



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:08 AM UTC

PDB ID : 6DDA / pdb_00006dda
Title : Nurr1 Covalently Modified by a Dopamine Metabolite
Authors : Bruning, J.M.; Wang, Y.; Otrabella, F.; Boxue, T.; Liu, H.; Bhattacharya, P.;
Guo, S.; Holton, J.M.; Fletterick, R.J.; Jacobson, M.P.; England, P.M.
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

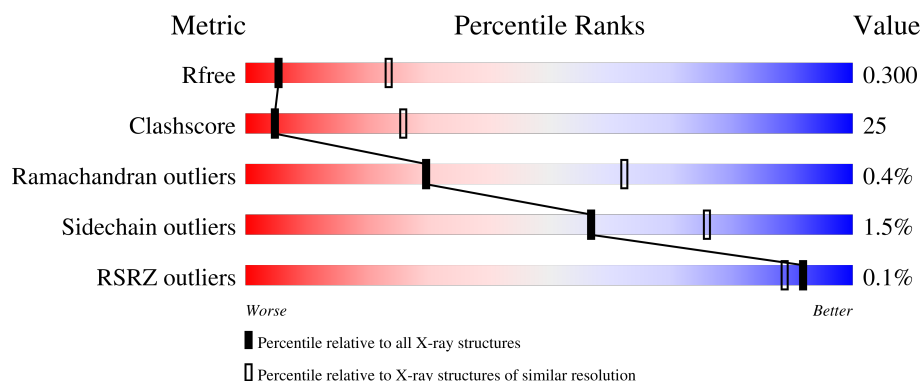
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 ≥ 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			

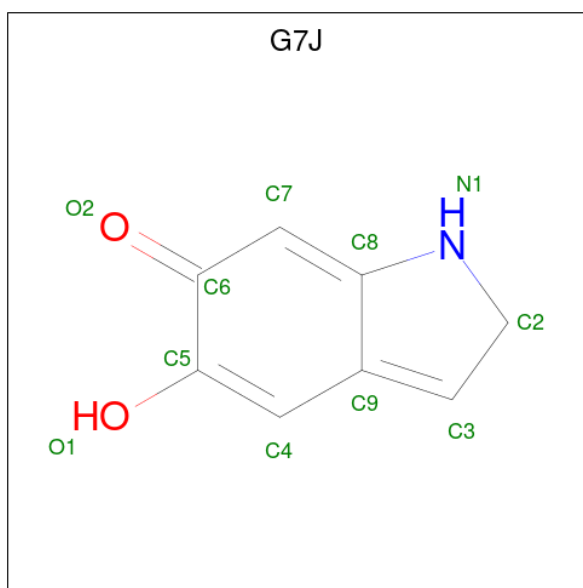
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is POTASSIUM ION (CCD ID: 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 (CCD ID: 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		

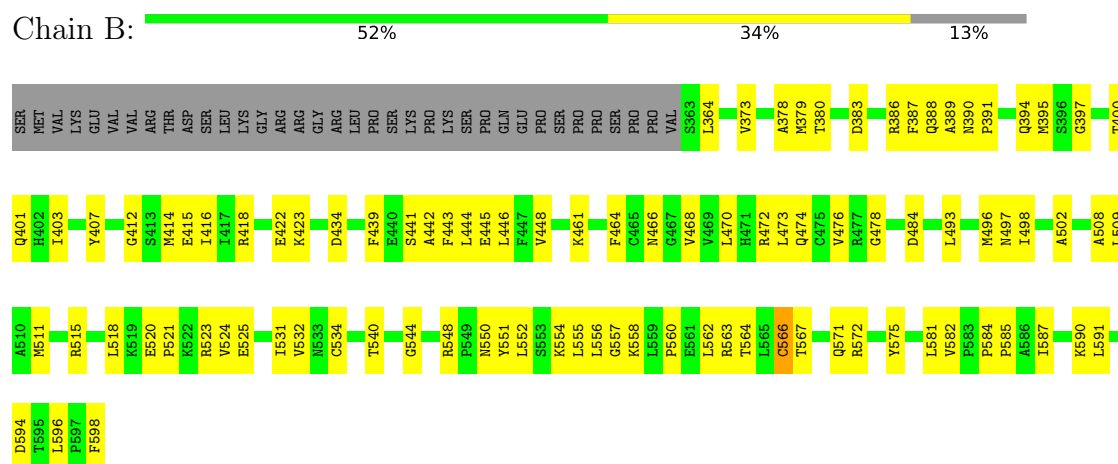
- Molecule 5 is BROMIDE ION (CCD ID: BR) (formula: Br).

