



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:47 AM UTC

PDB ID : 1XVP / pdb_00001xvp
Title : crystal structure of CAR/RXR heterodimer bound with SRC1 peptide, fatty acid and CITCO
Authors : Xu, R.X.; Lambert, M.H.; Wisely, B.B.; Warren, E.N.; Weinert, E.E.; Waitt, G.M.; Williams, J.D.; Moore, L.B.; Willson, T.M.; Moore, J.T.
Deposited on : 2004-10-28
Resolution : 2.60 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

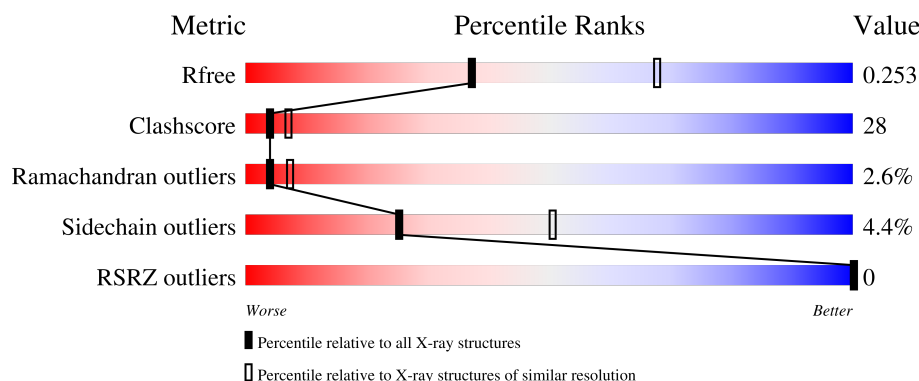
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

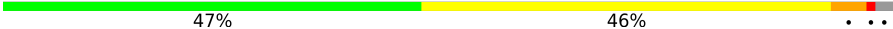
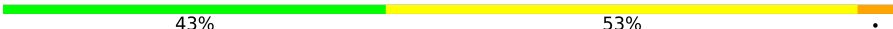
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 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	236	
1	C	236	
2	B	246	
2	D	246	

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Mol	Chain	Length	Quality of chain
3	E	13	23%46%8%23%
3	F	13	31%46%15%8%
3	G	13	54%38%8%
3	H	13	54%31%8%8%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8307 atoms, of which 58 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	232	Total	C	N	O	S	0	0	0
			1824	1166	311	336	11			
1	C	236	Total	C	N	O	S	0	0	0
			1859	1186	318	343	12			

- Molecule 2 is a protein called Orphan nuclear receptor NR1I3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	246	Total	C	N	O	S	0	0	0
			1990	1287	341	351	11			
2	D	246	Total	C	N	O	S	0	0	0
			1990	1287	341	351	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	VAL	deletion	UNP Q14994
B	?	-	SER	deletion	UNP Q14994
B	?	-	PRO	deletion	UNP Q14994
B	?	-	THR	deletion	UNP Q14994
D	?	-	VAL	deletion	UNP Q14994
D	?	-	SER	deletion	UNP Q14994
D	?	-	PRO	deletion	UNP Q14994
D	?	-	THR	deletion	UNP Q14994

- Molecule 3 is a protein called nuclear receptor coactivator 1 isoform 1.

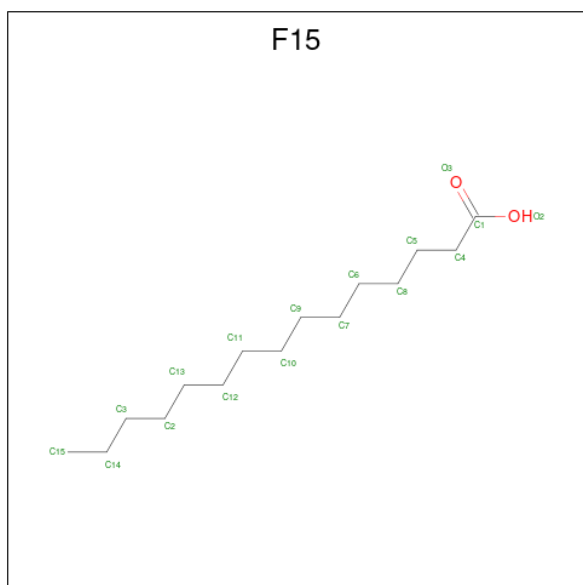
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	10	Total	C	N	O	0	0	0
			86	55	18	13			
3	F	12	Total	C	N	O	0	0	0
			102	63	23	16			

