



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 5, 2016 – 06:36 AM EDT

PDB ID : 5IZ0  
Title : RORgamma in complex with agonist BIO592 and Coactivator EBI96  
Authors : Marcotte, D.J.  
Deposited on : 2016-03-24  
Resolution : 2.63 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027674  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027674

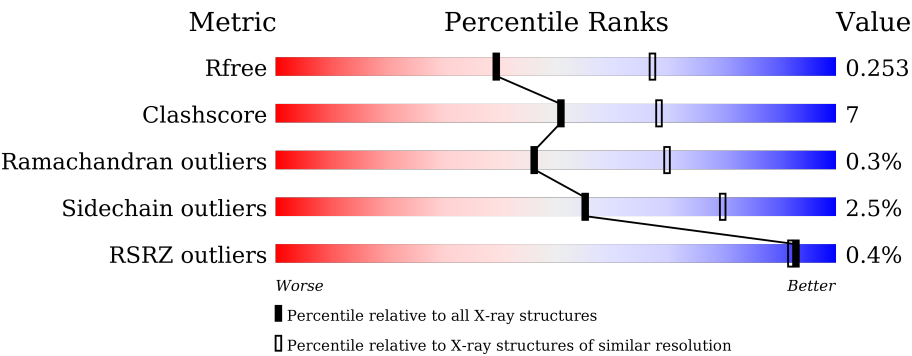
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.63 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))
$R_{free}$	91344	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	263	<div><div></div><div>81%11%• 7%</div></div>
1	B	263	<div><div></div><div>82%10%• 7%</div></div>
1	D	263	<div><div></div><div>82%8%• 8%</div></div>
1	G	263	<div><div>%</div><div>81%11%• 6%</div></div>
2	C	15	<div><div></div><div>60%7%33%</div></div>
2	E	15	<div><div></div><div>53%13%33%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	15	
2	H	15	

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	CL	A	604	-	-	-	X
4	CL	A	605	-	-	-	X
4	CL	A	606	-	-	X	X
4	CL	A	608	-	-	-	X
4	CL	A	609	-	-	-	X
4	CL	B	604	-	-	-	X
4	CL	B	605	-	-	X	X
4	CL	B	606	-	-	-	X
4	CL	B	607	-	-	-	X
4	CL	D	603	-	-	-	X
4	CL	D	604	-	-	X	-
4	CL	G	602	-	-	-	X
4	CL	G	603	-	-	X	X
4	CL	G	605	-	-	X	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8532 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Nuclear receptor ROR-gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1981	1263	352	352	14			
1	B	245	Total	C	N	O	S	0	0	0
			1997	1274	357	352	14			
1	D	243	Total	C	N	O	S	0	0	0
			1957	1246	348	349	14			
1	G	246	Total	C	N	O	S	0	0	0
			1997	1274	355	354	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	GLY	-	expression tag	UNP P51449
A	258	PRO	-	expression tag	UNP P51449
A	508	THR	-	insertion	UNP P51449
B	257	GLY	-	expression tag	UNP P51449
B	258	PRO	-	expression tag	UNP P51449
B	508	THR	-	insertion	UNP P51449
D	257	GLY	-	expression tag	UNP P51449
D	258	PRO	-	expression tag	UNP P51449
D	508	THR	-	insertion	UNP P51449
G	257	GLY	-	expression tag	UNP P51449
G	258	PRO	-	expression tag	UNP P51449
G	508	THR	-	insertion	UNP P51449

- Molecule 2 is a protein called GLU-PHE-PRO-TYR-LEU-LEU-SER-LEU-LEU-GLY-GLU-VAL-SER-PRO-GLN.

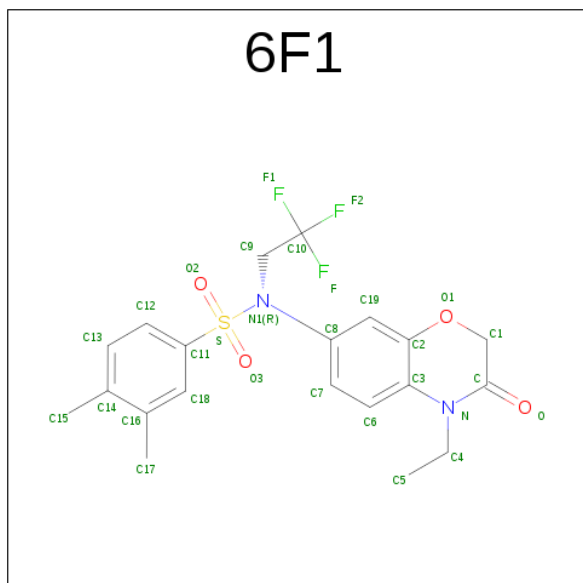
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			77	55	10	12			
2	E	10	Total	C	N	O	0	0	0
			81	57	10	14			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	10	Total	C	N	O	0	0	0
			77	55	10	12			
2	H	9	Total	C	N	O	0	0	0
			72	52	9	11			

