



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:00 PM UTC

PDB ID : 3DZU / pdb_00003dzu
Title : Intact PPAR gamma - RXR alpha Nuclear Receptor Complex on DNA bound with BVT.13, 9-cis Retinoic Acid and NCOA2 Peptide
Authors : Chandra, V.; Huang, P.; Hamuro, Y.; Raghuram, S.; Wang, Y.; Burris, T.P.; Rastinejad, F.
Deposited on : 2008-07-30
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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

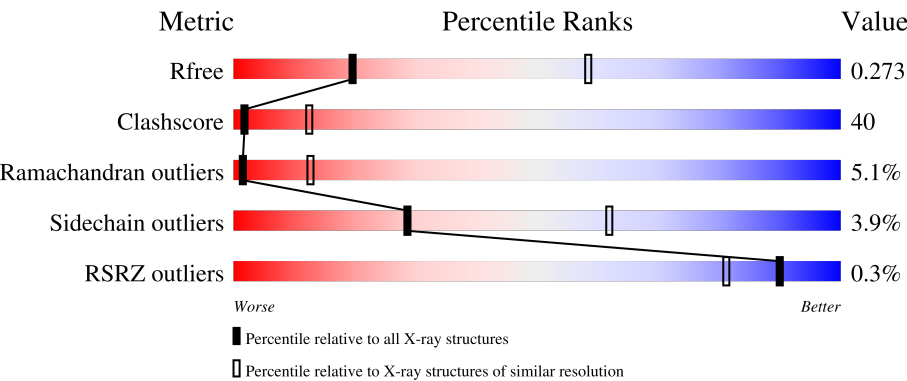
1 Overall quality at a glance i

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	A	467	25%33%•38%
2	D	419	33%44%8%•14%
3	C	20	15%70%5%10%
4	F	20	10%85%5%

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Mol	Chain	Length	Quality of chain
5	E	13	54% 8% 38%
5	G	13	8% 38% 23% 8% 31%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6204 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 Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2308	1457	417	413	21			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	expression tag	UNP P19793
A	-3	ALA	-	expression tag	UNP P19793
A	-2	HIS	-	expression tag	UNP P19793
A	-1	HIS	-	expression tag	UNP P19793
A	0	HIS	-	expression tag	UNP P19793
A	1	HIS	-	expression tag	UNP P19793
A	2	HIS	-	expression tag	UNP P19793
A	3	HIS	-	expression tag	UNP P19793
A	4	VAL	-	expression tag	UNP P19793
A	5	ASP	-	expression tag	UNP P19793
A	6	ASP	-	expression tag	UNP P19793
A	7	ASP	-	expression tag	UNP P19793
A	8	ASP	-	expression tag	UNP P19793
A	9	LYS	-	expression tag	UNP P19793
A	10	MET	-	expression tag	UNP P19793

- Molecule 2 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	359	Total	C	N	O	S	0	0	0
			2879	1840	492	526	21			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	59	MET	-	expression tag	UNP P37231

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Chain	Residue	Modelled	Actual	Comment	Reference
D	60	ALA	-	expression tag	UNP P37231
D	61	HIS	-	expression tag	UNP P37231
D	62	HIS	-	expression tag	UNP P37231
D	63	HIS	-	expression tag	UNP P37231
D	64	HIS	-	expression tag	UNP P37231
D	65	HIS	-	expression tag	UNP P37231
D	66	HIS	-	expression tag	UNP P37231
D	67	VAL	-	expression tag	UNP P37231
D	68	ASP	-	expression tag	UNP P37231
D	69	ASP	-	expression tag	UNP P37231
D	70	ASP	-	expression tag	UNP P37231
D	71	ASP	-	expression tag	UNP P37231
D	72	LYS	-	expression tag	UNP P37231
D	73	MET	-	expression tag	UNP P37231

- Molecule 3 is a DNA chain called DNA (5'-D(*DCP*DAP*DAP*DAP*DCP*DTP*DAP*DG*GDP*DTP*DCP*DAP*DAP*DAP*GDP*GDP*DTP*DCP*DAP*DG)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	20	Total	C	N	O	P	0	0	0
			411	196	83	113	19			

- Molecule 4 is a DNA chain called DNA (5'-D(*DCP*DTP*GDP*DAP*DCP*DCP*DTP*DT*DT*GDP*DAP*DCP*DCP*DT*DT*GDP*DT*DT*DT*DG)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	20	Total	C	N	O	P	0	0	0
			403	195	66	123	19			

- Molecule 5 is a protein called NCOA2 Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	9	Total	C	N	O	0	0	0
			79	51	16	12			
5	E	8	Total	C	N	O	0	0	0
			71	47	15	9			

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

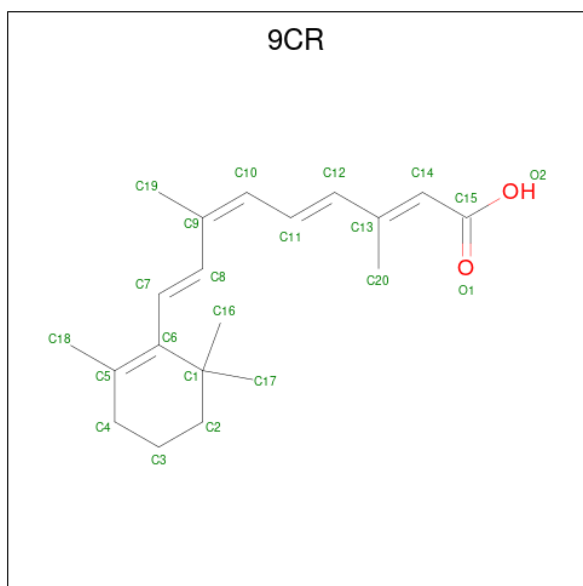
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Zn	0	0
			2	2		

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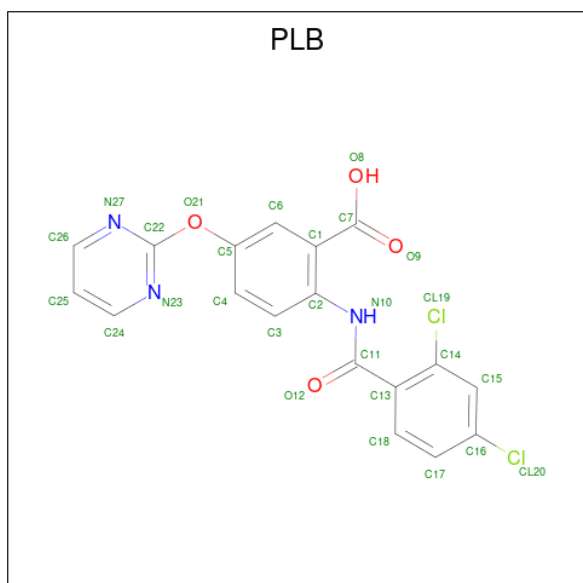
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total	Zn	0	0
			2	2		

- Molecule 7 is (9cis)-retinoic acid (CCD ID: 9CR) (formula: $C_{20}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			22	20	2		

- Molecule 8 is 2-[(2,4-DICHLOROBENZOYL)AMINO]-5-(PYRIMIDIN-2-YLOXY)BENZOIC ACID (CCD ID: PLB) (formula: $C_{18}H_{11}Cl_2N_3O_4$).