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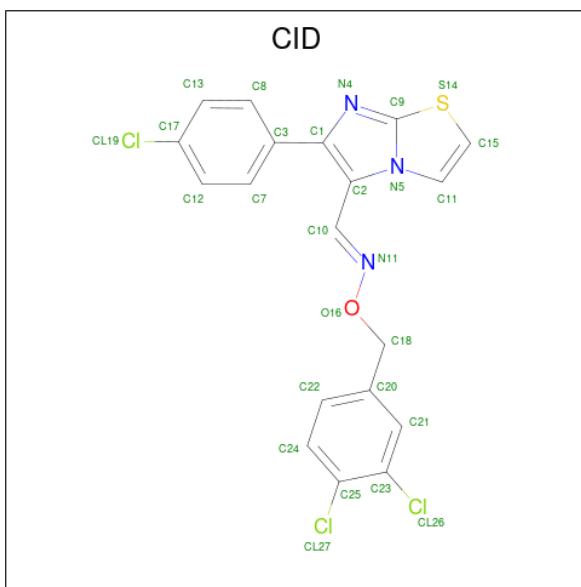
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	12	Total	C	N	O	0	0	0
			106	66	23	17			
3	H	12	Total	C	N	O	0	0	0
			106	66	23	17			

- Molecule 4 is PENTADECANOIC ACID (CCD ID: F15) (formula: $C_{15}H_{30}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			46	15	29	2		
4	C	1	Total	C	H	O	0	0
			46	15	29	2		

- Molecule 5 is 6-(4-CHLOROPHENYL)IMIDAZO[2,1-B][1,3]THIAZOLE-5-CARBALDEHYDE O-(3,4-DICHLOROBENZYL)OXIME (CCD ID: CID) (formula: $C_{19}H_{12}Cl_3N_3OS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	Cl	N	O	S	
			54	38	6	6	2	2	0
									1

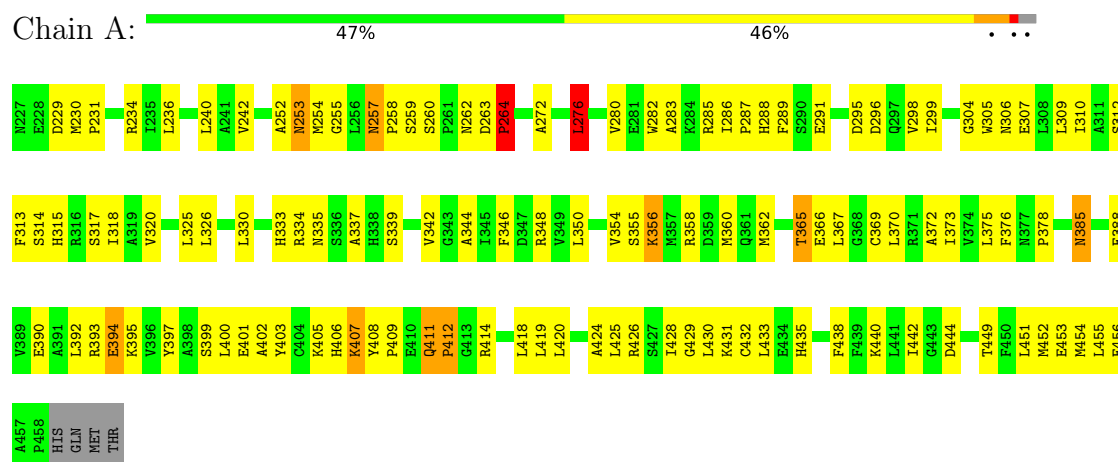
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	22	Total	O		
			22	22	0	0
6	B	21	Total	O		
			21	21	0	0
6	C	26	Total	O		
			26	26	0	0
6	D	24	Total	O		
			24	24	0	0
6	E	1	Total	O		
			1	1	0	0
6	F	1	Total	O		
			1	1	0	0
6	G	2	Total	O		
			2	2	0	0
6	H	1	Total	O		
			1	1	0	0

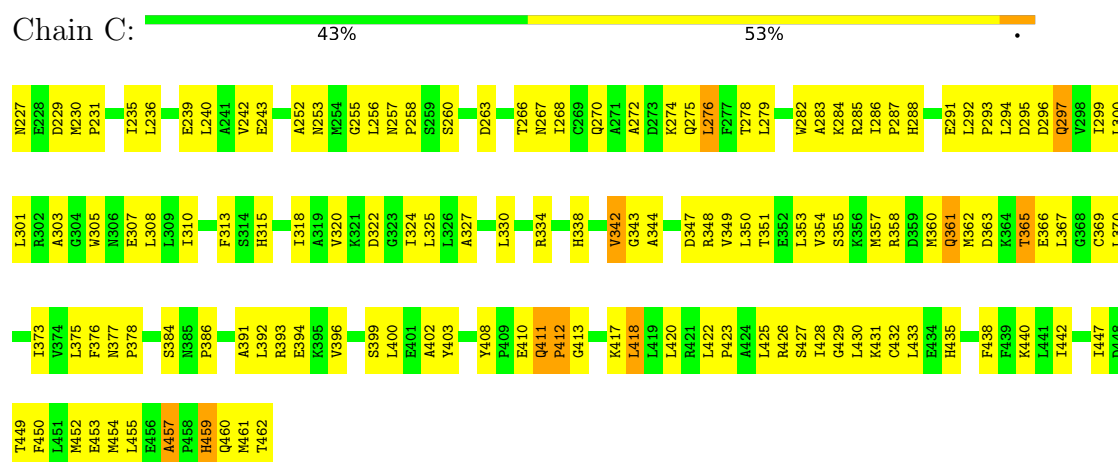
3 Residue-property plots

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.