- Molecule 3 is N-(4-ethyl-3-oxo-3,4-dihydro-2H-1,4-benzoxazin-7-yl)-3,4-dimethyl-N-(2,2,2-trifluoroethyl)benzene-1-sulfonamide (three-letter code: 6F1) (formula: C<sub>20</sub>H<sub>21</sub>F<sub>3</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			30	20	3	2	4	1		
3	B	1	Total	C	F	N	O	S	0	0
			30	20	3	2	4	1		
3	D	1	Total	C	F	N	O	S	0	0
			30	20	3	2	4	1		
3	G	1	Total	C	F	N	O	S	0	0
			30	20	3	2	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	5	Total 5 Cl 5	0	0
4	B	6	Total 6 Cl 6	0	0
4	A	8	Total 8 Cl 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	4	Total Cl 4 4	0	0

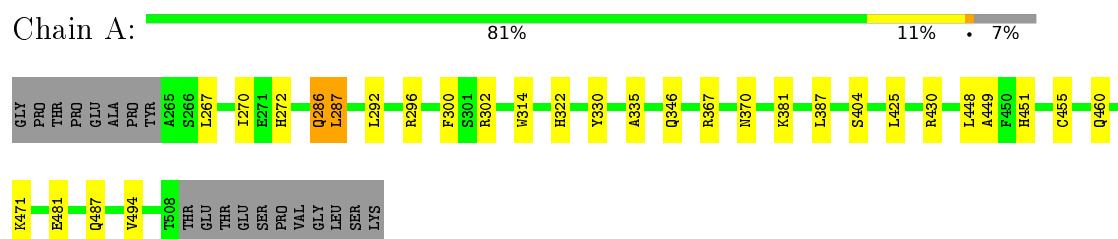
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	39	Total O 39 39	0	0
5	C	1	Total O 1 1	0	0
5	B	41	Total O 41 41	0	0
5	E	2	Total O 2 2	0	0
5	D	39	Total O 39 39	0	0
5	G	27	Total O 27 27	0	0
5	H	1	Total O 1 1	0	0

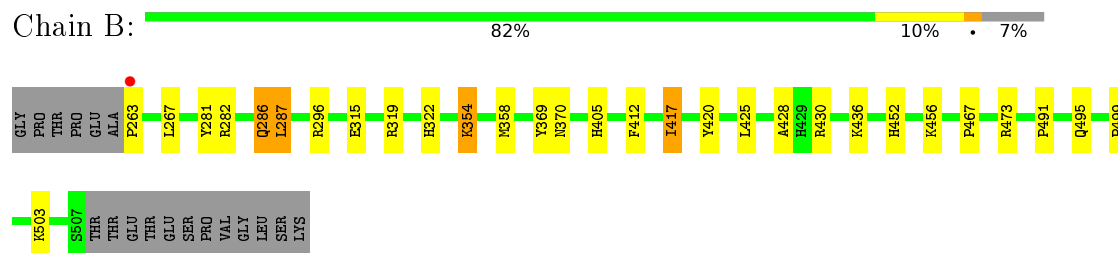
### 3 Residue-property plots [i](#)

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.

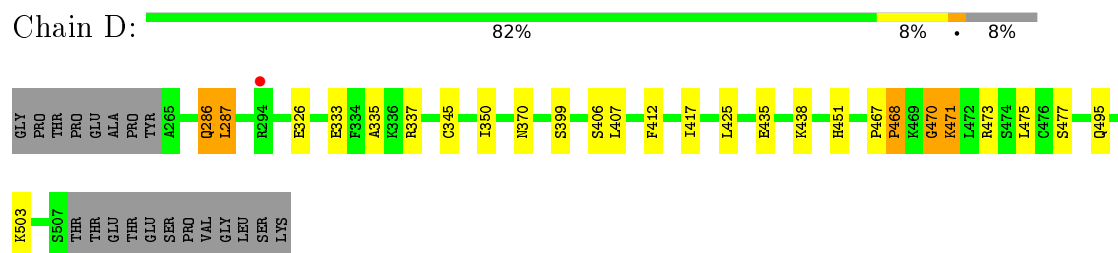
- Molecule 1: Nuclear receptor ROR-gamma



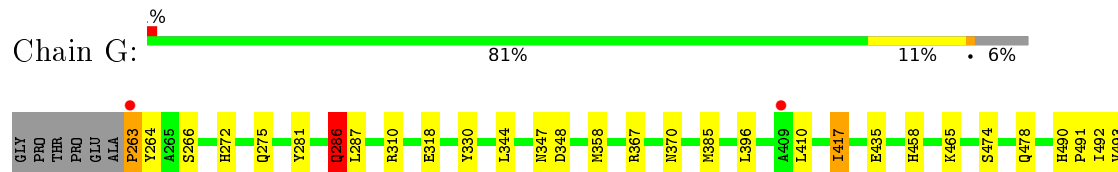
- Molecule 1: Nuclear receptor ROR-gamma