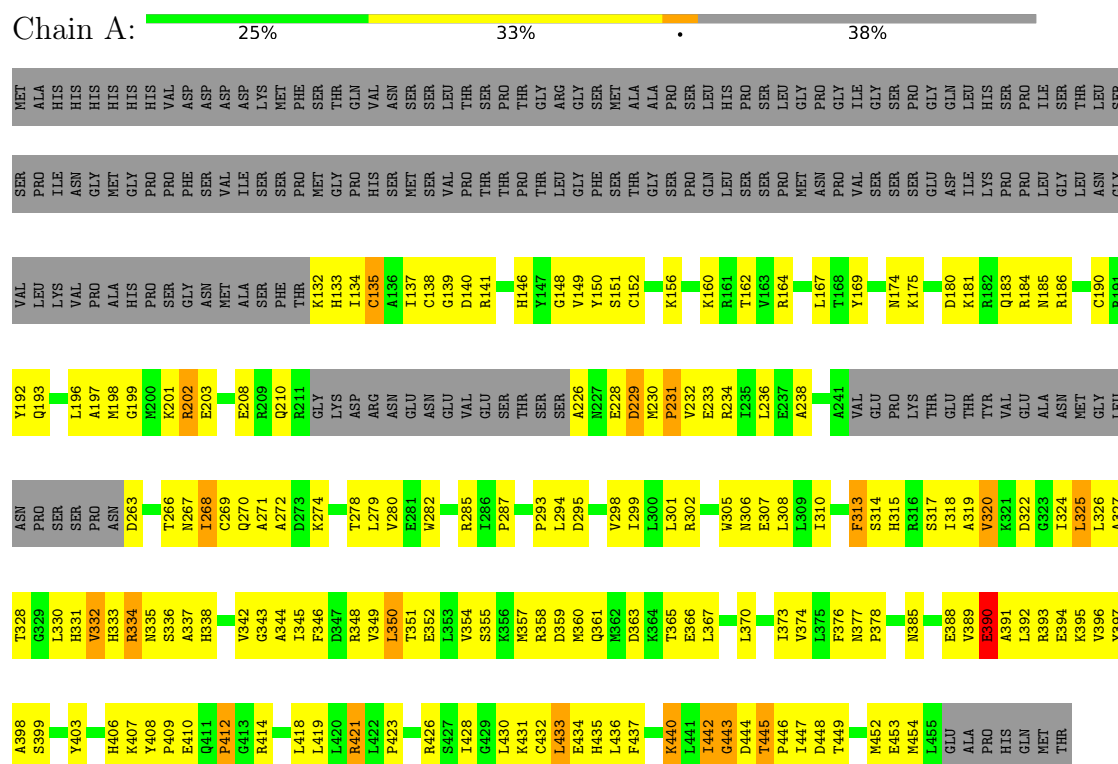


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	Cl	N	O	0	0
			27	18	2	3	4		

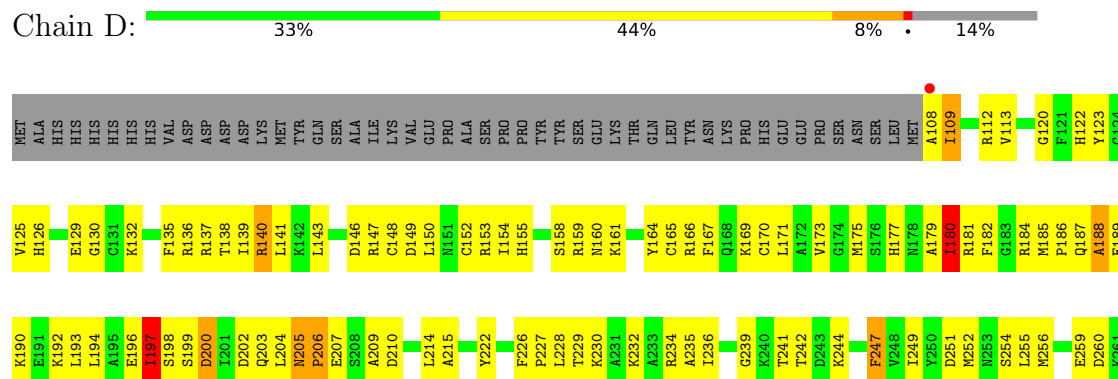
3 Residue-property plots

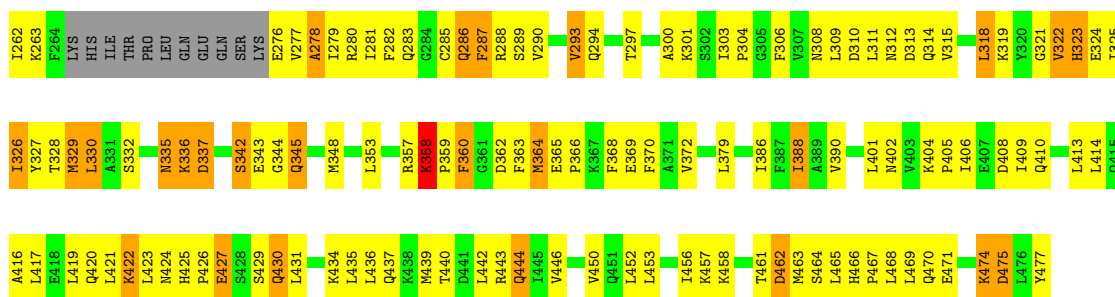
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Retinoic acid receptor RXR-alpha



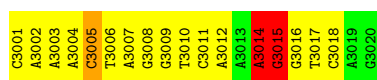
• Molecule 2: Peroxisome proliferator-activated receptor gamma





- Molecule 3: DNA (5'-D(*DCP*DAP*DAP*DAP*DCP*DTP*DAP*DGP*DGP*DTP*DCP*DAP*DAP*DAP*DGP*DGP*DTP*DCP*DAP*DG)-3')

Chain C: 15% 70% 5% 10%



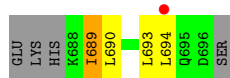
- Molecule 4: DNA (5'-D(*DCP*DTP*DGP*DAP*DCP*DCP*DTP*DTP*DTP*DGP*DAP*DCP*DCP*DTP*DAP*DGP*DTP*DTP*DTP*DG)-3')

Chain F: 10% 85% 5%



- Molecule 5: NCOA2 Peptide

Chain G: 8% 38% 23% 8% 31%



- Molecule 5: NCOA2 Peptide

Chain E: 54% 8% 38%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.19Å 66.91Å 78.46Å 70.95° 82.56° 62.88°	Depositor
Resolution (Å)	38.93 – 3.20 38.93 – 3.21	Depositor EDS
% Data completeness (in resolution range)	92.0 (38.93-3.20) 92.0 (38.93-3.21)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.55 (at 3.18Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.201 , 0.272 0.201 , 0.273	Depositor DCC
R_{free} test set	853 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6204	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 9CR, ZN, PLB

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	0.45	0/2348	1.01	13/3153 (0.4%)
2	D	0.47	0/2928	1.01	17/3931 (0.4%)
3	C	0.36	0/463	0.87	3/713 (0.4%)
4	F	0.36	0/449	0.88	1/691 (0.1%)
5	E	0.43	0/71	0.83	0/93
5	G	0.37	0/79	0.86	0/104
All	All	0.45	0/6338	0.99	34/8685 (0.4%)

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
3	C	0	3

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	252	MET	N-CA-C	-13.43	96.57	113.23
1	A	229	ASP	N-CA-C	-10.62	99.79	113.17
2	D	475	ASP	N-CA-C	8.99	121.43	110.91
2	D	332	SER	N-CA-C	-8.33	103.24	113.41
1	A	443	GLY	N-CA-C	-7.83	104.51	115.32
2	D	149	ASP	N-CA-C	-7.21	104.48	113.28
3	C	3014	DA	N9-C1'-C2'	-6.96	103.06	113.50
2	D	427	GLU	N-CA-C	6.69	119.18	111.02
1	A	433	LEU	N-CA-C	-6.43	104.69	112.54
2	D	337	ASP	N-CA-C	6.29	121.11	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	449	THR	N-CA-C	6.22	118.06	111.28
1	A	181	LYS	N-CA-C	-6.18	105.59	113.01
2	D	190	LYS	N-CA-C	-5.83	105.00	111.71
2	D	210	ASP	N-CA-C	-5.80	105.03	111.36
1	A	390	GLU	N-CA-C	-5.68	104.29	111.11
1	A	198	MET	N-CA-C	-5.65	106.42	113.15
1	A	319	ALA	N-CA-C	5.64	117.24	111.14
2	D	458	LYS	N-CA-C	5.62	117.26	111.03
2	D	293	VAL	N-CA-C	-5.51	103.95	111.89
1	A	377	ASN	CA-C-N	5.50	125.59	119.87
1	A	377	ASN	C-N-CA	5.50	125.59	119.87
2	D	458	LYS	CB-CA-C	-5.50	102.43	110.95
2	D	247	PHE	N-CA-C	-5.49	102.76	110.50
1	A	328	THR	N-CA-C	-5.20	106.24	112.59
2	D	364	MET	N-CA-C	5.20	118.88	112.54
2	D	345	GLN	N-CA-C	-5.17	106.82	113.23
2	D	215	ALA	N-CA-C	-5.17	105.34	110.97
4	F	4010	DG	N9-C1'-C2'	5.13	121.19	113.50
1	A	421	ARG	N-CA-C	-5.11	106.20	112.90
2	D	360	PHE	N-CA-C	5.06	118.23	111.75
3	C	3014	DA	C4'-C3'-O3'	5.06	117.59	110.00
3	C	3015	DG	C4'-C3'-O3'	5.04	117.56	110.00
1	A	328	THR	CB-CA-C	-5.01	102.95	111.02
2	D	278	ALA	N-CA-C	-5.01	105.51	110.97

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	3005	DC	Sidechain
3	C	3014	DA	Sidechain
3	C	3015	DG	Sidechain

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	2308	0	2335	187	0
2	D	2879	0	2935	250	0
3	C	411	0	225	29	0
4	F	403	0	230	30	0
5	E	71	0	84	20	0
5	G	79	0	88	5	0
6	A	2	0	0	0	0
6	D	2	0	0	0	0
7	A	22	0	27	4	0
8	D	27	0	10	2	0
All	All	6204	0	5934	487	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 40.