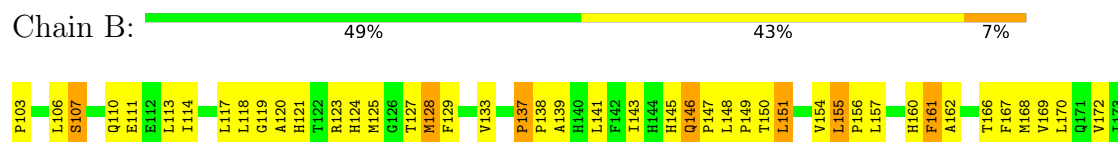
• Molecule 1: Retinoic acid receptor RXR-alpha

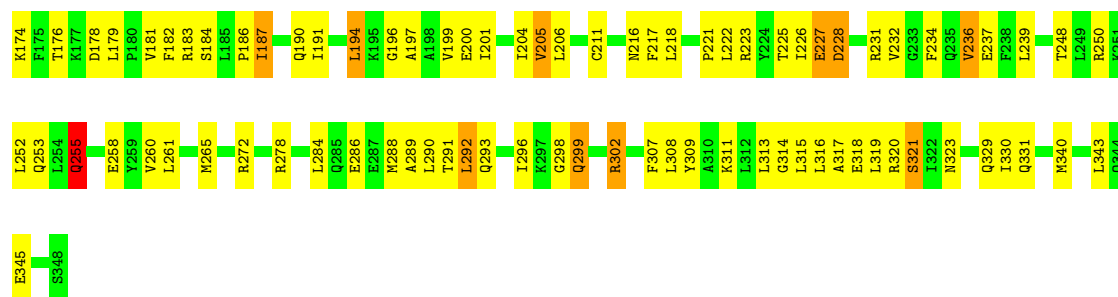


• Molecule 1: Retinoic acid receptor RXR-alpha



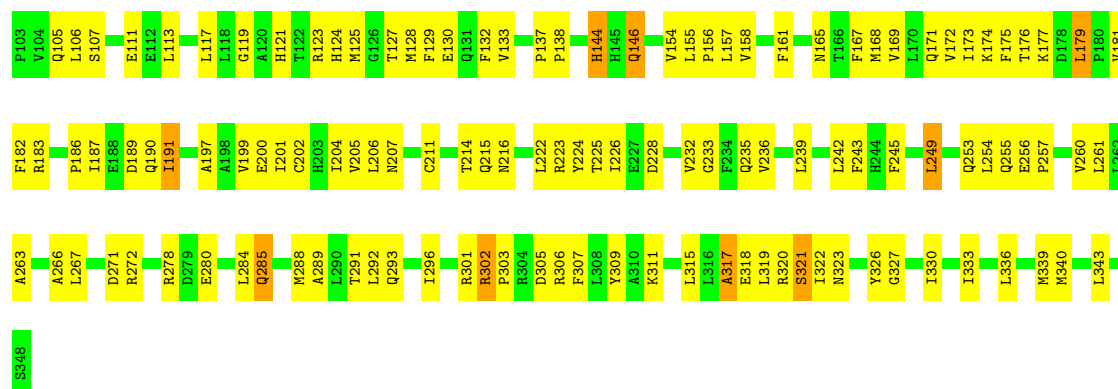
• Molecule 2: Orphan nuclear receptor NR1I3





- Molecule 2: Orphan nuclear receptor NR1I3

Chain D: 51% 46%



- Molecule 3: nuclear receptor coactivator 1 isoform 1

Chain E: 23% 46% 8% 23%



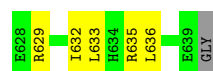
- Molecule 3: nuclear receptor coactivator 1 isoform 1

Chain F: 31% 46% 15% 8%



- Molecule 3: nuclear receptor coactivator 1 isoform 1

Chain G: 54% 38% 8%



- Molecule 3: nuclear receptor coactivator 1 isoform 1

Chain H: 54% 31% 8% 8%

E685	
I689	
I690	
H691	
R692	
L693	
L694	
Q695	
E696	
GLY	

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.02Å 128.02Å 212.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.3 (50.00-2.60) 89.7 (50.00-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.180 , 0.234 0.202 , 0.253	Depositor DCC
R_{free} test set	3356 reflections (5.68%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 79.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.425 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8307	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 2.56% 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: CID, F15