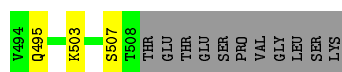


- Molecule 1: Nuclear receptor ROR-gamma

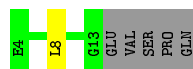


- Molecule 1: Nuclear receptor ROR-gamma

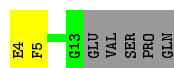




- Molecule 2: GLU-PHE-PRO-TYR-LEU-LEU-SER-LEU-LEU-GLY-GLU-VAL-SER-PRO-GLN



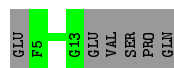
- Molecule 2: GLU-PHE-PRO-TYR-LEU-LEU-SER-LEU-LEU-GLY-GLU-VAL-SER-PRO-GLN



- Molecule 2: GLU-PHE-PRO-TYR-LEU-LEU-SER-LEU-LEU-GLY-GLU-VAL-SER-PRO-GLN



- Molecule 2: GLU-PHE-PRO-TYR-LEU-LEU-SER-LEU-LEU-GLY-GLU-VAL-SER-PRO-GLN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.67Å 68.11Å 96.06Å 90.00° 109.90° 90.00°	Depositor
Resolution (Å)	80.56 – 2.63 80.56 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.6 (80.56-2.63) 99.6 (80.56-2.63)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 2.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.199 , 0.255 0.206 , 0.253	Depositor DCC
$R_{free}$ test set	1557 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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 52.99 % 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 4.4969e-05. 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 6F1, CL

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	0.66	0/2024	0.85	4/2729 (0.1%)
1	B	0.73	0/2041	0.96	6/2749 (0.2%)
1	D	0.66	0/1999	0.90	5/2698 (0.2%)
1	G	0.69	0/2041	0.90	6/2751 (0.2%)
2	C	0.50	0/79	0.58	0/107
2	E	0.75	0/83	0.85	0/112
2	F	1.46	0/79	0.96	0/107
2	H	0.83	0/74	0.69	0/100
All	All	0.70	0/8420	0.90	21/11353 (0.2%)