All (487) 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:C:3007:DA:H2''	3:C:3008:DG:H5'	1.22	1.12
2:D:262:ILE:HG12	2:D:288:ARG:HH12	1.14	1.08
2:D:244:LYS:H	2:D:244:LYS:HD2	1.24	1.00
3:C:3007:DA:H2''	3:C:3008:DG:C5'	1.93	0.98
2:D:184:ARG:HD2	3:C:3004:DA:O4'	1.64	0.97
3:C:3009:DG:H1'	3:C:3010:DT:H5'	1.48	0.95
2:D:251:ASP:HB2	2:D:254:SER:H	1.29	0.94
1:A:160:LYS:HE3	1:A:164:ARG:HH12	1.31	0.94
4:F:4001:DC:HO5'	4:F:4001:DC:H6	1.14	0.92
2:D:309:LEU:HD21	2:D:405:PRO:HB2	1.50	0.91
2:D:135:PHE:HB2	2:D:175:MET:HE3	1.54	0.90
2:D:457:LYS:HE3	2:D:463:MET:HE1	1.52	0.90
2:D:229:THR:HG23	2:D:232:LYS:HE2	1.52	0.89
1:A:164:ARG:HH21	1:A:208:GLU:HA	1.38	0.86
2:D:262:ILE:CG1	2:D:288:ARG:HH12	1.88	0.85
1:A:325:LEU:N	1:A:325:LEU:HD12	1.95	0.82
1:A:320:VAL:CG1	1:A:325:LEU:HD11	2.11	0.81
2:D:260:ASP:HB2	2:D:342:SER:HB2	1.62	0.81
2:D:181:ARG:HH22	2:D:185:MET:CE	1.93	0.81
2:D:321:GLY:O	2:D:325:ILE:HG12	1.80	0.81
1:A:315:HIS:O	1:A:318:ILE:HG12	1.80	0.80
2:D:109:ILE:HD12	2:D:109:ILE:H	1.47	0.80
1:A:320:VAL:HG11	1:A:325:LEU:HD11	1.64	0.79
2:D:262:ILE:HG12	2:D:288:ARG:NH1	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:309:LEU:CD2	2:D:405:PRO:HB2	2.11	0.78
2:D:301:LYS:HE3	5:E:694:LEU:HA	1.63	0.78
2:D:290:VAL:HG13	2:D:468:LEU:HD23	1.65	0.78
4:F:4008:DT:H2''	4:F:4009:DT:H5'	1.64	0.77
1:A:306:ASN:ND2	1:A:433:LEU:HG	1.99	0.77
1:A:135:CYS:HA	1:A:151:SER:HA	1.64	0.77
5:E:690:LEU:HA	5:E:693:LEU:HD13	1.67	0.77
4:F:4018:DT:H2''	4:F:4019:DT:O5'	1.85	0.76
2:D:353:LEU:HD13	2:D:364:MET:HG2	1.67	0.76
1:A:318:ILE:HG23	1:A:358:ARG:HG3	1.67	0.76
4:F:4017:DT:H2''	4:F:4018:DT:H5''	1.66	0.76
2:D:138:THR:HG21	2:D:167:PHE:CE1	2.21	0.76
4:F:4008:DT:H2''	4:F:4009:DT:C5'	2.16	0.75
3:C:3004:DA:H1'	3:C:3005:DC:H5''	1.68	0.74
2:D:288:ARG:HG2	2:D:288:ARG:HH11	1.51	0.74
2:D:244:LYS:HD2	2:D:244:LYS:N	2.02	0.73
2:D:199:SER:HB3	2:D:203:GLN:HB2	1.69	0.73
2:D:187:GLN:O	2:D:187:GLN:HG2	1.88	0.73
1:A:160:LYS:HE3	1:A:164:ARG:NH1	2.04	0.73
1:A:406:HIS:O	1:A:409:PRO:HD3	1.88	0.73
2:D:286:GLN:OE1	2:D:465:LEU:HD23	1.89	0.73
4:F:4001:DC:H2''	4:F:4002:DT:H5'	1.71	0.72
2:D:322:VAL:HG23	2:D:323:HIS:H	1.55	0.71
2:D:181:ARG:NH2	2:D:185:MET:HE2	2.04	0.71
2:D:196:GLU:C	2:D:198:SER:H	1.99	0.71
2:D:309:LEU:HD13	2:D:406:ILE:HG12	1.72	0.71
1:A:310:ILE:O	1:A:314:SER:HB2	1.90	0.70
1:A:314:SER:HB3	1:A:357:MET:HE1	1.73	0.70
2:D:147:ARG:HG2	2:D:148:CYS:H	1.56	0.70
2:D:189:GLU:HA	2:D:192:LYS:HB3	1.72	0.70
1:A:133:HIS:O	1:A:134:ILE:HD13	1.92	0.70
1:A:268:ILE:HG21	7:A:7223:9CR:H7	1.74	0.70
1:A:315:HIS:CG	1:A:367:LEU:HD22	2.27	0.70
1:A:385:ASN:CG	1:A:388:GLU:HG3	2.18	0.69
2:D:289:SER:O	2:D:293:VAL:HG23	1.93	0.68
1:A:302:ARG:HG3	1:A:302:ARG:HH11	1.57	0.68
2:D:194:LEU:HB2	2:D:197:ILE:HG23	1.76	0.68
2:D:181:ARG:NH2	2:D:185:MET:CE	2.56	0.68
1:A:231:PRO:HB2	1:A:234:ARG:HD3	1.75	0.68
2:D:122:HIS:HA	3:C:3007:DA:OP1	1.92	0.67
2:D:193:LEU:HB2	2:D:197:ILE:HG12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ILE:HG22	1:A:269:CYS:N	2.10	0.67
2:D:188:ALA:O	2:D:192:LYS:HB2	1.95	0.67
2:D:288:ARG:HG3	8:D:701:PLB:O9	1.95	0.67
1:A:393:ARG:HD3	1:A:397:TYR:OH	1.95	0.67
1:A:442:ILE:CG2	1:A:444:ASP:HB2	2.25	0.67
2:D:205:ASN:HA	2:D:206:PRO:C	2.20	0.66
2:D:184:ARG:HD2	3:C:3004:DA:C4'	2.24	0.66
2:D:277:VAL:O	2:D:281:ILE:HG13	1.95	0.66
2:D:135:PHE:HB2	2:D:175:MET:CE	2.24	0.66
2:D:260:ASP:HB2	2:D:342:SER:CB	2.24	0.66
2:D:109:ILE:HD12	2:D:109:ILE:N	2.11	0.66
1:A:233:GLU:H	1:A:233:GLU:CD	2.03	0.66
1:A:326:LEU:O	1:A:327:ALA:HB3	1.96	0.65
1:A:442:ILE:HG22	1:A:444:ASP:N	2.11	0.65
2:D:181:ARG:HH22	2:D:185:MET:HE2	1.59	0.65
1:A:348:ARG:HH11	1:A:428:ILE:HG12	1.62	0.65
2:D:461:THR:O	2:D:462:ASP:HB2	1.97	0.65
2:D:135:PHE:CB	2:D:175:MET:HE3	2.25	0.65
4:F:4013:DC:H2''	4:F:4014:DT:OP2	1.94	0.65
4:F:4004:DA:H1'	4:F:4005:DC:H5'	1.79	0.65
5:E:689:ILE:HG23	5:E:690:LEU:HD12	1.80	0.64
1:A:370:LEU:O	1:A:374:VAL:HG23	1.98	0.64
1:A:164:ARG:NH2	1:A:208:GLU:HA	2.13	0.64
2:D:244:LYS:H	2:D:244:LYS:CD	2.04	0.64
1:A:358:ARG:C	1:A:360:MET:H	2.03	0.63
2:D:112:ARG:HG3	2:D:125:VAL:CG2	2.27	0.63
3:C:3005:DC:H2'	3:C:3006:DT:H72	1.80	0.63
2:D:434:LYS:O	2:D:437:GLN:HB3	1.97	0.63
1:A:388:GLU:O	1:A:392:LEU:HD13	1.98	0.63
5:E:694:LEU:N	5:E:694:LEU:HD12	2.14	0.63
2:D:136:ARG:HG2	2:D:136:ARG:HH11	1.64	0.63
3:C:3014:DA:H2''	3:C:3015:DG:H8	1.64	0.63
2:D:370:PHE:CZ	2:D:442:LEU:HD21	2.34	0.63
2:D:310:ASP:OD2	2:D:312:ASN:HB2	1.99	0.62
3:C:3014:DA:H5'	3:C:3014:DA:H8	1.64	0.62
1:A:442:ILE:HG22	1:A:444:ASP:H	1.63	0.62
1:A:238:ALA:HA	1:A:285:ARG:HD2	1.79	0.62
4:F:4017:DT:C2'	4:F:4018:DT:H5''	2.28	0.62
2:D:453:LEU:O	2:D:453:LEU:HD23	1.99	0.62
2:D:113:VAL:HG13	2:D:169:LYS:HG2	1.82	0.62
2:D:194:LEU:HD13	2:D:200:ASP:OD2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LEU:HD11	2:D:444:GLN:OE1	1.98	0.62
1:A:306:ASN:HD22	1:A:433:LEU:HG	1.64	0.62
5:E:690:LEU:HD12	5:E:690:LEU:H	1.65	0.61
2:D:199:SER:HA	2:D:203:GLN:H	1.65	0.61
1:A:305:TRP:CD1	1:A:454:MET:HE2	2.36	0.61
2:D:141:LEU:HB3	2:D:143:LEU:HD21	1.82	0.61
2:D:189:GLU:HA	2:D:192:LYS:CB	2.31	0.61
1:A:167:LEU:HD12	1:A:169:TYR:OH	1.99	0.61
1:A:295:ASP:O	1:A:299:ILE:HG12	2.01	0.61
2:D:322:VAL:HG23	2:D:323:HIS:N	2.16	0.61
3:C:3005:DC:C2'	3:C:3006:DT:H72	2.31	0.61
2:D:232:LYS:H	2:D:232:LYS:HD2	1.65	0.61
2:D:187:GLN:C	2:D:189:GLU:H	2.09	0.60
2:D:471:GLU:HG2	5:E:689:ILE:HG22	1.84	0.60
2:D:167:PHE:O	2:D:170:CYS:HB2	2.01	0.60