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	0.49	0/1862	1.09	10/2523 (0.4%)
1	C	0.54	0/1898	1.15	14/2570 (0.5%)
2	B	0.50	0/2036	1.05	8/2758 (0.3%)
2	D	0.50	0/2036	1.10	15/2758 (0.5%)
3	E	0.42	0/87	0.88	1/116 (0.9%)
3	F	0.46	0/103	1.28	2/135 (1.5%)
3	G	0.38	0/107	0.87	0/142
3	H	0.54	0/107	0.94	1/142 (0.7%)
All	All	0.50	0/8236	1.09	51/11144 (0.5%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	411	GLN	CA-C-N	10.06	132.41	119.84
1	C	411	GLN	C-N-CA	10.06	132.41	119.84
1	C	457	ALA	CA-C-N	8.43	130.38	119.84
1	C	457	ALA	C-N-CA	8.43	130.38	119.84
2	D	305	ASP	N-CA-C	7.58	120.36	110.43
1	C	449	THR	N-CA-C	7.52	120.43	111.33
2	D	179	LEU	CA-C-N	7.47	127.34	119.05
2	D	179	LEU	C-N-CA	7.47	127.34	119.05
1	C	297	GLN	N-CA-C	-7.17	103.40	111.14
2	D	146	GLN	CA-C-N	7.16	128.79	119.84
2	D	146	GLN	C-N-CA	7.16	128.79	119.84
1	C	408	TYR	CA-C-N	6.80	128.34	119.84
1	C	408	TYR	C-N-CA	6.80	128.34	119.84
2	B	187	ILE	N-CA-C	6.71	117.33	110.82
1	A	411	GLN	CA-C-N	6.52	127.99	119.84
1	A	411	GLN	C-N-CA	6.52	127.99	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	ASN	CA-C-N	6.43	127.87	119.84
1	A	385	ASN	C-N-CA	6.43	127.87	119.84
2	D	266	ALA	N-CA-C	-6.33	102.93	112.04
3	F	693	LEU	N-CA-C	6.27	119.09	111.82
2	B	143	ILE	N-CA-C	6.17	112.82	106.21
1	C	402	ALA	N-CA-C	-6.15	104.20	111.03
2	B	227	GLU	N-CA-C	-6.14	105.61	113.23
1	C	276	LEU	N-CA-C	-6.07	105.54	113.12
2	D	144	HIS	N-CA-C	6.05	120.16	113.21
1	A	356	LYS	N-CA-C	6.00	117.49	111.07
1	A	394	GLU	N-CA-C	-5.92	106.60	113.88
1	C	303	ALA	N-CA-C	5.85	118.61	111.82
2	B	172	VAL	N-CA-C	-5.75	104.00	112.04
2	D	278	ARG	N-CA-C	5.71	118.23	111.33
2	D	191	ILE	N-CA-C	5.70	116.43	110.62
1	C	459	HIS	N-CA-C	-5.66	98.75	110.80
2	D	130	GLU	N-CA-C	-5.65	105.65	112.54
3	H	689	ILE	N-CA-C	5.61	115.80	110.53
1	C	433	LEU	N-CA-C	-5.61	104.66	112.45
2	D	255	GLN	N-CA-C	-5.56	102.52	110.59
3	F	696	GLU	N-CA-C	5.56	115.72	107.88
1	A	276	LEU	N-CA-C	-5.51	105.19	111.14
2	B	141	LEU	N-CA-C	-5.49	106.42	113.23
3	E	632	ILE	N-CA-C	5.47	120.72	109.34
2	B	137	PRO	N-CA-C	5.42	117.31	110.70
1	C	351	THR	N-CA-C	5.41	117.88	111.33
2	B	228	ASP	N-CA-C	-5.37	105.50	111.36
2	D	340	MET	CA-C-N	5.27	125.07	119.28
2	D	340	MET	C-N-CA	5.27	125.07	119.28
1	A	257	ASN	CA-C-N	5.26	125.34	119.87
1	A	257	ASN	C-N-CA	5.26	125.34	119.87
2	B	139	ALA	N-CA-C	5.22	117.65	111.33
2	D	317	ALA	N-CA-C	-5.22	105.67	111.36
1	A	433	LEU	N-CA-C	-5.20	105.51	111.07
2	D	321	SER	N-CA-C	-5.05	105.90	111.71

There are no chirality outliers.

There are no planarity outliers.