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	D	0	1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	GLN	CB-CA-C	-12.00	86.40	110.40
1	G	286	GLN	CB-CA-C	-10.39	89.62	110.40
1	D	286	GLN	CB-CA-C	-10.16	90.09	110.40
1	B	263	PRO	CA-N-CD	-9.82	97.75	111.50
1	G	263	PRO	CA-N-CD	-9.63	98.02	111.50
1	A	286	GLN	CB-CA-C	-9.24	91.91	110.40
1	D	471	LYS	N-CA-C	8.42	133.72	111.00
1	G	385	MET	CB-CA-C	-7.23	95.94	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	LEU	N-CA-CB	6.95	124.29	110.40
1	G	287	LEU	N-CA-CB	6.68	123.75	110.40
1	B	473	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	G	286	GLN	N-CA-C	6.11	127.51	111.00
1	D	471	LYS	CB-CA-C	-6.04	98.31	110.40
1	D	287	LEU	N-CA-CB	5.90	122.20	110.40
1	A	451	HIS	CB-CA-C	-5.84	98.72	110.40
1	G	367	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	287	LEU	N-CA-CB	5.63	121.66	110.40
1	A	367	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	319	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	282	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	D	286	GLN	N-CA-C	5.03	124.57	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	470	GLY	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1981	0	1970	28	0
1	B	1997	0	2000	22	0
1	D	1957	0	1933	25	0
1	G	1997	0	1991	25	0
2	C	77	0	78	0	0
2	E	81	0	82	3	0
2	F	77	0	78	3	0
2	H	72	0	76	0	0
3	A	30	0	0	3	0
3	B	30	0	0	4	0
3	D	30	0	0	3	0
3	G	30	0	0	4	0
4	A	8	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	0	2	0
4	D	4	0	0	2	0
4	G	5	0	0	5	0
5	A	39	0	0	0	0
5	B	41	0	0	0	0
5	C	1	0	0	0	0
5	D	39	0	0	0	0
5	E	2	0	0	0	0
5	G	27	0	0	1	0
5	H	1	0	0	0	0
All	All	8532	0	8208	114	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (114) 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)
3:B:601:6F1:S	3:B:601:6F1:N1	1.99	1.33
3:G:601:6F1:S	3:G:601:6F1:N1	2.00	1.33
3:A:601:6F1:S	3:A:601:6F1:N1	2.03	1.30
1:A:270:ILE:HD11	1:A:448:LEU:C	1.53	1.29
3:D:601:6F1:S	3:D:601:6F1:N1	2.08	1.26
1:B:286:GLN:CG	1:B:286:GLN:O	1.92	1.11
1:A:270:ILE:CD1	1:A:448:LEU:HB3	1.82	1.09
1:G:286:GLN:HG2	1:G:286:GLN:O	1.45	1.09
1:D:286:GLN:HG2	1:D:286:GLN:O	1.44	1.08
1:G:263:PRO:HD2	1:G:264:TYR:H	1.13	1.08
1:A:270:ILE:HD12	1:A:448:LEU:CB	1.87	1.03
1:A:270:ILE:CD1	1:A:448:LEU:CB	2.36	1.03
1:D:467:PRO:O	1:D:468:PRO:O	1.74	1.02
1:A:286:GLN:HG2	1:A:286:GLN:O	1.63	0.98
1:B:286:GLN:HG2	1:B:286:GLN:O	1.15	0.95
1:A:270:ILE:HD11	1:A:449:ALA:N	1.83	0.92
1:A:270:ILE:HD12	1:A:448:LEU:HB2	1.52	0.90
1:G:490:HIS:O	1:G:493:VAL:HG12	1.72	0.90
1:A:270:ILE:HD12	1:A:448:LEU:HB3	1.52	0.88
1:G:263:PRO:HD2	1:G:264:TYR:N	1.84	0.88
1:G:491:PRO:O	1:G:495:GLN:OE1	1.92	0.86
1:D:286:GLN:O	1:D:286:GLN:CG	2.19	0.83
1:G:263:PRO:CD	1:G:264:TYR:H	1.91	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLN:CG	1:A:286:GLN:O	2.31	0.77
1:D:286:GLN:O	1:D:287:LEU:HG	1.84	0.77
3:B:601:6F1:C8	3:B:601:6F1:S	2.77	0.72
1:D:345:CYS:N	4:D:604:CL:CL	2.57	0.70
1:A:430:ARG:NE	4:A:608:CL:CL	2.60	0.69
1:B:452:HIS:NE2	1:B:456:LYS:HD2	2.08	0.69
3:A:601:6F1:C8	3:A:601:6F1:S	2.81	0.68
3:G:601:6F1:S	3:G:601:6F1:C8	2.81	0.68
1:D:399:SER:HB3	1:D:475:LEU:HD21	1.76	0.67
1:G:263:PRO:CD	1:G:264:TYR:N	2.52	0.67
1:A:270:ILE:HD11	1:A:448:LEU:CA	2.26	0.66
1:B:281:TYR:CE1	1:B:417:ILE:HD11	2.32	0.64
1:A:270:ILE:CD1	1:A:448:LEU:C	2.48	0.64
1:G:318:GLU:HB3	4:G:605:CL:CL	2.36	0.63
1:G:281:TYR:CE1	1:G:417:ILE:HD11	2.36	0.61
1:B:420:TYR:OH	1:B:467:PRO:HD2	2.02	0.59
1:D:470:GLY:CA	1:D:473:ARG:HB2	2.33	0.58
1:A:270:ILE:HD11	1:A:448:LEU:CB	2.24	0.58
1:D:470:GLY:HA2	1:D:473:ARG:H	1.68	0.58
1:D:337:ARG:HG3	1:D:337:ARG:HH11	1.70	0.57