1:A:410:GLU:O	1:A:412:PRO:HD3	2.02	0.60
1:A:338:HIS:ND1	1:A:343:GLY:HA3	2.17	0.60
1:A:426:ARG:HD3	2:D:444:GLN:HB2	1.83	0.60
2:D:330:LEU:HD12	2:D:330:LEU:O	2.01	0.60
2:D:474:LYS:HG2	2:D:475:ASP:OD1	2.02	0.60
2:D:192:LYS:C	2:D:194:LEU:H	2.10	0.60
1:A:210:GLN:O	2:D:161:LYS:HB3	2.01	0.59
1:A:342:VAL:HG12	1:A:435:HIS:HD2	1.67	0.59
3:C:3007:DA:C2'	3:C:3008:DG:C5'	2.74	0.59
1:A:134:ILE:HG23	1:A:139:GLY:O	2.01	0.59
2:D:204:LEU:HB3	2:D:209:ALA:HB2	1.84	0.59
2:D:228:LEU:HD12	2:D:232:LYS:HB2	1.85	0.59
2:D:232:LYS:O	2:D:236:ILE:HG13	2.01	0.59
5:E:693:LEU:HD12	5:E:693:LEU:N	2.18	0.59
2:D:276:GLU:HG2	2:D:277:VAL:H	1.66	0.59
1:A:423:PRO:CD	2:D:440:THR:HG22	2.33	0.59
2:D:421:LEU:HD13	2:D:431:LEU:HG	1.85	0.58
4:F:4006:DC:H2''	4:F:4007:DT:OP2	2.04	0.58
2:D:193:LEU:O	2:D:197:ILE:HG12	2.03	0.58
2:D:249:ILE:HG21	2:D:348:MET:HE2	1.85	0.58
2:D:282:PHE:O	2:D:285:CYS:HB3	2.03	0.58
2:D:309:LEU:HD21	2:D:405:PRO:CB	2.28	0.58
1:A:132:LYS:HA	1:A:141:ARG:HH22	1.68	0.58
1:A:135:CYS:SG	1:A:137:ILE:HB	2.44	0.58
3:C:3001:DC:H2''	3:C:3002:DA:C8	2.39	0.58
1:A:326:LEU:O	1:A:327:ALA:CB	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ARG:HD2	1:A:454:MET:HE1	1.85	0.58
2:D:288:ARG:NH1	2:D:288:ARG:HG2	2.14	0.58
1:A:320:VAL:HG13	1:A:325:LEU:HD11	1.84	0.58
2:D:286:GLN:NE2	2:D:469:LEU:HD12	2.18	0.58
2:D:230:LYS:HE2	2:D:379:LEU:O	2.03	0.57
3:C:3007:DA:H8	3:C:3007:DA:OP2	1.87	0.57
2:D:277:VAL:HG13	2:D:278:ALA:N	2.19	0.57
2:D:158:SER:HB2	2:D:161:LYS:HG3	1.85	0.57
2:D:368:PHE:O	2:D:372:VAL:HG23	2.03	0.57
1:A:348:ARG:NE	1:A:431:LYS:HZ3	2.02	0.57
2:D:194:LEU:HD12	2:D:197:ILE:CG2	2.35	0.57
2:D:335:ASN:C	2:D:335:ASN:OD1	2.47	0.57
1:A:423:PRO:HD3	2:D:440:THR:HG22	1.87	0.57
1:A:446:PRO:C	1:A:447:ILE:HD12	2.30	0.57
2:D:461:THR:HG22	2:D:462:ASP:N	2.20	0.57
2:D:259:GLU:HA	2:D:259:GLU:OE2	2.05	0.57
2:D:138:THR:HG21	2:D:167:PHE:CD1	2.40	0.56
4:F:4016:DG:H2''	4:F:4017:DT:OP2	2.05	0.56
2:D:423:LEU:HD12	2:D:424:ASN:N	2.19	0.56
1:A:230:MET:HE3	1:A:396:VAL:CG2	2.35	0.56
2:D:452:LEU:HG	2:D:456:ILE:HD11	1.88	0.56
3:C:3008:DG:H1'	3:C:3009:DG:H5'	1.88	0.56
2:D:300:ALA:O	2:D:303:ILE:HG12	2.06	0.56
1:A:395:LYS:O	1:A:398:ALA:N	2.38	0.56
5:E:691:HIS:HB3	5:E:695:GLN:OE1	2.05	0.56
1:A:322:ASP:O	1:A:333:HIS:HA	2.07	0.55
2:D:154:ILE:HG12	2:D:166:ARG:HA	1.87	0.55
2:D:239:GLY:C	2:D:241:THR:H	2.15	0.55
1:A:238:ALA:HB2	1:A:285:ARG:HG2	1.89	0.55
2:D:277:VAL:CG1	2:D:278:ALA:N	2.70	0.55
2:D:326:ILE:O	2:D:327:TYR:C	2.50	0.55
4:F:4008:DT:H1'	4:F:4009:DT:H5''	1.88	0.55
1:A:326:LEU:HD23	1:A:330:LEU:O	2.06	0.55
1:A:432:CYS:HB3	7:A:7223:9CR:H24	1.89	0.55
1:A:440:LYS:O	1:A:443:GLY:N	2.39	0.55
2:D:421:LEU:O	2:D:423:LEU:N	2.39	0.55
2:D:194:LEU:HD12	2:D:197:ILE:HG22	1.89	0.54
2:D:386:ILE:HB	2:D:417:LEU:HD13	1.90	0.54
4:F:4001:DC:H2'	4:F:4002:DT:H72	1.88	0.54
4:F:4001:DC:H2'	4:F:4002:DT:C7	2.37	0.54
1:A:442:ILE:HG21	1:A:444:ASP:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:VAL:HG11	5:G:693:LEU:HD22	1.90	0.54
2:D:329:MET:HE3	2:D:388:ILE:HD11	1.90	0.54
2:D:152:CYS:HB2	2:D:165:CYS:SG	2.46	0.54
1:A:184:ARG:NH2	4:F:4003:DG:OP1	2.34	0.54
1:A:230:MET:HE3	1:A:396:VAL:HG23	1.90	0.54
1:A:363:ASP:HB3	1:A:366:GLU:CD	2.33	0.53
2:D:181:ARG:CZ	2:D:185:MET:HE2	2.38	0.53
2:D:310:ASP:OD2	2:D:401:LEU:HD12	2.08	0.53
1:A:426:ARG:CD	2:D:444:GLN:HB2	2.38	0.53
2:D:228:LEU:CD1	2:D:232:LYS:HB2	2.38	0.53
1:A:298:VAL:HG13	5:G:690:LEU:HD23	1.90	0.53
2:D:184:ARG:HB2	3:C:3004:DA:N3	2.23	0.53
5:E:688:LYS:HA	5:E:691:HIS:ND1	2.22	0.53
1:A:385:ASN:OD1	1:A:388:GLU:HG3	2.08	0.53
1:A:180:ASP:O	1:A:184:ARG:HB3	2.08	0.53
2:D:196:GLU:C	2:D:198:SER:N	2.66	0.53
2:D:167:PHE:CE2	2:D:171:LEU:HD11	2.44	0.53
2:D:421:LEU:O	2:D:422:LYS:C	2.52	0.53
1:A:174:ASN:O	1:A:175:LYS:C	2.52	0.53
1:A:228:GLU:OE1	1:A:231:PRO:HA	2.09	0.53
2:D:309:LEU:CD1	2:D:406:ILE:HG12	2.39	0.53
2:D:199:SER:CB	2:D:203:GLN:HB2	2.39	0.52
1:A:447:ILE:HG22	1:A:448:ASP:N	2.24	0.52
2:D:358:LYS:HB2	2:D:358:LYS:NZ	2.24	0.52
1:A:203:GLU:CD	2:D:234:ARG:HH22	2.18	0.52
1:A:431:LYS:HD2	2:D:477:TYR:OXT	2.10	0.52
2:D:436:LEU:O	2:D:439:MET:HB2	2.10	0.52
1:A:149:VAL:HG22	1:A:150:TYR:N	2.25	0.52
2:D:205:ASN:HD22	2:D:205:ASN:C	2.17	0.52
4:F:4005:DC:H2''	4:F:4006:DC:OP2	2.10	0.52
2:D:159:ARG:HG3	2:D:160:ASN:N	2.24	0.52
2:D:311:LEU:O	2:D:315:VAL:HG23	2.10	0.52
4:F:4008:DT:H2'	4:F:4009:DT:H71	1.92	0.52
1:A:326:LEU:CD2	1:A:330:LEU:O	2.58	0.52
2:D:108:ALA:HB3	2:D:109:ILE:HD12	1.92	0.52
2:D:207:GLU:C	2:D:209:ALA:H	2.18	0.52
1:A:313:PHE:C	1:A:313:PHE:CD2	2.88	0.52
1:A:394:GLU:HA	1:A:397:TYR:CD2	2.44	0.52
2:D:135:PHE:CG	2:D:175:MET:HE3	2.45	0.52
2:D:457:LYS:HE3	2:D:463:MET:CE	2.32	0.52
1:A:325:LEU:N	1:A:325:LEU:CD1	2.65	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ARG:HG3	1:A:302:ARG:NH1	2.25	0.51
1:A:453:GLU:OE1	5:G:689:ILE:HB	2.10	0.51
1:A:135:CYS:CA	1:A:151:SER:HA	2.38	0.51
1:A:358:ARG:O	1:A:360:MET:N	2.43	0.51
5:G:693:LEU:O	5:G:693:LEU:HD23	2.10	0.51
2:D:283:GLN:O	2:D:286:GLN:HB2	2.11	0.51
2:D:155:HIS:HD2	2:D:427:GLU:HG3	1.75	0.51
1:A:184:ARG:HH21	4:F:4003:DG:P	2.34	0.51
1:A:193:GLN:NE2	1:A:196:LEU:HD12	2.26	0.51
1:A:351:THR:HA	1:A:355:SER:HB2	1.93	0.51
1:A:358:ARG:C	1:A:360:MET:N	2.69	0.51
2:D:229:THR:OG1	2:D:232:LYS:HD2	2.11	0.51
5:E:692:ARG:HH11	5:E:692:ARG:HB2	1.76	0.50
1:A:365:THR:HG21	1:A:403:TYR:CE2	2.46	0.50
2:D:148:CYS:HB3	2:D:164:TYR:HD2	1.75	0.50