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	1824	0	1849	109	0
1	C	1859	0	1880	132	0
2	B	1990	0	2023	120	0
2	D	1990	0	2023	104	0
3	E	86	0	86	5	0
3	F	102	0	102	6	0
3	G	106	0	105	5	0
3	H	106	0	105	7	0
4	A	17	29	29	6	0
4	C	17	29	29	7	0
5	D	54	0	24	2	0
6	A	22	0	0	2	0
6	B	21	0	0	1	0
6	C	26	0	0	3	0
6	D	24	0	0	3	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	2	0	0	0	0
6	H	1	0	0	0	0
All	All	8249	58	8255	457	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 28.

All (457) 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:C:362:MET:HE3	1:C:367:LEU:HB2	1.42	1.00
1:A:414:ARG:O	1:A:418:LEU:HD12	1.68	0.93
1:C:236:LEU:HB2	1:C:365:THR:HG23	1.50	0.90
1:A:236:LEU:O	1:A:240:LEU:HG	1.71	0.90
1:A:411:GLN:HG3	1:A:414:ARG:HB2	1.54	0.88
1:C:344:ALA:HB3	6:C:24:HOH:O	1.74	0.87
1:C:275:GLN:HG3	4:C:1001:F15:O2	1.76	0.85
1:A:360:MET:HE2	1:A:362:MET:HB2	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:VAL:HG11	3:E:636:LEU:HB3	1.59	0.82
1:A:259:SER:HA	3:H:685:GLU:HG2	1.61	0.81
1:A:231:PRO:HG3	1:A:234:ARG:HD2	1.62	0.81
1:C:276:LEU:HB3	1:C:450:PHE:CD2	2.16	0.81
2:B:113:LEU:HD23	2:B:291:THR:HG21	1.62	0.80
1:A:313:PHE:HB3	4:A:1002:F15:O3	1.82	0.80
2:D:113:LEU:HD23	2:D:291:THR:HG21	1.62	0.80
1:A:318:ILE:HG23	1:A:358:ARG:HB2	1.65	0.78
2:B:200:GLU:HG2	2:B:319:LEU:HB3	1.66	0.78
2:B:169:VAL:HG21	2:B:343:LEU:HD21	1.64	0.78
2:B:103:PRO:HA	2:B:298:GLY:HA2	1.67	0.77
3:G:632:ILE:O	3:G:636:LEU:HD13	1.84	0.77
1:A:252:ALA:HB2	1:A:330:LEU:HD11	1.65	0.76
2:D:200:GLU:HG2	2:D:319:LEU:HB3	1.67	0.76
1:A:378:PRO:HD3	1:A:393:ARG:HD3	1.67	0.76
2:B:345:GLU:CD	3:F:689:ILE:HG22	2.10	0.76
1:A:406:HIS:O	1:A:409:PRO:HD3	1.86	0.74
1:A:230:MET:HB3	1:A:399:SER:OG	1.88	0.74
2:B:289:ALA:O	2:B:293:GLN:HG3	1.87	0.73
2:D:200:GLU:HG3	2:D:323:ASN:HD22	1.55	0.72
1:C:384:SER:O	1:C:386:PRO:HD3	1.89	0.71
1:C:276:LEU:HB3	1:C:450:PHE:CE2	2.26	0.71
1:A:272:ALA:HB2	4:A:1002:F15:H29	1.71	0.71
1:A:315:HIS:O	1:A:318:ILE:HG13	1.91	0.71
1:C:426:ARG:HG2	2:D:317:ALA:O	1.91	0.71
1:A:438:PHE:CB	1:C:442:ILE:HD11	2.21	0.71
1:A:344:ALA:HB3	6:A:41:HOH:O	1.91	0.70
1:C:300:LEU:HD22	1:C:375:LEU:O	1.91	0.70
1:A:310:ILE:HA	1:A:313:PHE:CE2	2.27	0.69
1:C:295:ASP:O	1:C:299:ILE:HG13	1.92	0.69
2:D:107:SER:O	2:D:111:GLU:HG2	1.93	0.68
1:C:296:ASP:HA	1:C:299:ILE:HD12	1.76	0.68
2:B:227:GLU:O	2:B:231:ARG:HG2	1.94	0.68
1:C:362:MET:CE	1:C:367:LEU:HB2	2.21	0.68
2:B:155:LEU:HB3	2:B:156:PRO:HD3	1.76	0.68
1:C:362:MET:HE3	1:C:367:LEU:CB	2.23	0.68