1:A:270:ILE:CD1	1:A:448:LEU:HB2	2.22	0.56
1:G:490:HIS:HB3	1:G:493:VAL:CG1	2.37	0.55
3:D:601:6F1:S	3:D:601:6F1:C8	2.92	0.55
1:D:470:GLY:HA3	1:D:473:ARG:HB2	1.87	0.55
1:A:270:ILE:HD13	1:A:448:LEU:HB3	1.80	0.55
1:A:322:HIS:HB2	4:A:606:CL:CL	2.45	0.54
1:B:354:LYS:HE2	2:E:5:PHE:CE2	2.42	0.54
1:D:435:GLU:OE1	1:D:438:LYS:NZ	2.25	0.54
1:D:495:GLN:HA	1:D:503:LYS:CE	2.38	0.54
1:B:452:HIS:CE1	1:B:456:LYS:HD2	2.43	0.53
1:G:286:GLN:CG	1:G:286:GLN:O	2.26	0.53
1:A:455:CYS:HB2	1:A:460:GLN:NE2	2.23	0.53
1:G:396:LEU:HD13	1:G:478:GLN:HB3	1.90	0.53
1:A:387:LEU:O	4:A:609:CL:CL	2.64	0.53
1:A:270:ILE:HD11	1:A:448:LEU:O	2.04	0.53
1:A:455:CYS:HB2	1:A:460:GLN:HE21	1.74	0.52
1:B:286:GLN:O	1:B:287:LEU:HG	2.10	0.52
1:A:287:LEU:HD13	1:A:292:LEU:HD21	1.92	0.52
3:B:601:6F1:S	3:B:601:6F1:C9	2.94	0.52
3:G:601:6F1:S	3:G:601:6F1:C9	2.93	0.51
1:A:335:ALA:HB2	1:A:425:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:435:GLU:HB2	4:G:603:CL:CL	2.47	0.51
1:G:347:ASN:ND2	1:G:348:ASP:OD1	2.44	0.51
3:D:601:6F1:N1	3:D:601:6F1:C11	2.73	0.50
1:D:470:GLY:HA2	1:D:473:ARG:N	2.26	0.50
1:B:491:PRO:O	1:B:495:GLN:OE1	2.29	0.50
1:B:495:GLN:HG3	1:B:503:LYS:NZ	2.27	0.50
1:B:354:LYS:CE	2:E:5:PHE:CZ	2.95	0.50
1:D:407:LEU:HD11	1:D:467:PRO:HG2	1.93	0.49
1:D:435:GLU:HB2	4:D:604:CL:CL	2.50	0.49
1:D:412:PHE:HB3	1:D:417:ILE:HG13	1.95	0.49
1:G:344:LEU:HB3	4:G:603:CL:CL	2.49	0.49
1:G:490:HIS:HB3	1:G:493:VAL:HG12	1.95	0.48
1:G:272:HIS:O	1:G:275:GLN:HG2	2.14	0.48
1:A:300:PHE:CZ	1:A:381:LYS:HB2	2.48	0.48
4:A:606:CL:CL	1:B:499:PRO:HG3	2.51	0.48
1:D:467:PRO:C	1:D:468:PRO:O	2.43	0.48
1:D:495:GLN:HA	1:D:503:LYS:HE3	1.96	0.48
3:G:601:6F1:C11	3:G:601:6F1:N1	2.74	0.48
2:F:11:LEU:HD23	1:G:492:ILE:CD1	2.43	0.47
1:A:404:SER:HA	4:A:605:CL:CL	2.53	0.46
3:A:601:6F1:N1	3:A:601:6F1:C11	2.79	0.45
1:B:425:LEU:O	4:B:605:CL:CL	2.72	0.45
3:B:601:6F1:C11	3:B:601:6F1:N1	2.79	0.44
1:G:458:HIS:CG	1:G:458:HIS:O	2.70	0.44
1:G:310:ARG:NH1	5:G:702:HOH:O	2.50	0.44
1:D:407:LEU:CD1	1:D:467:PRO:HG2	2.47	0.44
1:B:354:LYS:HE3	2:E:5:PHE:CZ	2.53	0.44
1:D:333:GLU:OE1	1:D:337:ARG:NH1	2.51	0.43
1:B:296:ARG:HD3	1:B:370:ASN:ND2	2.34	0.43
1:A:330:TYR:OH	1:B:315:GLU:OE1	2.35	0.43
1:B:369:TYR:OH	1:B:405:HIS:HD2	2.01	0.43
1:B:267:LEU:HD11	1:B:452:HIS:CE1	2.54	0.43
1:D:470:GLY:HA2	1:D:473:ARG:HB2	2.01	0.43
1:D:350:ILE:HD11	2:F:9:LEU:HD13	2.00	0.42
1:B:428:ALA:O	1:B:436:LYS:HE3	2.20	0.42
1:D:337:ARG:CG	1:D:337:ARG:HH11	2.28	0.42
1:G:410:LEU:HD11	1:G:465:LYS:HB3	2.01	0.42
1:G:458:HIS:HA	4:G:604:CL:CL	2.57	0.42
2:F:7:TYR:O	2:F:10:SER:OG	2.32	0.41
1:D:335:ALA:HB2	1:D:425:LEU:HD21	2.02	0.41
1:A:267:LEU:HA	1:A:270:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:GLN:HG3	1:A:494:VAL:HG21	2.02	0.41
1:D:326:GLU:OE2	4:G:605:CL:CL	2.76	0.41
1:G:490:HIS:HB3	1:G:493:VAL:HG11	2.02	0.41
1:B:495:GLN:N	1:B:495:GLN:OE1	2.46	0.41
1:G:503:LYS:O	1:G:507:SER:HB2	2.21	0.41
1:A:296:ARG:NE	4:A:604:CL:CL	2.88	0.40
1:G:286:GLN:HG3	1:G:330:TYR:CE1	2.56	0.40
1:B:412:PHE:HB3	1:B:417:ILE:HG22	2.02	0.40
1:B:430:ARG:NE	4:B:605:CL:CL	2.75	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	242/263 (92%)	238 (98%)	4 (2%)	0	100	100
1	B	243/263 (92%)	238 (98%)	5 (2%)	0	100	100
1	D	241/263 (92%)	232 (96%)	7 (3%)	2 (1%)	24	44
1	G	244/263 (93%)	239 (98%)	4 (2%)	1 (0%)	39	63
2	C	8/15 (53%)	8 (100%)	0	0	100	100
2	E	8/15 (53%)	8 (100%)	0	0	100	100
2	F	8/15 (53%)	8 (100%)	0	0	100	100
2	H	7/15 (47%)	7 (100%)	0	0	100	100
All	All	1001/1112 (90%)	978 (98%)	20 (2%)	3 (0%)	46	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	468	PRO