5:E:689:ILE:HD13	5:E:692:ARG:NH2	2.26	0.50
1:A:230:MET:SD	1:A:287:PRO:HG2	2.51	0.50
1:A:146:HIS:CE1	1:A:156:LYS:HD2	2.47	0.50
1:A:393:ARG:HD3	1:A:397:TYR:CZ	2.47	0.50
1:A:444:ASP:OD1	1:A:445:THR:HG23	2.12	0.50
2:D:283:GLN:HA	2:D:286:GLN:HG3	1.94	0.50
2:D:324:GLU:HG2	2:D:442:LEU:HB3	1.93	0.50
1:A:132:LYS:HA	1:A:141:ARG:NH2	2.27	0.49
1:A:146:HIS:ND1	1:A:156:LYS:HD2	2.27	0.49
1:A:210:GLN:H	2:D:161:LYS:HD2	1.77	0.49
1:A:226:ALA:O	1:A:229:ASP:OD1	2.30	0.49
2:D:413:LEU:O	2:D:416:ALA:HB3	2.12	0.49
3:C:3014:DA:H2''	3:C:3015:DG:C8	2.47	0.49
1:A:135:CYS:HB2	1:A:152:CYS:H	1.77	0.49
1:A:175:LYS:HA	1:A:190:CYS:SG	2.53	0.49
1:A:342:VAL:HG12	1:A:435:HIS:CD2	2.46	0.49
1:A:447:ILE:HD12	1:A:447:ILE:N	2.27	0.49
1:A:135:CYS:HB2	1:A:152:CYS:N	2.28	0.49
1:A:332:VAL:O	1:A:346:PHE:CZ	2.66	0.49
1:A:373:ILE:HD13	1:A:397:TYR:CE1	2.48	0.49
1:A:370:LEU:HD11	1:A:418:LEU:HD13	1.95	0.49
2:D:181:ARG:NH1	2:D:185:MET:HE2	2.28	0.49
2:D:363:PHE:CZ	2:D:456:ILE:HD13	2.47	0.49
2:D:140:ARG:NH1	2:D:140:ARG:HG3	2.28	0.49
2:D:169:LYS:O	2:D:173:VAL:HG22	2.11	0.49
2:D:466:HIS:ND1	2:D:467:PRO:HD2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLN:O	1:A:274:LYS:HG3	2.13	0.49
1:A:322:ASP:HB3	1:A:334:ARG:HG3	1.94	0.49
2:D:197:ILE:HG22	2:D:200:ASP:HB2	1.95	0.48
2:D:313:ASP:O	2:D:314:GLN:C	2.56	0.48
2:D:358:LYS:HB2	2:D:359:PRO:CD	2.43	0.48
1:A:376:PHE:O	1:A:378:PRO:HD3	2.13	0.48
2:D:286:GLN:HE22	2:D:466:HIS:H	1.61	0.48
2:D:297:THR:O	2:D:300:ALA:HB3	2.14	0.48
2:D:471:GLU:CG	5:E:689:ILE:HG22	2.43	0.48
5:E:692:ARG:HB2	5:E:692:ARG:NH1	2.28	0.48
4:F:4011:DA:H1'	4:F:4012:DC:H5'	1.96	0.48
1:A:234:ARG:HD2	1:A:234:ARG:N	2.29	0.48
2:D:285:CYS:O	2:D:286:GLN:C	2.57	0.48
2:D:189:GLU:C	2:D:192:LYS:H	2.22	0.48
4:F:4018:DT:H2'	4:F:4019:DT:H71	1.95	0.48
1:A:338:HIS:CE1	1:A:343:GLY:HA3	2.48	0.48
2:D:262:ILE:HG23	2:D:288:ARG:NH1	2.29	0.48
1:A:230:MET:HB3	1:A:399:SER:OG	2.14	0.48
1:A:414:ARG:O	1:A:418:LEU:HB2	2.13	0.48
2:D:466:HIS:CG	2:D:467:PRO:HD2	2.48	0.48
2:D:193:LEU:HB2	2:D:197:ILE:CG1	2.43	0.47
2:D:419:LEU:O	2:D:420:GLN:C	2.57	0.47
1:A:348:ARG:NH1	1:A:428:ILE:HG12	2.27	0.47
1:A:363:ASP:OD2	1:A:403:TYR:OH	2.32	0.47
2:D:192:LYS:HG2	2:D:192:LYS:O	2.14	0.47
2:D:405:PRO:O	2:D:408:ASP:HB3	2.14	0.47
2:D:423:LEU:O	2:D:426:PRO:HD3	2.14	0.47
2:D:443:ARG:HG3	2:D:443:ARG:HH11	1.79	0.47
1:A:324:ILE:C	1:A:325:LEU:HD12	2.38	0.47
1:A:345:ILE:HG23	1:A:346:PHE:N	2.29	0.47
2:D:198:SER:O	2:D:202:ASP:HB2	2.14	0.47
2:D:365:GLU:O	2:D:366:PRO:C	2.56	0.47
2:D:187:GLN:C	2:D:189:GLU:N	2.73	0.47
2:D:463:MET:HG3	2:D:464:SER:N	2.30	0.47
1:A:197:ALA:C	1:A:199:GLY:H	2.21	0.47
1:A:298:VAL:O	1:A:299:ILE:C	2.57	0.47
1:A:394:GLU:O	1:A:397:TYR:HB2	2.15	0.47
1:A:442:ILE:HG22	1:A:444:ASP:HB2	1.96	0.47
2:D:109:ILE:H	2:D:109:ILE:CD1	2.23	0.47
2:D:404:LYS:N	2:D:405:PRO:CD	2.77	0.47
1:A:306:ASN:ND2	1:A:433:LEU:CG	2.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:TYR:HE2	1:A:196:LEU:HD11	1.79	0.47
2:D:130:GLY:HA2	4:F:4010:DG:H2'	1.98	0.47
2:D:306:PHE:C	2:D:308:ASN:H	2.23	0.47
1:A:448:ASP:O	1:A:452:MET:HG2	2.15	0.46
2:D:196:GLU:O	2:D:198:SER:N	2.48	0.46
2:D:241:THR:OG1	2:D:242:THR:N	2.41	0.46
3:C:3014:DA:H5'	3:C:3014:DA:C8	2.47	0.46
1:A:184:ARG:HG3	1:A:185:ASN:OD1	2.15	0.46
2:D:154:ILE:HD12	2:D:154:ILE:N	2.29	0.46
5:E:689:ILE:CD1	5:E:692:ARG:NH2	2.78	0.46
2:D:321:GLY:O	2:D:322:VAL:C	2.58	0.46
1:A:271:ALA:O	1:A:272:ALA:C	2.59	0.46
2:D:421:LEU:HD22	2:D:425:HIS:HD2	1.81	0.46
3:C:3005:DC:C2'	3:C:3006:DT:C7	2.93	0.46
3:C:3014:DA:H2''	3:C:3015:DG:O5'	2.14	0.46
2:D:146:ASP:O	2:D:164:TYR:HB2	2.15	0.46
1:A:314:SER:CB	1:A:357:MET:HE1	2.42	0.46
2:D:461:THR:O	2:D:462:ASP:CB	2.63	0.46
1:A:363:ASP:HB3	1:A:366:GLU:CG	2.46	0.46
2:D:205:ASN:HA	2:D:206:PRO:O	2.15	0.46
2:D:474:LYS:NZ	2:D:474:LYS:HB3	2.31	0.46
1:A:148:GLY:HA3	1:A:201:LYS:HE3	1.99	0.45
1:A:360:MET:O	1:A:361:GLN:C	2.59	0.45
2:D:136:ARG:HG2	2:D:136:ARG:NH1	2.31	0.45
2:D:279:ILE:O	2:D:283:GLN:HG2	2.17	0.45
2:D:362:ASP:O	2:D:363:PHE:C	2.59	0.45
2:D:402:ASN:ND2	2:D:405:PRO:HG2	2.31	0.45
2:D:442:LEU:O	2:D:446:VAL:HG23	2.17	0.45
3:C:3002:DA:H1'	3:C:3003:DA:H5'	1.97	0.45
1:A:325:LEU:O	1:A:326:LEU:HD13	2.16	0.45
2:D:280:ARG:O	8:D:701:PLB:H24	2.16	0.45
1:A:279:LEU:O	1:A:282:TRP:HB3	2.16	0.45
1:A:419:LEU:C	1:A:421:ARG:H	2.23	0.45
1:A:435:HIS:HB2	7:A:7223:9CR:H17	1.98	0.45
2:D:306:PHE:C	2:D:308:ASN:N	2.74	0.45
2:D:182:PHE:CD1	4:F:4017:DT:H4'	2.51	0.45
2:D:327:TYR:O	2:D:328:THR:C	2.58	0.45
1:A:436:LEU:O	1:A:437:PHE:C	2.60	0.45
2:D:122:HIS:CE1	2:D:132:LYS:HD2	2.52	0.45
1:A:332:VAL:O	1:A:346:PHE:HZ	1.99	0.45
2:D:139:ILE:HD11	2:D:177:HIS:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:ILE:HG22	3:C:3007:DA:O5'	2.17	0.45
2:D:322:VAL:O	2:D:323:HIS:C	2.60	0.45
2:D:466:HIS:ND1	2:D:467:PRO:CD	2.80	0.45
1:A:263:ASP:O	1:A:267:ASN:ND2	2.50	0.45
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.84	0.45
2:D:200:ASP:HA	2:D:204:LEU:HD12	1.97	0.45
1:A:318:ILE:CG2	1:A:358:ARG:HG3	2.43	0.45
1:A:348:ARG:NH1	1:A:352:GLU:OE1	2.50	0.45
1:A:346:PHE:O	1:A:349:VAL:HB	2.16	0.44
2:D:120:GLY:O	2:D:126:HIS:HA	2.17	0.44
2:D:358:LYS:HB2	2:D:359:PRO:HD3	1.98	0.44
1:A:134:ILE:CG2	1:A:139:GLY:O	2.63	0.44
2:D:153:ARG:HH11	2:D:153:ARG:HG2	1.82	0.44
1:A:192:TYR:CE2	1:A:196:LEU:HD11	2.51	0.44
2:D:435:LEU:HD12	2:D:435:LEU:O	2.17	0.44
3:C:3011:DC:H2''	3:C:3012:DA:OP2	2.17	0.44
1:A:403:TYR:CD1	1:A:403:TYR:C	2.95	0.44