2:D:124:HIS:HD2	2:D:174:LYS:HD3	1.59	0.67
2:D:197:ALA:O	2:D:201:ILE:HG13	1.94	0.67
1:A:289:PHE:HD1	1:A:376:PHE:HE1	1.41	0.67
2:D:327:GLY:O	2:D:330:ILE:HG12	1.95	0.67
1:A:288:HIS:HA	1:A:291:GLU:OE1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:LEU:HB3	2:D:111:GLU:OE2	1.95	0.66
1:A:339:SER:HB2	1:C:338:HIS:O	1.96	0.66
1:C:293:PRO:O	1:C:297:GLN:HG3	1.95	0.66
1:A:438:PHE:HB2	1:C:442:ILE:HD11	1.76	0.66
2:D:138:PRO:HG2	2:D:157:LEU:HA	1.78	0.66
1:C:230:MET:SD	1:C:287:PRO:HG2	2.35	0.66
1:C:440:LYS:HB2	1:C:447:ILE:CD1	2.26	0.65
1:A:253:ASN:H	1:A:262:ASN:HB2	1.62	0.65
1:A:401:GLU:O	1:A:405:LYS:HG2	1.95	0.65
2:D:261:LEU:HD13	2:D:292:LEU:HA	1.78	0.65
2:B:138:PRO:HG2	2:B:157:LEU:HA	1.78	0.65
1:C:376:PHE:O	1:C:393:ARG:HD2	1.97	0.65
1:A:365:THR:HG21	1:A:403:TYR:CE2	2.32	0.65
1:A:230:MET:SD	1:A:287:PRO:HG2	2.37	0.65
1:C:369:CYS:HB3	1:C:400:LEU:HD22	1.78	0.65
1:C:440:LYS:HB2	1:C:447:ILE:HD12	1.78	0.64
1:A:229:ASP:OD2	1:A:395:LYS:HD3	1.98	0.64
1:C:370:LEU:HD23	1:C:373:ILE:HD12	1.78	0.64
2:B:284:LEU:O	2:B:288:MET:HG2	1.97	0.64
1:A:403:TYR:HE1	1:A:408:TYR:HE2	1.47	0.63
1:C:318:ILE:HG23	1:C:358:ARG:HB2	1.79	0.63
2:D:301:ARG:HB3	2:D:303:PRO:HD3	1.81	0.63
2:B:169:VAL:HG21	2:B:343:LEU:CD2	2.29	0.62
1:A:369:CYS:O	1:A:373:ILE:HG13	2.00	0.62
1:A:255:GLY:HA2	1:A:264:PRO:HD2	1.80	0.62
2:B:190:GLN:O	2:B:194:LEU:HD22	2.00	0.62
1:C:266:THR:O	1:C:270:GLN:HG3	2.00	0.61
2:D:296:ILE:HD12	2:D:309:TYR:HB2	1.83	0.61
2:B:103:PRO:CA	2:B:298:GLY:HA2	2.31	0.61
1:C:432:CYS:HB3	4:C:1001:F15:H5	1.83	0.61
1:A:360:MET:O	1:A:360:MET:HG2	1.99	0.61
2:D:169:VAL:O	2:D:173:ILE:HG13	2.00	0.61
2:B:117:LEU:HB3	2:B:260:VAL:HG11	1.81	0.60
2:B:179:LEU:HB2	2:B:182:PHE:HB3	1.82	0.60
2:D:182:PHE:CE1	2:D:267:LEU:HD11	2.36	0.60
2:B:121:HIS:HD2	2:B:125:MET:HE3	1.66	0.60
2:B:176:THR:HA	2:B:179:LEU:HG	1.83	0.60
1:A:362:MET:HE3	1:A:367:LEU:HA	1.84	0.60
1:C:391:ALA:O	1:C:394:GLU:HB2	2.01	0.60
3:F:695:GLN:O	3:F:696:GLU:HG2	2.01	0.60
2:B:248:THR:HG21	2:B:315:LEU:HD21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:SER:OG	2:D:320:ARG:HD3	2.01	0.60
1:C:366:GLU:HB3	1:C:418:LEU:HD21	1.83	0.60
1:A:365:THR:HG21	1:A:403:TYR:CD2	2.36	0.60
1:A:385:ASN:HB3	1:A:388:GLU:OE2	2.02	0.60
1:A:369:CYS:HB3	1:A:400:LEU:HD22	1.84	0.60
2:D:161:PHE:O	2:D:165:ASN:HB2	2.01	0.60
2:D:326:TYR:CZ	5:D:1003[B]:CID:S14	2.94	0.60
1:C:360:MET:O	1:C:361:GLN:C	2.45	0.60
1:C:453:GLU:O	1:C:453:GLU:HG2	2.01	0.59
2:D:165:ASN:OD1	2:D:343:LEU:HG	2.03	0.59
1:A:307:GLU:HB3	1:A:425:LEU:HD21	1.85	0.59