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Mol	Chain	Res	Type
1	G	286	GLN
1	D	471	LYS

### 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	215/234 (92%)	208 (97%)	7 (3%)	45	72
1	B	218/234 (93%)	214 (98%)	4 (2%)	66	86
1	D	211/234 (90%)	207 (98%)	4 (2%)	65	85
1	G	217/234 (93%)	212 (98%)	5 (2%)	58	81
2	C	8/14 (57%)	7 (88%)	1 (12%)	6	10
2	E	9/14 (64%)	8 (89%)	1 (11%)	8	13
2	F	8/14 (57%)	8 (100%)	0	100	100
2	H	8/14 (57%)	8 (100%)	0	100	100
All	All	894/992 (90%)	872 (98%)	22 (2%)	55	80

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	HIS
1	A	302	ARG
1	A	314	TRP
1	A	346	GLN
1	A	370	ASN
1	A	471	LYS
1	A	481	GLU
2	C	8	LEU
1	B	322	HIS
1	B	354	LYS
1	B	358	MET
1	B	417	ILE
2	E	4	GLU

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Mol	Chain	Res	Type
1	D	370	ASN
1	D	406	SER
1	D	451	HIS
1	D	477	SER
1	G	266	SER
1	G	358	MET
1	G	370	ASN
1	G	417	ILE
1	G	474	SER

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

Mol	Chain	Res	Type
1	A	370	ASN
1	A	487	GLN
1	B	405	HIS
1	B	484	GLN
1	D	322	HIS
1	D	370	ASN
1	D	405	HIS
1	D	460	GLN
1	D	478	GLN
1	D	487	GLN
1	D	488	HIS
1	G	298	ASN
1	G	370	ASN
1	G	460	GLN
1	G	484	GLN
1	G	495	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 23 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	6F1	A	601	-	32,32,32	5.88	10 (31%)	46,49,49	2.86	15 (32%)
3	6F1	B	601	-	32,32,32	5.62	12 (37%)	46,49,49	2.61	15 (32%)
3	6F1	D	601	-	32,32,32	6.34	8 (25%)	46,49,49	3.53	20 (43%)
3	6F1	G	601	-	32,32,32	5.65	11 (34%)	46,49,49	2.48	13 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6F1	A	601	-	-	0/22/36/36	0/3/3/3
3	6F1	B	601	-	-	0/22/36/36	0/3/3/3
3	6F1	D	601	-	-	0/22/36/36	0/3/3/3
3	6F1	G	601	-	-	0/22/36/36	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	6F1	C1-C	-9.35	1.39	1.51
3	A	601	6F1	C1-C	-9.34	1.39	1.51
3	B	601	6F1	C8-N1	-9.10	1.33	1.44
3	B	601	6F1	C1-C	-8.92	1.39	1.51
3	G	601	6F1	C1-C	-8.74	1.39	1.51
3	G	601	6F1	C8-N1	-8.68	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	6F1	C8-N1	-7.70	1.34	1.44
3	D	601	6F1	C8-N1	-6.17	1.36	1.44
3	D	601	6F1	C15-C14	-5.68	1.39	1.51
3	B	601	6F1	C15-C14	-5.63	1.39	1.51
3	A	601	6F1	C17-C16	-5.56	1.40	1.51
3	A	601	6F1	C15-C14	-5.45	1.40	1.51
3	G	601	6F1	C15-C14	-5.35	1.40	1.51
3	G	601	6F1	C17-C16	-5.11	1.40	1.51
3	D	601	6F1	C17-C16	-5.10	1.40	1.51
3	B	601	6F1	C17-C16	-5.01	1.41	1.51
3	D	601	6F1	F1-C10	-3.95	1.16	1.33
3	G	601	6F1	C11-S	-3.77	1.71	1.76
3	A	601	6F1	F-C10	-3.56	1.18	1.33
3	A	601	6F1	C3-N	-3.12	1.35	1.41
3	B	601	6F1	C9-N1	-2.92	1.42	1.47
3	A	601	6F1	C9-N1	-2.90	1.42	1.47
3	B	601	6F1	C11-S	-2.84	1.72	1.76
3	G	601	6F1	C9-N1	-2.78	1.42	1.47
3	B	601	6F1	O1-C2	-2.57	1.34	1.37
3	G	601	6F1	C3-N	-2.27	1.36	1.41
3	G	601	6F1	F-C10	-2.24	1.23	1.33
3	B	601	6F1	C3-N	-2.00	1.37	1.41
3	B	601	6F1	F2-C10	2.48	1.43	1.33
3	A	601	6F1	O3-S	7.47	1.52	1.43
3	D	601	6F1	O3-S	7.59	1.53	1.43
3	B	601	6F1	O2-S	7.65	1.53	1.43
3	A	601	6F1	O2-S	7.88	1.53	1.43
3	G	601	6F1	O3-S	8.33	1.54	1.43
3	D	601	6F1	O2-S	8.38	1.54	1.43
3	G	601	6F1	O2-S	8.77	1.54	1.43
3	B	601	6F1	O3-S	9.01	1.54	1.43
3	B	601	6F1	S-N1	24.69	1.99	1.65
3	G	601	6F1	S-N1	25.05	2.00	1.65
3	A	601	6F1	S-N1	27.08	2.03	1.65
3	D	601	6F1	S-N1	30.58	2.08	1.65