2:D:154:ILE:HD12	2:D:154:ILE:H	1.82	0.44
4:F:4008:DT:C2'	4:F:4009:DT:H5''	2.47	0.44
1:A:233:GLU:CD	1:A:233:GLU:N	2.74	0.44
1:A:266:THR:O	1:A:267:ASN:C	2.60	0.44
1:A:306:ASN:HD22	1:A:433:LEU:CG	2.28	0.44
1:A:334:ARG:O	1:A:336:SER:N	2.51	0.44
2:D:249:ILE:O	2:D:249:ILE:HG22	2.18	0.44
1:A:301:LEU:HD12	5:G:694:LEU:HD11	2.00	0.44
1:A:354:VAL:O	1:A:355:SER:C	2.61	0.44
2:D:360:PHE:HA	2:D:363:PHE:CD1	2.53	0.44
2:D:423:LEU:HD12	2:D:423:LEU:C	2.42	0.44
1:A:202:ARG:CZ	2:D:336:LYS:HG2	2.47	0.44
1:A:203:GLU:OE2	2:D:234:ARG:NH2	2.51	0.44
2:D:318:LEU:O	2:D:319:LYS:C	2.61	0.44
2:D:359:PRO:HG2	2:D:360:PHE:H	1.82	0.44
1:A:149:VAL:CG2	1:A:150:TYR:N	2.80	0.43
2:D:137:ARG:CB	2:D:137:ARG:HH11	2.31	0.43
2:D:247:PHE:CD1	2:D:345:GLN:O	2.71	0.43
1:A:389:VAL:O	1:A:390:GLU:C	2.59	0.43
1:A:414:ARG:HG3	1:A:414:ARG:HH11	1.83	0.43
2:D:141:LEU:O	2:D:143:LEU:HD23	2.18	0.43
2:D:180:ILE:HG22	3:C:3007:DA:C5'	2.49	0.43
1:A:414:ARG:HG3	1:A:414:ARG:NH1	2.33	0.43
2:D:179:ALA:O	2:D:181:ARG:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:192:LYS:C	2:D:194:LEU:N	2.70	0.43
2:D:232:LYS:O	2:D:235:ALA:HB3	2.19	0.43
4:F:4001:DC:H2''	4:F:4002:DT:C5'	2.45	0.43
1:A:310:ILE:HA	1:A:313:PHE:CE1	2.54	0.43
1:A:348:ARG:NH1	1:A:428:ILE:CG1	2.82	0.43
2:D:229:THR:CG2	2:D:232:LYS:HE2	2.37	0.43
2:D:251:ASP:H	2:D:254:SER:CB	2.31	0.43
2:D:294:GLN:O	2:D:297:THR:HB	2.18	0.43
1:A:232:VAL:HG11	1:A:403:TYR:CD2	2.54	0.43
1:A:236:LEU:HD23	1:A:365:THR:HA	2.01	0.43
1:A:307:GLU:O	1:A:308:LEU:C	2.61	0.43
1:A:388:GLU:O	1:A:391:ALA:HB3	2.18	0.43
2:D:471:GLU:HG2	5:E:689:ILE:CG2	2.48	0.43
3:C:3005:DC:H2''	3:C:3006:DT:C7	2.48	0.43
1:A:348:ARG:HG3	1:A:352:GLU:OE2	2.19	0.43
2:D:139:ILE:C	2:D:141:LEU:H	2.27	0.43
3:C:3016:DG:C2'	3:C:3017:DT:H72	2.48	0.43
1:A:351:THR:HA	1:A:355:SER:CB	2.49	0.43
2:D:357:ARG:O	2:D:358:LYS:C	2.62	0.43
2:D:471:GLU:HG2	5:E:690:LEU:CD1	2.49	0.43
1:A:135:CYS:SG	1:A:138:CYS:N	2.80	0.42
2:D:122:HIS:O	2:D:123:TYR:C	2.61	0.42
1:A:418:LEU:HD13	1:A:418:LEU:O	2.19	0.42
1:A:432:CYS:C	1:A:434:GLU:N	2.77	0.42
5:E:690:LEU:HD12	5:E:690:LEU:N	2.32	0.42
1:A:320:VAL:HG11	1:A:325:LEU:CD1	2.44	0.42
1:A:348:ARG:HH11	1:A:428:ILE:CG1	2.30	0.42
1:A:350:LEU:O	1:A:354:VAL:HB	2.20	0.42
2:D:255:LEU:O	2:D:256:MET:C	2.61	0.42
4:F:4008:DT:H2''	4:F:4009:DT:H5''	1.96	0.42
2:D:300:ALA:O	2:D:301:LYS:C	2.62	0.42
2:D:335:ASN:O	2:D:337:ASP:N	2.52	0.42
2:D:365:GLU:HB3	2:D:366:PRO:HD3	2.01	0.42
2:D:467:PRO:HA	2:D:470:GLN:HB2	2.01	0.42
2:D:287:PHE:O	2:D:288:ARG:C	2.62	0.42
2:D:443:ARG:HG3	2:D:443:ARG:NH1	2.35	0.42
1:A:202:ARG:NE	2:D:337:ASP:OD2	2.43	0.42
2:D:222:TYR:CD1	2:D:222:TYR:C	2.97	0.42
2:D:452:LEU:HG	2:D:456:ILE:CD1	2.49	0.42
1:A:344:ALA:O	1:A:345:ILE:C	2.61	0.42
2:D:335:ASN:O	2:D:336:LYS:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:150:LEU:O	2:D:152:CYS:N	2.49	0.41
5:E:694:LEU:N	5:E:694:LEU:CD1	2.83	0.41
1:A:184:ARG:C	1:A:186:ARG:H	2.29	0.41
1:A:317:SER:HA	1:A:325:LEU:HD13	2.02	0.41
1:A:331:HIS:O	1:A:332:VAL:CG2	2.67	0.41
1:A:406:HIS:O	1:A:409:PRO:CD	2.64	0.41
2:D:140:ARG:HH11	2:D:140:ARG:CG	2.34	0.41
2:D:342:SER:C	2:D:344:GLY:N	2.76	0.41
2:D:436:LEU:HD23	2:D:439:MET:HE3	2.03	0.41
2:D:410:GLN:O	2:D:414:LEU:HG	2.20	0.41
4:F:4008:DT:H5'	4:F:4008:DT:H6	1.85	0.41
1:A:423:PRO:HG3	2:D:440:THR:HG22	2.00	0.41
2:D:129:GLU:O	2:D:132:LYS:HB3	2.21	0.41
2:D:129:GLU:HG2	4:F:4011:DA:C8	2.55	0.41
2:D:430:GLN:O	2:D:434:LYS:HG3	2.20	0.41
1:A:294:LEU:O	1:A:298:VAL:HG23	2.21	0.41
1:A:345:ILE:HD13	1:A:431:LYS:HB3	2.01	0.41
3:C:3014:DA:H1'	3:C:3015:DG:H5'	2.03	0.41
5:E:690:LEU:CA	5:E:693:LEU:HD13	2.45	0.41
1:A:370:LEU:HD11	1:A:418:LEU:CD1	2.50	0.41
2:D:286:GLN:HE21	2:D:286:GLN:HB3	1.55	0.41
1:A:278:THR:O	1:A:279:LEU:C	2.63	0.41
1:A:331:HIS:C	1:A:332:VAL:HG23	2.46	0.41
2:D:408:ASP:OD1	2:D:408:ASP:C	2.63	0.41
2:D:429:SER:C	2:D:431:LEU:H	2.28	0.41
2:D:435:LEU:HD12	2:D:435:LEU:C	2.46	0.41
3:C:3018:DC:O5'	3:C:3018:DC:H2'	2.21	0.41
1:A:293:PRO:O	1:A:294:LEU:C	2.64	0.41
1:A:334:ARG:O	1:A:337:ALA:N	2.50	0.41
1:A:445:THR:HB	1:A:446:PRO:HD2	2.02	0.41
2:D:137:ARG:HB2	2:D:137:ARG:NH1	2.36	0.41
2:D:199:SER:HA	2:D:203:GLN:N	2.34	0.41
2:D:369:GLU:OE2	2:D:369:GLU:HA	2.19	0.41
2:D:390:VAL:CG1	2:D:414:LEU:HD21	2.51	0.41
2:D:430:GLN:O	2:D:431:LEU:C	2.64	0.41
5:E:694:LEU:HD12	5:E:694:LEU:H	1.84	0.41
2:D:239:GLY:C	2:D:241:THR:N	2.78	0.41
2:D:290:VAL:HG21	2:D:466:HIS:CD2	2.56	0.41
2:D:461:THR:HG22	2:D:462:ASP:OD1	2.21	0.41
4:F:4001:DC:C6	4:F:4002:DT:H72	2.56	0.41
1:A:180:ASP:HB2	1:A:183:GLN:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LEU:HD21	7:A:7223:9CR:H8	2.04	0.40
1:A:408:TYR:N	1:A:409:PRO:HD3	2.37	0.40
1:A:447:ILE:CG2	1:A:448:ASP:N	2.83	0.40
2:D:180:ILE:CG2	3:C:3007:DA:H5'	2.51	0.40
2:D:226:PHE:HA	2:D:227:PRO:HD2	1.90	0.40
1:A:162:THR:HG23	1:A:169:TYR:CE1	2.55	0.40
2:D:140:ARG:HG3	2:D:140:ARG:HH11	1.87	0.40
2:D:214:LEU:HD21	2:D:413:LEU:HD23	2.03	0.40
2:D:426:PRO:HG2	2:D:427:GLU:H	1.86	0.40
4:F:4008:DT:C2'	4:F:4009:DT:C5'	2.94	0.40
2:D:363:PHE:HD1	2:D:363:PHE:H	1.69	0.40
4:F:4017:DT:H2''	4:F:4018:DT:C5'	2.43	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	283/467 (61%)	225 (80%)	46 (16%)	12 (4%)	2	16
2	D	355/419 (85%)	276 (78%)	59 (17%)	20 (6%)	1	11
5	E	6/13 (46%)	6 (100%)	0	0	100	100
5	G	7/13 (54%)	4 (57%)	2 (29%)	1 (14%)	0	1
All	All	651/912 (71%)	511 (78%)	107 (16%)	33 (5%)	1	13