1:A:348:ARG:HD2	6:A:100:HOH:O	2.02	0.59
1:C:357:MET:HE2	1:C:362:MET:HE1	1.83	0.59
2:B:117:LEU:HD22	2:B:260:VAL:HG12	1.85	0.58
1:C:236:LEU:HD22	1:C:365:THR:OG1	2.03	0.58
1:C:384:SER:C	1:C:386:PRO:HD3	2.27	0.58
1:C:320:VAL:HG11	1:C:325:LEU:HD21	1.83	0.58
1:A:342:VAL:HG12	1:A:435:HIS:CD2	2.39	0.58
2:B:167:PHE:HA	2:B:170:LEU:HD12	1.83	0.58
2:B:181:VAL:O	2:B:184:SER:HB3	2.02	0.58
1:C:350:LEU:HA	1:C:354:VAL:HB	1.85	0.58
2:D:186:PRO:HG2	2:D:189:ASP:CG	2.27	0.58
2:B:120:ALA:HB2	2:B:178:ASP:HB3	1.84	0.58
2:B:124:HIS:CD2	2:B:174:LYS:HD3	2.38	0.58
1:A:257:ASN:HD21	1:A:260:SER:HB3	1.68	0.58
2:B:226:ILE:HG22	2:B:227:GLU:OE2	2.04	0.58
1:C:230:MET:HG2	1:C:396:VAL:HG22	1.85	0.58
1:C:313:PHE:CD2	4:C:1001:F15:H22	2.38	0.58
1:A:378:PRO:HB3	1:A:390:GLU:HB2	1.86	0.57
2:B:296:ILE:HD12	2:B:309:TYR:HB2	1.86	0.57
1:C:440:LYS:HE3	1:C:452:MET:CE	2.33	0.57
2:B:117:LEU:HB3	2:B:260:VAL:CG1	2.35	0.57
2:B:145:HIS:O	2:B:146:GLN:HB2	2.05	0.57
1:C:236:LEU:HD22	1:C:365:THR:HG23	1.86	0.57
2:D:200:GLU:O	2:D:204:ILE:HG13	2.05	0.57
2:D:186:PRO:HG2	2:D:189:ASP:HB2	1.85	0.57
1:A:407:LYS:HG2	1:A:408:TYR:CE2	2.40	0.56
2:D:177:LYS:HA	2:D:183:ARG:HD3	1.87	0.56
2:B:179:LEU:O	2:B:183:ARG:HG2	2.05	0.56
1:C:268:ILE:HG21	4:C:1001:F15:H6	1.87	0.56
1:C:275:GLN:HA	1:C:278:THR:OG1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:SER:HA	1:A:325:LEU:HD12	1.86	0.56
1:A:366:GLU:HB3	1:A:418:LEU:CD2	2.35	0.56
2:B:129:PHE:CE2	2:B:206:LEU:HA	2.40	0.56
2:D:201:ILE:O	2:D:205:VAL:HG23	2.05	0.56
1:A:425:LEU:O	1:A:425:LEU:HG	2.05	0.56
2:B:124:HIS:HD2	2:B:174:LYS:HD3	1.71	0.56
2:B:316:LEU:O	2:B:320:ARG:HG2	2.06	0.56
2:D:216:ASN:CG	2:D:225:THR:HG22	2.31	0.56
1:A:231:PRO:CG	1:A:234:ARG:HD2	2.36	0.56
1:C:413:GLY:O	1:C:417:LYS:HB2	2.06	0.56
1:A:289:PHE:HD1	1:A:376:PHE:CE1	2.24	0.56
1:C:428:ILE:HG13	6:D:1008:HOH:O	2.06	0.56
2:B:200:GLU:O	2:B:204:ILE:HG13	2.05	0.55
2:B:292:LEU:HD23	2:B:292:LEU:C	2.30	0.55
1:A:306:ASN:HD21	1:A:429:GLY:C	2.15	0.55
2:D:307:PHE:O	2:D:311:LYS:HG3	2.07	0.55
2:D:124:HIS:CD2	2:D:174:LYS:HB3	2.41	0.55
1:A:385:ASN:CG	1:A:388:GLU:HB2	2.31	0.55
2:D:191:ILE:HD11	3:H:691:HIS:HD2	1.71	0.55
1:C:288:HIS:HA	1:C:291:GLU:OE1	2.06	0.54
2:D:249:LEU:HD12	2:D:249:LEU:O	2.07	0.54
2:B:197:ALA:O	2:B:201:ILE:HG13	2.07	0.54
1:C:230:MET:HB3	1:C:399:SER:OG	2.06	0.54
1:A:452:MET:O	1:A:455:LEU:HD23	2.07	0.54
1:C:236:LEU:HD22	1:C:365:THR:CG2	2.38	0.54
1:A:255:GLY:CA	1:A:264:PRO:HD2	2.36	0.54
2:D:124:HIS:CD2	2:D:174:LYS:HD3	2.41	0.54