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	6F1	C9-N1-C8	-11.29	105.66	117.46
3	D	601	6F1	C11-S-N1	-10.00	91.10	106.75
3	B	601	6F1	C9-N1-C8	-9.27	107.77	117.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	6F1	C9-N1-C8	-9.04	108.02	117.46
3	G	601	6F1	C9-N1-C8	-8.91	108.14	117.46
3	A	601	6F1	C11-S-N1	-8.03	94.18	106.75
3	G	601	6F1	C11-S-N1	-7.56	94.92	106.75
3	B	601	6F1	C11-S-N1	-6.24	96.99	106.75
3	B	601	6F1	O3-S-O2	-5.10	110.73	119.47
3	D	601	6F1	O3-S-O2	-4.94	111.00	119.47
3	A	601	6F1	F-C10-C9	-4.04	105.24	112.08
3	D	601	6F1	C18-C11-S	-4.00	114.55	119.39
3	D	601	6F1	O1-C1-C	-3.48	106.26	115.95
3	A	601	6F1	C3-N-C	-3.44	113.66	121.12
3	A	601	6F1	C8-N1-S	-3.44	111.17	118.19
3	B	601	6F1	O1-C1-C	-3.33	106.69	115.95
3	A	601	6F1	O3-S-O2	-3.31	113.80	119.47
3	G	601	6F1	O3-S-O2	-3.31	113.80	119.47
3	B	601	6F1	F2-C10-C9	-3.27	106.53	112.08
3	A	601	6F1	C1-O1-C2	-3.26	106.21	115.87
3	B	601	6F1	C8-N1-S	-3.24	111.56	118.19
3	D	601	6F1	F2-C10-C9	-3.23	106.61	112.08
3	G	601	6F1	O1-C1-C	-2.88	107.94	115.95
3	D	601	6F1	C17-C16-C18	-2.66	114.55	119.49
3	B	601	6F1	F-C10-C9	-2.62	107.64	112.08
3	A	601	6F1	F1-C10-C9	-2.58	107.71	112.08
3	G	601	6F1	F2-C10-C9	-2.57	107.72	112.08
3	D	601	6F1	F1-C10-C9	-2.44	107.95	112.08
3	G	601	6F1	C8-N1-S	-2.43	113.22	118.19
3	A	601	6F1	O1-C1-C	-2.40	109.27	115.95
3	D	601	6F1	C3-N-C	-2.35	116.02	121.12
3	D	601	6F1	F-C10-C9	-2.32	108.15	112.08
3	G	601	6F1	F1-C10-C9	-2.24	108.28	112.08
3	G	601	6F1	O1-C2-C3	-2.13	117.04	121.78
3	A	601	6F1	O-C-N	-2.10	119.52	122.52
3	B	601	6F1	C18-C11-S	-2.05	116.92	119.39
3	B	601	6F1	O-C-N	-2.02	119.63	122.52
3	A	601	6F1	O1-C2-C19	2.16	119.83	116.69
3	B	601	6F1	C4-N-C3	2.19	122.54	120.18
3	G	601	6F1	C17-C16-C14	2.28	125.63	120.73
3	D	601	6F1	F-C10-F2	2.48	115.83	106.46
3	B	601	6F1	C6-C3-N	2.50	124.76	121.41
3	D	601	6F1	C17-C16-C14	2.51	126.12	120.73
3	B	601	6F1	C12-C11-S	2.68	122.60	119.79
3	G	601	6F1	O1-C2-C19	2.74	120.66	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	6F1	O2-S-C11	2.94	111.73	108.01
3	A	601	6F1	O3-S-N1	2.96	110.71	106.86
3	D	601	6F1	C6-C3-N	3.04	125.48	121.41
3	D	601	6F1	C7-C8-N1	3.14	125.12	120.35
3	G	601	6F1	O3-S-C11	3.20	112.06	108.01
3	G	601	6F1	O3-S-N1	3.37	111.25	106.86
3	A	601	6F1	C9-N1-S	3.58	124.60	117.62
3	B	601	6F1	O3-S-N1	3.68	111.65	106.86
3	D	601	6F1	O2-S-C11	4.07	113.16	108.01
3	D	601	6F1	C4-N-C3	4.24	124.75	120.18
3	D	601	6F1	O3-S-N1	4.39	112.58	106.86
