484:ASP:OD1	2.11	0.50
1:B:548:ARG:HH11	1:B:550:ASN:HB2	1.76	0.50
1:B:395:MET:O	1:B:397:GLY:N	2.42	0.50
2:A:446:LEU:HD11	2:A:511:MET:HB2	1.93	0.50
1:C:580:ASP:OD1	1:C:583:PRO:HG3	2.12	0.50
1:C:587:ILE:HD12	1:C:587:ILE:H	1.76	0.49
2:A:455:SER:O	2:A:494:GLN:NE2	2.43	0.49
2:A:412:GLY:O	2:A:416:ILE:HG12	2.13	0.49
2:A:453:TYR:HB2	2:A:503:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:LEU:O	1:C:539:VAL:HG23	2.12	0.49
1:B:407:TYR:OH	1:B:584:PRO:HG3	2.12	0.49
1:B:497:ASN:CB	2:A:541:PHE:CE2	2.94	0.49
2:A:551:TYR:CE2	2:A:555:LEU:HD22	2.48	0.49
1:B:590:LYS:HG2	1:B:594:ASP:OD2	2.13	0.49
2:A:387:PHE:CZ	2:A:461:LYS:HE2	2.48	0.48
2:A:559:LEU:HB2	2:A:560:PRO:HD3	1.94	0.48
2:A:522:LYS:O	2:A:526:GLU:HG2	2.12	0.48
2:A:464:PHE:C	2:A:466:ASN:H	2.17	0.48
2:A:365:ILE:HG23	2:A:534:CYS:HB3	1.94	0.48
2:A:558:LYS:HD3	2:A:561:GLU:OE1	2.14	0.48
2:A:506:ILE:HG13	2:A:555:LEU:HG	1.95	0.48
2:A:490:SER:O	2:A:494:GLN:HG3	2.14	0.48
2:A:388:GLN:H	2:A:474:GLN:NE2	2.11	0.48
1:B:548:ARG:CG	1:B:551:TYR:CB	2.92	0.47
1:C:581:LEU:HD12	1:C:582:VAL:HG23	1.95	0.47
1:B:548:ARG:CG	1:B:551:TYR:HB3	2.44	0.47
2:A:489:PHE:CG	2:A:565:LEU:HD11	2.49	0.47
1:B:423:LYS:HE2	1:B:423:LYS:HA	1.97	0.47
1:B:587:ILE:HD12	1:B:587:ILE:H	1.80	0.47
1:B:414:MET:CA	1:B:443:PHE:CE1	2.97	0.47
2:A:548:ARG:HA	2:A:548:ARG:NE	2.30	0.47
1:B:383:ASP:OD1	1:B:383:ASP:O	2.33	0.47
2:A:376:ASN:HD22	2:A:454:ARG:HE	1.63	0.47
1:B:464:PHE:C	1:B:466:ASN:H	2.18	0.47
2:A:444:LEU:HD23	2:A:444:LEU:HA	1.46	0.46
1:B:590:LYS:CG	1:B:594:ASP:OD2	2.64	0.46
2:A:364:LEU:HB2	2:A:534:CYS:SG	2.56	0.46
1:B:403:ILE:CG2	1:B:582:VAL:HB	2.45	0.46
1:C:470:LEU:CD1	1:C:474:GLN:OE1	2.64	0.46
1:C:591:LEU:HD13	1:C:591:LEU:C	2.36	0.46
1:C:554:LYS:HE2	1:C:558:LYS:NZ	2.31	0.46
1:B:445:GLU:CB	1:B:562:LEU:HG	2.40	0.46
1:B:400:THR:HG23	1:B:401:GLN:H	1.81	0.45
1:B:493:LEU:O	1:B:496:MET:HG2	2.17	0.45
1:B:540:THR:O	1:B:544:GLY:O	2.34	0.45
1:B:598:PHE:CD1	1:B:598:PHE:N	2.84	0.45
2:A:457:PRO:HD2	2:A:494:GLN:OE1	2.16	0.45
1:C:482:TRP:O	1:C:486:ILE:HG13	2.17	0.45
1:C:368:LEU:HB3	1:C:504:SER:HB3	1.99	0.45
1:B:445:GLU:HB3	1:B:562:LEU:CG	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:ALA:CB	5:C:601:BR:BR	3.20	0.45
1:C:438:LEU:CD2	1:C:515:ARG:HG3	2.40	0.45
1:B:596:LEU:HG	1:B:598:PHE:CE1	2.52	0.45
1:B:364:LEU:HB2	1:B:534:CYS:SG	2.57	0.45