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	206	PRO
2	D	358	LYS
1	A	334	ARG

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Mol	Chain	Res	Type
1	A	335	ASN
1	A	359	ASP
1	A	407	LYS
2	D	186	PRO
2	D	197	ILE
2	D	336	LYS
2	D	422	LYS
1	A	412	PRO
2	D	323	HIS
1	A	140	ASP
2	D	188	ALA
2	D	200	ASP
2	D	263	LYS
2	D	330	LEU
2	D	343	GLU
2	D	462	ASP
1	A	231	PRO
1	A	320	VAL
1	A	332	VAL
1	A	440	LYS
2	D	287	PHE
2	D	342	SER
2	D	430	GLN
1	A	445	THR
2	D	304	PRO
2	D	326	ILE
5	G	689	ILE
1	A	268	ILE
2	D	180	ILE
2	D	322	VAL

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	250/405 (62%)	243 (97%)	7 (3%)	38 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	318/375 (85%)	303 (95%)	15 (5%)	23	57
5	E	8/13 (62%)	7 (88%)	1 (12%)	4	21
5	G	9/13 (69%)	9 (100%)	0	100	100
All	All	585/806 (73%)	562 (96%)	23 (4%)	28	62

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	CYS
1	A	202	ARG
1	A	313	PHE
1	A	325	LEU
1	A	350	LEU
1	A	390	GLU
1	A	442	ILE
2	D	109	ILE
2	D	140	ARG
2	D	180	ILE
2	D	197	ILE
2	D	205	ASN
2	D	286	GLN
2	D	318	LEU
2	D	329	MET
2	D	335	ASN
2	D	358	LYS
2	D	388	ILE
2	D	409	ILE
2	D	444	GLN
2	D	450	VAL
2	D	474	LYS
5	E	689	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	ASN
1	A	377	ASN
2	D	122	HIS
2	D	168	GLN
2	D	217	HIS

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Mol	Chain	Res	Type
2	D	375	ASN
5	G	691	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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$
8	PLB	D	701	-	29,29,29	2.29	15 (51%)	40,40,40	2.83	9 (22%)
7	9CR	A	7223	-	22,22,22	4.17	10 (45%)	30,30,30	2.35	12 (40%)

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
8	PLB	D	701	-	-	2/16/16/16	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	9CR	A	7223	-	-	7/15/32/32	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	7223	9CR	C1-C6	13.13	1.70	1.53
7	A	7223	9CR	C5-C6	9.32	1.50	1.34
8	D	701	PLB	C22-N23	4.71	1.38	1.32
7	A	7223	9CR	C2-C1	4.51	1.64	1.54
7	A	7223	9CR	C16-C1	4.33	1.61	1.53
7	A	7223	9CR	C20-C13	3.99	1.58	1.50
7	A	7223	9CR	C4-C5	3.61	1.57	1.51
8	D	701	PLB	C13-C14	3.46	1.44	1.39
7	A	7223	9CR	C2-C3	3.45	1.60	1.52
8	D	701	PLB	C6-C1	3.29	1.45	1.39
8	D	701	PLB	C22-N27	3.21	1.36	1.32
8	D	701	PLB	C1-C7	3.20	1.56	1.49
7	A	7223	9CR	C14-C13	3.19	1.39	1.35
7	A	7223	9CR	C10-C9	2.99	1.42	1.35
8	D	701	PLB	C15-C14	2.93	1.43	1.38
8	D	701	PLB	C18-C13	2.90	1.44	1.39
8	D	701	PLB	C15-C16	2.74	1.42	1.38
8	D	701	PLB	C13-C11	2.71	1.55	1.50
8	D	701	PLB	C18-C17	2.65	1.43	1.38
8	D	701	PLB	C17-C16	2.65	1.42	1.38
8	D	701	PLB	C1-C2	2.60	1.45	1.41
8	D	701	PLB	C2-N10	-2.36	1.37	1.41
8	D	701	PLB	C6-C5	2.33	1.42	1.39
8	D	701	PLB	C3-C2	2.30	1.43	1.39
7	A	7223	9CR	C14-C15	2.16	1.53	1.47

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	701	PLB	C24-N23-C22	10.89	121.67	114.46
8	D	701	PLB	C26-N27-C22	7.82	119.63	114.46
8	D	701	PLB	N23-C22-N27	-6.41	120.46	128.12
8	D	701	PLB	C22-O21-C5	6.06	133.81	118.72
7	A	7223	9CR	C7-C8-C9	5.30	134.08	126.23
7	A	7223	9CR	C17-C1-C6	4.75	117.69	110.24
7	A	7223	9CR	C19-C9-C10	-4.20	116.02	122.82
8	D	701	PLB	C15-C14-C13	-3.77	118.50	121.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	7223	9CR	C20-C13-C12	3.59	123.57	118.09
7	A	7223	9CR	C8-C7-C6	3.58	136.57	127.00
7	A	7223	9CR	C19-C9-C8	3.15	122.91	118.09
7	A	7223	9CR	C1-C6-C5	-3.02	118.51	122.64
7	A	7223	9CR	C15-C14-C13	3.01	132.88	128.40
8	D	701	PLB	C25-C24-N23	-2.60	119.31	123.42
7	A	7223	9CR	C18-C5-C6	2.32	127.01	124.48
8	D	701	PLB	O21-C5-C6	2.26	126.25	119.16
7	A	7223	9CR	C4-C5-C6	-2.22	119.70	122.70
7	A	7223	9CR	O2-C15-C14	2.21	119.98	113.40
7	A	7223	9CR	C7-C6-C5	2.21	126.64	121.56
8	D	701	PLB	C14-C15-C16	2.18	121.19	118.72
8	D	701	PLB	O21-C22-N27	2.17	123.01	115.87

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	7223	9CR	C7-C8-C9-C10
7	A	7223	9CR	C7-C8-C9-C19
8	D	701	PLB	N27-C22-O21-C5
8	D	701	PLB	N23-C22-O21-C5
7	A	7223	9CR	C6-C7-C8-C9
7	A	7223	9CR	C13-C14-C15-O2
7	A	7223	9CR	C11-C10-C9-C19
7	A	7223	9CR	C13-C14-C15-O1
7	A	7223	9CR	C11-C10-C9-C8

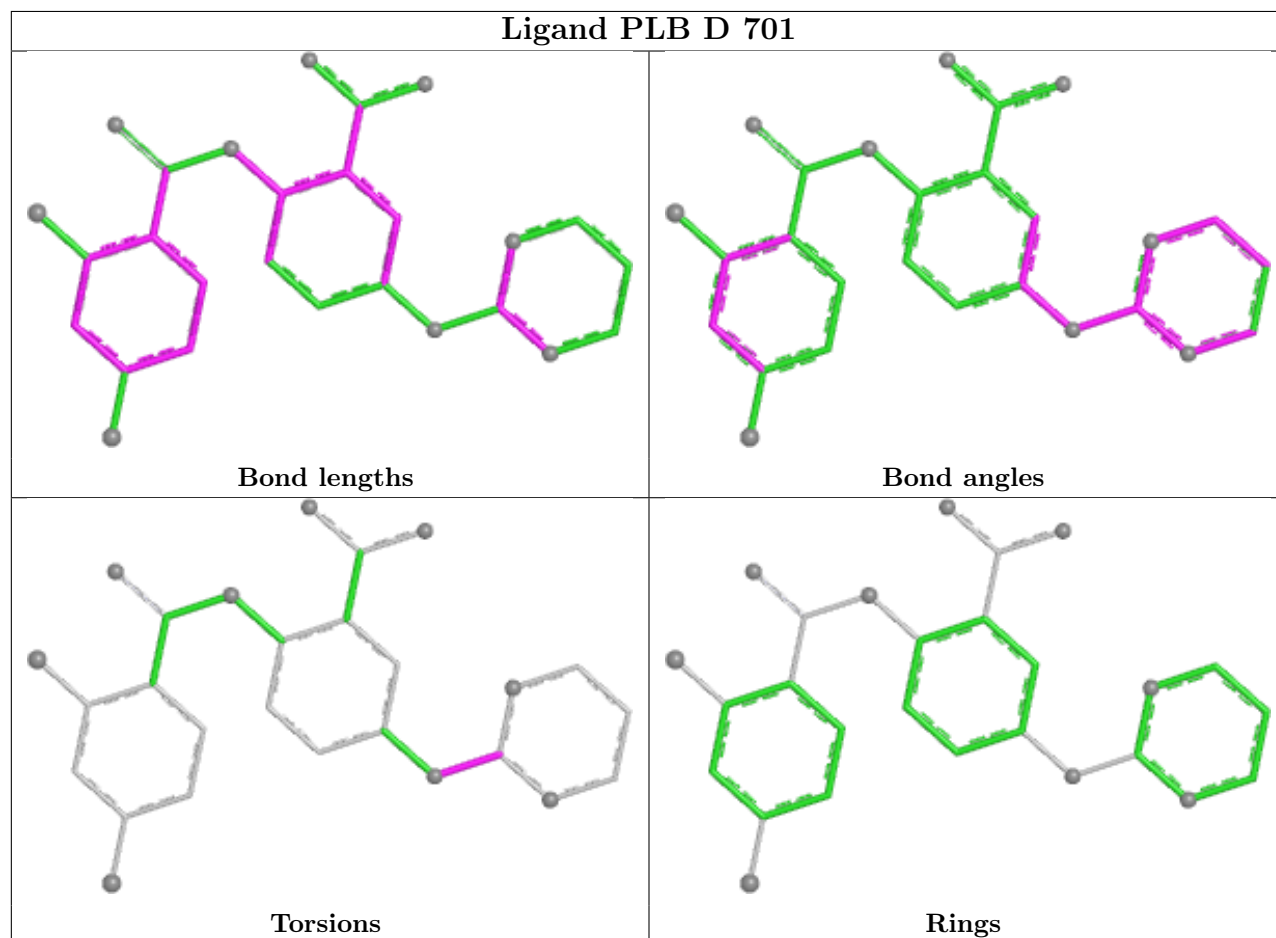
There are no ring outliers.