3	D	601	6F1	C12-C11-S	5.18	125.23	119.79
3	A	601	6F1	C4-N-C3	6.01	126.66	120.18
3	B	601	6F1	O2-S-N1	6.02	114.69	106.86
3	D	601	6F1	C9-N1-S	6.11	129.53	117.62
3	G	601	6F1	O2-S-N1	6.12	114.83	106.86
3	A	601	6F1	O2-S-N1	7.68	116.87	106.86
3	D	601	6F1	O2-S-N1	8.78	118.30	106.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	6F1	3	0
3	B	601	6F1	4	0
3	D	601	6F1	3	0
3	G	601	6F1	4	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, 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	244/263 (92%)	-0.30	0 100 100	18, 33, 49, 63	5 (2%)
1	B	245/263 (93%)	-0.34	1 (0%) 93 92	17, 27, 44, 58	7 (2%)
1	D	243/263 (92%)	-0.26	1 (0%) 93 92	18, 33, 57, 70	5 (2%)
1	G	246/263 (93%)	-0.17	2 (0%) 87 85	20, 35, 57, 72	7 (2%)
2	C	10/15 (66%)	-0.48	0 100 100	33, 35, 44, 48	0
2	E	10/15 (66%)	-0.21	0 100 100	25, 31, 46, 65	0
2	F	10/15 (66%)	-0.45	0 100 100	27, 32, 43, 58	0
2	H	9/15 (60%)	-0.30	0 100 100	24, 27, 45, 58	0
All	All	1017/1112 (91%)	-0.27	4 (0%) 93 92	17, 32, 53, 72	24 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	PRO	3.3
1	G	263	PRO	3.0
1	G	409	ALA	2.1
1	D	294	ARG	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CL	A	605	1/1	0.94	0.48	26.77	97,97,97,97	0
4	CL	A	608	1/1	0.95	0.44	16.26	60,60,60,60	0
4	CL	B	605	1/1	0.97	0.36	15.23	57,57,57,57	0
4	CL	B	607	1/1	0.98	0.52	9.79	69,69,69,69	0
4	CL	A	609	1/1	0.97	0.38	9.44	54,54,54,54	0
4	CL	B	604	1/1	0.99	0.39	8.00	54,54,54,54	0
4	CL	G	602	1/1	0.96	0.38	6.97	66,66,66,66	0
4	CL	G	603	1/1	0.97	0.35	6.17	65,65,65,65	0
4	CL	G	605	1/1	0.88	0.34	5.05	63,63,63,63	0
4	CL	A	604	1/1	0.82	0.32	3.93	83,83,83,83	0
4	CL	D	603	1/1	0.94	0.23	3.77	64,64,64,64	0
4	CL	B	606	1/1	0.91	0.31	3.54	60,60,60,60	0
4	CL	A	606	1/1	0.85	0.23	3.23	73,73,73,73	0
3	6F1	A	601	30/30	0.95	0.19	1.52	22,30,35,38	0
4	CL	D	604	1/1	0.95	0.21	0.81	71,71,71,71	0
3	6F1	G	601	30/30	0.93	0.18	0.71	37,41,45,45	0
3	6F1	B	601	30/30	0.96	0.17	0.25	32,36,40,41	0
3	6F1	D	601	30/30	0.95	0.16	0.13	23,30,33,35	0
4	CL	D	602	1/1	0.81	0.15	-0.05	54,54,54,54	0
4	CL	D	605	1/1	0.83	0.14	-0.48	62,62,62,62	0
4	CL	B	602	1/1	0.94	0.14	-0.53	31,31,31,31	0
4	CL	G	604	1/1	0.95	0.14	-1.01	58,58,58,58	0
4	CL	A	603	1/1	0.94	0.09	-2.00	44,44,44,44	0
4	CL	B	603	1/1	0.91	0.13	-	48,48,48,48	0
4	CL	A	607	1/1	0.83	0.13	-	57,57,57,57	0
4	CL	G	606	1/1	0.97	0.10	-	37,37,37,37	0
4	CL	A	602	1/1	0.91	0.36	-	67,67,67,67	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.