1:C:479:PHE:CB	1:C:483:ILE:HB	2.47	0.45
1:B:441:SER:CB	1:B:515:ARG:HE	2.30	0.44
2:A:406:PHE:CZ	2:A:410:LEU:HD11	2.52	0.44
2:A:439:PHE:HD1	2:A:511:MET:HE1	1.82	0.44
1:C:365:ILE:HG13	1:C:366:SER:N	2.32	0.44
1:B:434:ASP:OD1	1:B:518:LEU:HD12	2.17	0.44
2:A:402:HIS:CD2	2:A:477:ARG:HB3	2.51	0.44
1:C:502:ALA:HA	1:C:535:LEU:HD13	1.98	0.44
1:B:509:LEU:CD2	1:B:532:VAL:HG23	2.47	0.44
2:A:436:ASP:O	2:A:440:GLU:HG3	2.18	0.44
1:B:524:VAL:HG13	1:B:525:GLU:N	2.33	0.44
2:A:518:LEU:CD1	2:A:524:VAL:HG11	2.43	0.44
2:A:589:ASP:O	2:A:593:LEU:HG	2.17	0.44
1:B:388:GLN:N	1:B:474:GLN:NE2	2.58	0.44
1:B:473:LEU:O	1:B:476:VAL:HG12	2.17	0.44
2:A:378:ALA:O	2:A:380:THR:N	2.50	0.44
1:C:375:SER:HB2	1:C:420:TRP:HB2	1.99	0.43
1:C:383:ASP:OD1	1:C:468:VAL:HA	2.18	0.43
1:C:470:LEU:HD13	1:C:474:GLN:OE1	2.18	0.43
1:C:471:HIS:CE1	1:C:473:LEU:HG	2.53	0.43
1:B:567:THR:O	1:B:571:GLN:HG3	2.18	0.43
2:A:409:LEU:HD13	2:A:464:PHE:CE2	2.53	0.43
1:B:591:LEU:C	1:B:591:LEU:HD13	2.38	0.43
2:A:550:ASN:O	2:A:552:LEU:N	2.47	0.43
1:C:364:LEU:HB2	1:C:534:CYS:SG	2.59	0.43
2:A:426:GLY:C	2:A:527:LEU:HD11	2.39	0.43
1:C:454:ARG:HD2	1:C:463:ILE:O	2.17	0.43
1:B:407:TYR:CD2	1:B:585:PRO:HD3	2.53	0.43
1:C:388:GLN:HB3	1:C:474:GLN:NE2	2.33	0.43
2:A:574:PHE:CZ	2:A:578:LEU:HD11	2.54	0.43
1:C:493:LEU:O	1:C:496:MET:HG2	2.19	0.43
2:A:555:LEU:HD12	2:A:555:LEU:HA	1.89	0.43
1:C:399:ASP:OD1	1:C:400:THR:N	2.52	0.43
2:A:412:GLY:O	2:A:415:GLU:HG2	2.19	0.43
1:C:462:LEU:HD13	1:C:462:LEU:HA	1.88	0.43
1:C:479:PHE:HB2	1:C:483:ILE:HB	2.01	0.43
1:C:554:LYS:HA	1:C:554:LYS:HD2	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:418:ARG:HB2	2:A:439:PHE:CZ	2.53	0.42
2:A:479:PHE:HB2	2:A:483:ILE:HB	1.99	0.42
1:C:452:ALA:HB1	1:C:490:SER:CA	2.48	0.42
2:A:482:TRP:O	2:A:486:ILE:HG13	2.20	0.42
2:A:386:ARG:HH21	2:A:468:VAL:CG1	2.32	0.42
2:A:473:LEU:O	2:A:476:VAL:HG12	2.19	0.42
1:C:469:VAL:O	1:C:470:LEU:HD22	2.19	0.42
1:B:498:ILE:HG23	1:B:502:ALA:HB3	2.02	0.42
2:A:475:CYS:HB2	2:A:483:ILE:HG12	2.01	0.42
1:B:548:ARG:HG2	1:B:551:TYR:HB2	2.01	0.42
2:A:583:PRO:HA	2:A:584:PRO:HD3	1.92	0.42
1:B:563:ARG:HH21	1:B:567:THR:CG2	2.22	0.42
2:A:475:CYS:CB	2:A:483:ILE:HG12	2.50	0.42
1:C:418:ARG:O	1:C:422:GLU:HG3	2.20	0.42
1:C:429:ASP:O	1:C:523:ARG:NH2	2.53	0.42
2:A:493:LEU:O	2:A:496:MET:HG2	2.18	0.42
1:C:430:LEU:CD2	1:C:523:ARG:HG2	2.50	0.41
1:C:464:PHE:C	1:C:466:ASN:H	2.23	0.41