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

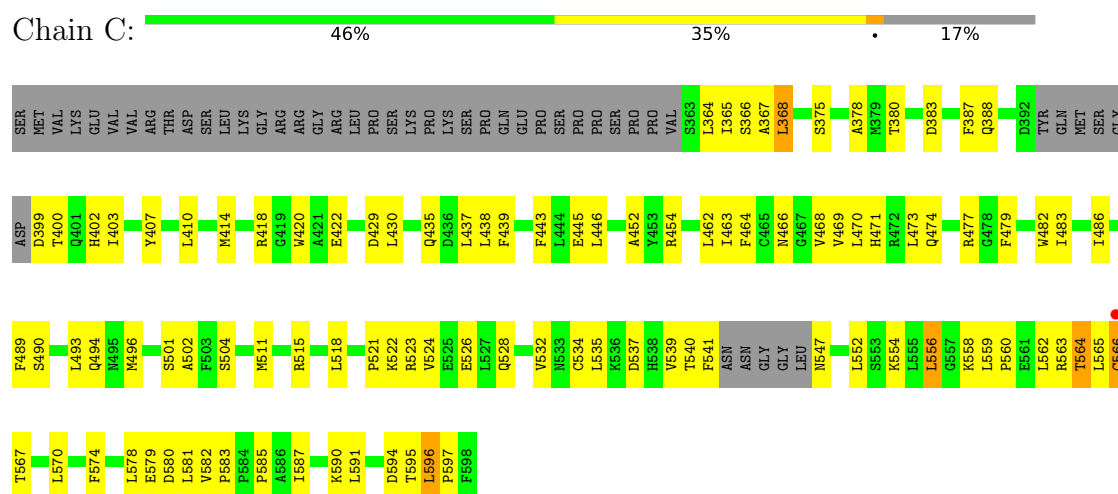
3 Residue-property plots

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



L556	G557	K558	L559	P560	E561	L562	R563	T564	L565	C566	T567	Q568		R572	I573	F574	Y575	L576	K577	L578		L581	V582	P583	P584		I587	I588	D589	K590		L593	F598																										
G478	F479		W482	I483		I486	F489	S490	S491	N492	L493	Q494	N495	M496		D499		F503		I506		L509	A510	M511		L518	R519	E520	P521	K522	R523	V524	E525	E526	L527	Q528		V532	N533	C534		H538		F541	ASN	ASN	GLY	GLY	LEU	ASN	R548	P549	N550	Y551	L552	S553	K554	L555	
SER	MET	SER	GLY	ASP	D399	Q401	H402		F406		L409	L410	T411	G412	S413	M414	E415	I416	I417	R418		G426		D436		F439	E440		F443	L444	E445	L446		L449		A452	Y453	R454	S455	N456	P457		K461	L462	I463	F464	C465	N466	G467	V468		V469	L470		L473	Q474	C475	V476	R477
SER	MET	VAL	LYS	GLU	VAL	VAL	ARG	THR	ASP	SER	SER	LEU	LYS	ARG	ARG	GLY	GLY	LEU	PRO	SER	LYS	PRO	LYS	SER	PRO	GLN	GLU	PRO	PRO	PRO	PRO	SER	PRO	PRO	VAL	S363	L364	I365		V369	R370		N376	F377	A378	R379	T380	S381	L382	D383	Y384	S385	R386	F387	Q388		P391	D392	TYR