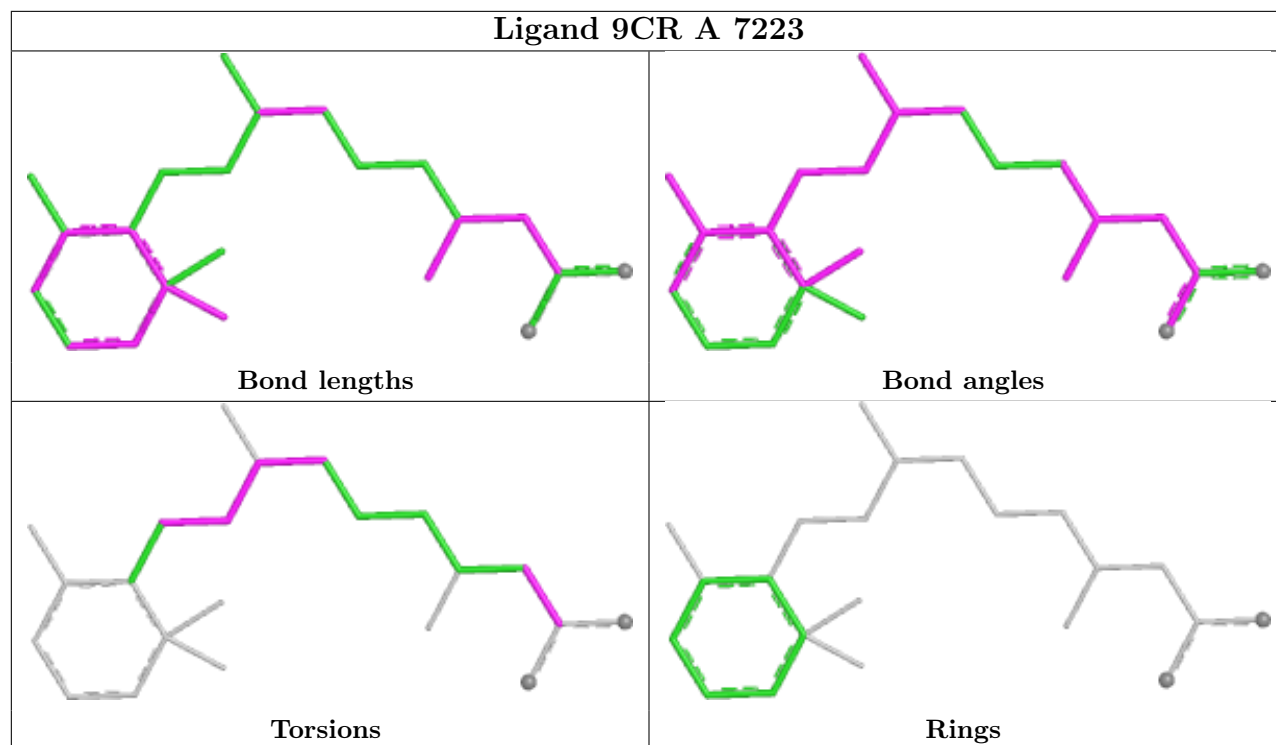
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	701	PLB	2	0
7	A	7223	9CR	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 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	A	289/467 (61%)	-0.41	0 100 100	37, 80, 118, 155	0
2	D	359/419 (85%)	-0.29	1 (0%) 90 81	33, 78, 138, 176	0
3	C	20/20 (100%)	-0.02	0 100 100	45, 68, 95, 99	0
4	F	20/20 (100%)	0.05	0 100 100	45, 70, 94, 97	0
5	E	8/13 (61%)	0.01	0 100 100	86, 104, 114, 126	0
5	G	9/13 (69%)	0.14	1 (11%) 10 7	82, 98, 134, 135	0
All	All	705/952 (74%)	-0.32	2 (0%) 90 81	33, 79, 127, 176	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	G	694	LEU	3.1
2	D	108	ALA	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](#)

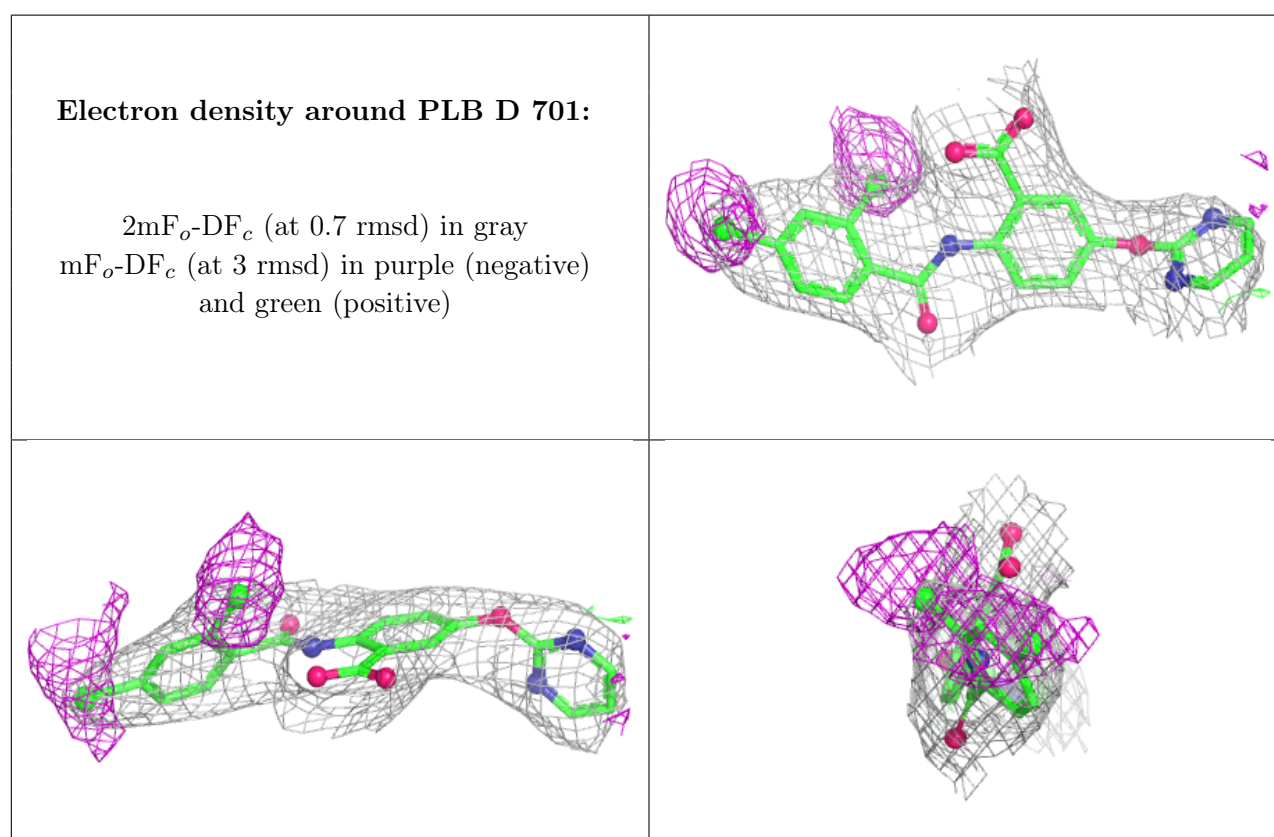
There are no oligosaccharides in this entry.

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.

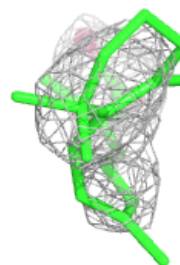
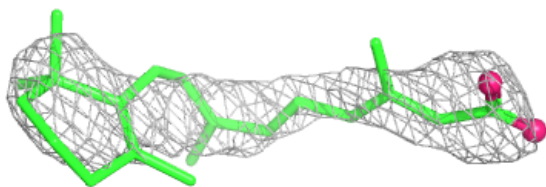
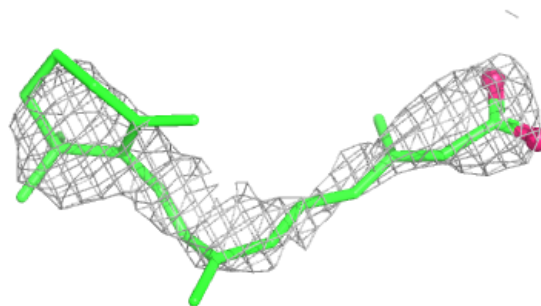
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	PLB	D	701	27/27	0.87	0.12	54,71,77,78	0
7	9CR	A	7223	22/22	0.95	0.15	96,98,100,100	0
6	ZN	A	7222	1/1	0.99	0.02	69,69,69,69	0
6	ZN	D	7122	1/1	1.00	0.04	83,83,83,83	0
6	ZN	A	7221	1/1	1.00	0.04	74,74,74,74	0
6	ZN	D	7121	1/1	1.00	0.02	70,70,70,70	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around 9CR A 7223:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.