2:A:388:GLN:HB3	2:A:474:GLN:NE2	2.34	0.41
2:A:391:PRO:HG3	2:A:473:LEU:HD13	2.03	0.41
1:B:444:LEU:O	1:B:448:VAL:HG23	2.21	0.41
1:B:520:GLU:OE1	1:B:523:ARG:HD3	2.20	0.41
1:C:552:LEU:HD13	1:C:552:LEU:C	2.41	0.41
1:C:490:SER:O	1:C:494:GLN:HG3	2.21	0.41
1:B:581:LEU:HD13	1:B:582:VAL:HG23	2.01	0.41
2:A:478:GLY:O	2:A:572:ARG:NH2	2.54	0.41
2:A:581:LEU:HD12	2:A:581:LEU:HA	1.79	0.41
1:C:388:GLN:H	1:C:474:GLN:NE2	2.19	0.41
1:C:403:ILE:HD12	1:C:581:LEU:HD12	2.02	0.41
1:C:437:LEU:HD22	1:C:518:LEU:CD1	2.51	0.41
1:C:567:THR:HA	1:C:570:LEU:HD12	2.03	0.41
1:C:581:LEU:HD13	1:C:581:LEU:O	2.21	0.41
1:B:497:ASN:HB2	2:A:541:PHE:HE2	1.84	0.41
2:A:399:ASP:CA	2:A:477:ARG:HH11	2.33	0.41
1:C:410:LEU:HD23	1:C:410:LEU:HA	1.96	0.41
1:C:556:LEU:N	1:C:556:LEU:CD1	2.84	0.41
2:A:468:VAL:HG12	2:A:470:LEU:CD2	2.51	0.40
1:B:548:ARG:NH1	1:B:550:ASN:HB2	2.36	0.40
2:A:365:ILE:O	2:A:369:VAL:HG23	2.22	0.40
2:A:464:PHE:CE1	2:A:470:LEU:HD23	2.56	0.40
2:A:509:LEU:HD21	2:A:532:VAL:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:GLN:N	1:C:474:GLN:HE22	2.19	0.40
1:B:496:MET:HG3	1:B:498:ILE:HG13	2.04	0.40
2:A:563:ARG:O	2:A:567:THR:HG23	2.21	0.40

All (2) 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:C:501:SER:OG	5:C:603:BR:BR[5_555]	1.91	0.29
1:B:388:GLN:NE2	1:C:387:PHE:O[6_455]	2.19	0.01

## 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	B	234/272 (86%)	226 (97%)	7 (3%)	1 (0%)	30	64
1	C	219/272 (80%)	209 (95%)	10 (5%)	0	100	100
2	A	217/272 (80%)	209 (96%)	6 (3%)	2 (1%)	14	49
All	All	670/816 (82%)	644 (96%)	23 (3%)	3 (0%)	30	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	551	TYR
2	A	379	MET
1	B	379	MET

### 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	B	209/243 (86%)	207 (99%)	2 (1%)	73	87
1	C	201/243 (83%)	198 (98%)	3 (2%)	60	81
2	A	199/242 (82%)	197 (99%)	2 (1%)	73	87
All	All	609/728 (84%)	602 (99%)	7 (1%)	70	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	552	LEU
1	B	566	CYS
2	A	555	LEU
2	A	566	CYS
1	C	522	LYS
1	C	566	CYS
1	C	568	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	474	GLN
1	C	376	ASN
1	C	402	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is 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	OCS	A	465	2	6,8,9	0.70	0	7,11,13	1.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OCS	A	465	2	-	2/4/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	465	OCS	CA-CB-SG-OD1