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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	1450 reflections (9.85%)	wwPDB-VP
Wilson B-factor (Å ²)	85.7	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 96.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.47	3/1921 (0.2%)	0.82	0/2601
1	C	0.49	4/1839 (0.2%)	0.73	0/2488
2	A	0.55	4/1824 (0.2%)	0.82	1/2466 (0.0%)
All	All	0.50	11/5584 (0.2%)	0.79	1/7555 (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	C	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	566	CYS	N-CA	-11.55	1.31	1.46
1	C	566	CYS	N-CA	-11.53	1.31	1.46
1	B	566	CYS	N-CA	-11.50	1.31	1.46
2	A	567	THR	C-N	10.05	1.47	1.34
1	C	564	THR	C-N	9.67	1.48	1.33
1	C	566	CYS	CA-CB	-7.90	1.40	1.53
1	B	566	CYS	CA-CB	-7.88	1.40	1.53
2	A	566	CYS	CA-CB	-7.86	1.40	1.53
2	A	566	CYS	CA-C	-6.71	1.44	1.52
1	B	566	CYS	CA-C	-6.68	1.44	1.52
1	C	566	CYS	CA-C	-6.67	1.44	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	567	THR	O-C-N	-5.24	116.09	122.22

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

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	94	1
1	C	1802	3	1817	97	2
2	A	1797	3	1808	93	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	280	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 25.

All (280) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:446:LEU:HD11	1:B:511:MET:HE3	1.62	0.81
1:B:563:ARG:HH21	1:B:567:THR:HG21	1.44	0.81
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
2:A:439:PHE:HA	2:A:511:MET:HE2	1.66	0.77
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:B:439:PHE:HA	1:B:511:MET:HE2	1.72	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:LYS:HE2	1:B:558:LYS:HZ3	1.61	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
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:446:LEU:CD1	1:C:511:MET:HE3	2.33	0.58
1:C:407:TYR:CD2	1:C:585:PRO:HD3	2.38	0.58
1:C:446:LEU:HD11	1:C:511:MET:HE3	1.85	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
2:A:552:LEU:HD13	2:A:552:LEU:C	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:ARG:HG3	1:B:551:TYR:H	1.70	0.56
2:A:378:ALA:C	2:A:380:THR:H	2.13	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:B:575:TYR:CD1	1:B:575:TYR:C	2.84	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:C:439:PHE:HA	1:C:511:MET:HE2	1.89	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
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
2:A:399:ASP:HA	2:A:477:ARG:HH11	1.72	0.53
2:A:464:PHE:C	2:A:466:ASN:H	2.17	0.53
2:A:496:MET:HE1	2:A:554:LYS:HG3	1.90	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:551:TYR:CZ	1:B:555:LEU:HD11	2.45	0.52
1:C:387:PHE:CE1	1:C:471:HIS:HB2	2.45	0.52
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:464:PHE:C	1:B:466:ASN:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:LEU:HD13	1:C:591:LEU:C	2.36	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: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
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
1:B:496:MET:HE2	1:B:555:LEU:HD12	1.95	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
1:B:591:LEU:C	1:B:591:LEU:HD13	2.38	0.48
2:A:506:ILE:HG13	2:A:555:LEU:HG	1.95	0.48
2:A:426:GLY:C	2:A:527:LEU:HD11	2.39	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
2:A:444:LEU:HD23	2:A:444:LEU:HA	1.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:499:ASP:CG	2:A:538:HIS:HE2	2.20	0.46
1:B:590:LYS:CG	1:B:594:ASP:OD2	2.64	0.46
1:C:464:PHE:C	1:C:466:ASN:H	2.23	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:552:LEU:HD13	1:C:552:LEU:C	2.41	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:446:LEU:CD1	1:B:511:MET:HE3	2.40	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:B:496:MET:HE2	1:B:555:LEU:CD1	2.47	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
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
1:C:521:PRO:C	1:C:524:VAL:HG12	2.42	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:378:ALA:C	1:C:380:THR:H	2.25	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
2:A:575:TYR:CD1	2:A:575:TYR:C	2.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
2:A:503:PHE:CD1	2:A:503:PHE:C	2.97	0.42
1:C:452:ALA:HB1	1:C:490:SER:CA	2.48	0.42
1:B:442:ALA:O	1:B:443:PHE:C	2.62	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:439:PHE:HD1	1:C:511:MET:HE1	1.85	0.42
1:B:378:ALA:C	1:B:380:THR:H	2.28	0.41
1:C:430:LEU:CD2	1:C:523:ARG:HG2	2.50	0.41
2:A:388:GLN:HB3	2:A:474:GLN:NE2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:391:PRO:HG3	2:A:473:LEU:HD13	2.03	0.41
1:C:579:GLU:CD	1:C:581:LEU:HB2	2.45	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
2:A:378:ALA:C	2:A:380:THR:N	2.77	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
1:B:581:LEU:HD13	1:B:581:LEU:C	2.46	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:496:MET:HE1	2:A:554:LYS:CG	2.52	0.40
2:A:509:LEU:HD21	2:A:532:VAL:HG23	2.02	0.40
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
1:C:388:GLN:C	1:C:474:GLN:HE21	2.26	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 [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	B	234/272 (86%)	226 (97%)	7 (3%)	1 (0%)	30	62
1	C	219/272 (80%)	209 (95%)	10 (5%)	0	100	100
2	A	217/272 (80%)	209 (96%)	6 (3%)	2 (1%)	14	47
All	All	670/816 (82%)	644 (96%)	23 (3%)	3 (0%)	30	62