2	A	465	OCS	CA-CB-SG-OD2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 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
4	G7J	A	608	2	12,12,12	1.35	1 (8%)	11,17,17	1.42	2 (18%)
4	G7J	C	605	1	12,12,12	1.36	1 (8%)	11,17,17	1.43	2 (18%)
4	G7J	B	602	1	12,12,12	1.36	1 (8%)	11,17,17	1.43	2 (18%)

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
4	G7J	A	608	2	-	-	0/2/2/2
4	G7J	C	605	1	-	-	0/2/2/2
4	G7J	B	602	1	-	-	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	605	G7J	C2-C3	2.06	1.52	1.50
4	B	602	G7J	C2-C3	2.04	1.52	1.50
4	A	608	G7J	C2-C3	2.03	1.52	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	G7J	C3-C2-N1	-3.66	98.06	104.27
4	C	605	G7J	C3-C2-N1	-3.66	98.07	104.27
4	A	608	G7J	C3-C2-N1	-3.64	98.09	104.27
4	C	605	G7J	C9-C8-N1	-2.38	103.08	106.65
4	B	602	G7J	C9-C8-N1	-2.38	103.08	106.65
4	A	608	G7J	C9-C8-N1	-2.36	103.10	106.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	608	G7J	1	0
4	C	605	G7J	5	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	B	236/272 (86%)	-0.52	0 <span>100</span> <span>100</span>	59, 101, 147, 174	0
1	C	225/272 (82%)	-0.23	1 (0%) <span>89</span> <span>81</span>	59, 142, 191, 236	0
2	A	223/272 (81%)	-0.52	0 <span>100</span> <span>100</span>	59, 103, 171, 215	0
All	All	684/816 (83%)	-0.42	1 (0%) <span>92</span> <span>90</span>	59, 121, 176, 236	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	566	CYS	3.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	OCS	A	465	9/10	0.92	0.08	78,80,93,94	3

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	G7J	C	605	11/11	0.21	0.14	10,89,103,107	17
3	K	C	604	1/1	0.45	0.10	152,152,152,152	0
3	K	A	607	1/1	0.62	0.11	121,121,121,121	0
3	K	A	606	1/1	0.72	0.12	112,112,112,112	0
4	G7J	B	602	11/11	0.75	0.15	10,89,103,107	17
4	G7J	A	608	11/11	0.76	0.12	10,89,103,107	17
5	BR	C	602	1/1	0.85	0.07	132,132,132,132	1
5	BR	A	605	1/1	0.88	0.06	122,122,122,122	1
3	K	B	601	1/1	0.90	0.10	87,87,87,87	0
5	BR	C	601	1/1	0.91	0.06	135,135,135,135	1
5	BR	A	604	1/1	0.93	0.05	91,91,91,91	1
5	BR	A	603	1/1	0.93	0.06	95,95,95,95	1
5	BR	C	603	1/1	0.94	0.05	151,151,151,151	1
5	BR	A	602	1/1	0.95	0.05	78,78,78,78	1
3	K	A	601	1/1	0.98	0.04	48,48,48,48	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.