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%)	206 (99%)	3 (1%)	59	77
1	C	201/243 (83%)	197 (98%)	4 (2%)	48	72
2	A	199/242 (82%)	197 (99%)	2 (1%)	68	80
All	All	609/728 (84%)	600 (98%)	9 (2%)	57	76

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	552	LEU
1	B	556	LEU
1	B	566	CYS
2	A	555	LEU
2	A	566	CYS
1	C	368	LEU
1	C	556	LEU
1	C	566	CYS
1	C	596	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	376	ASN
1	B	474	GLN
1	B	568	GLN
2	A	388	GLN
2	A	402	HIS
2	A	404	GLN
1	C	376	ASN
1	C	402	HIS
1	C	404	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	C	605	1	12,12,12	1.36	1 (8%)	11,17,17	1.43	2 (18%)
4	G7J	A	608	2	12,12,12	1.35	1 (8%)	11,17,17	1.42	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	C	605	1	-	-	0/2/2/2
4	G7J	A	608	2	-	-	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	C	605	G7J	5	0
4	A	608	G7J	1	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 [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, 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	B	236/272 (86%)	-0.37	0 100 100	59, 101, 147, 174	0
1	C	225/272 (82%)	-0.08	1 (0%) 88 79	59, 142, 191, 236	0
2	A	223/272 (81%)	-0.37	0 100 100	59, 103, 171, 215	0
All	All	684/816 (83%)	-0.28	1 (0%) 92 89	59, 121, 176, 236	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	566	CYS	3.7

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	G7J	C	605	11/11	0.21	0.14	10,89,103,107	17
3	K	C	604	1/1	0.43	0.11	152,152,152,152	0
3	K	A	607	1/1	0.60	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
5	BR	C	601	1/1	0.91	0.06	135,135,135,135	1
3	K	B	601	1/1	0.91	0.10	87,87,87,87	0
5	BR	A	604	1/1	0.93	0.05	91,91,91,91	1
5	BR	A	603	1/1	0.94	0.06	95,95,95,95	1
5	BR	A	602	1/1	0.95	0.05	78,78,78,78	1
5	BR	C	603	1/1	0.95	0.05	151,151,151,151	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.