1:A:258:PRO:HA	1:A:263:ASP:OD1	2.07	0.54
2:B:200:GLU:HG3	2:B:323:ASN:HD22	1.73	0.53
2:B:299:GLN:O	2:B:299:GLN:HG3	2.09	0.53
1:C:307:GLU:HG2	1:C:425:LEU:HG	1.89	0.53
1:A:230:MET:SD	1:A:287:PRO:CG	2.97	0.53
1:A:298:VAL:HG13	3:E:633:LEU:HD23	1.90	0.53
1:A:424:ALA:O	1:A:428:ILE:HG13	2.08	0.53
2:D:186:PRO:O	2:D:190:GLN:HG3	2.09	0.53
1:A:370:LEU:HD21	1:A:419:LEU:HD23	1.89	0.53
2:B:125:MET:HA	2:B:128:MET:HG2	1.91	0.53
2:B:292:LEU:HD23	2:B:292:LEU:O	2.08	0.53
2:B:169:VAL:CG2	2:B:343:LEU:HD21	2.37	0.53
1:C:422:LEU:HB2	1:C:423:PRO:HD3	1.89	0.53
2:B:302:ARG:HD2	2:B:302:ARG:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:HIS:CD2	2:B:125:MET:HE3	2.44	0.52
3:F:689:ILE:HG13	3:F:692:ARG:CZ	2.39	0.52
1:A:280:VAL:O	1:A:283:ALA:HB3	2.10	0.52
1:C:230:MET:HG3	1:C:235:ILE:HD11	1.92	0.52
1:A:455:LEU:C	1:A:456:GLU:HG2	2.34	0.52
1:C:363:ASP:OD1	1:C:366:GLU:HG3	2.09	0.52
1:C:279:LEU:HD21	1:C:308:LEU:HD12	1.92	0.52
2:D:197:ALA:HB1	2:D:201:ILE:HD11	1.92	0.52
1:C:305:TRP:CD1	1:C:454:MET:HE3	2.44	0.52
2:D:128:MET:CE	2:D:168:MET:HG2	2.39	0.52
2:D:181:VAL:HG11	2:D:284:LEU:HD22	1.91	0.52
2:B:261:LEU:HD13	2:B:292:LEU:HA	1.92	0.51
1:C:276:LEU:HB3	1:C:450:PHE:HD2	1.68	0.51
1:C:267:ASN:ND2	1:C:330:LEU:HD22	2.25	0.51
2:B:114:ILE:O	2:B:118:LEU:HD13	2.10	0.51
2:B:345:GLU:OE1	3:F:689:ILE:HG22	2.10	0.51
3:H:691:HIS:O	3:H:695:GLN:HG2	2.11	0.51
1:A:276:LEU:CD2	1:A:451:LEU:HA	2.39	0.51
1:A:440:LYS:HE3	1:A:452:MET:HE2	1.93	0.51
1:C:240:LEU:C	1:C:242:VAL:H	2.18	0.51
2:D:280:GLU:O	2:D:284:LEU:HG	2.10	0.51
2:B:190:GLN:O	2:B:194:LEU:CD2	2.59	0.51
2:D:106:LEU:HB3	2:D:111:GLU:CD	2.35	0.51
1:A:253:ASN:H	1:A:262:ASN:CB	2.23	0.51
2:B:206:LEU:HG	2:B:217:PHE:CE2	2.46	0.51
2:B:128:MET:HE1	2:B:168:MET:HG2	1.92	0.51
2:B:261:LEU:HD13	2:B:292:LEU:CA	2.40	0.51
1:C:287:PRO:O	1:C:288:HIS:HB2	2.10	0.51
2:B:133:VAL:HG11	2:B:221:PRO:HG2	1.93	0.50
1:C:453:GLU:OE1	3:G:632:ILE:HB	2.11	0.50
1:C:338:HIS:HE1	1:C:347:ASP:OD1	1.94	0.50
2:D:144:HIS:HB2	2:D:223:ARG:HD2	1.93	0.50
2:B:236:VAL:HG13	2:B:237:GLU:HG3	1.92	0.50
1:C:462:THR:HG23	2:D:235:GLN:CD	2.36	0.50
2:D:173:ILE:HD13	3:H:693:LEU:HD12	1.93	0.50
2:D:226:ILE:HG22	6:D:1016:HOH:O	2.11	0.50
3:H:685:GLU:O	3:H:685:GLU:HG3	2.11	0.50
1:A:350:LEU:HA	1:A:354:VAL:HB	1.93	0.50
2:B:176:THR:HB	2:B:182:PHE:CD2	2.47	0.50
2:D:284:LEU:O	2:D:288:MET:HG2	2.11	0.50
1:A:426:ARG:HG2	2:B:317:ALA:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:129:PHE:HE2	2:D:206:LEU:HD13	1.76	0.50
2:D:182:PHE:CE2	2:D:190:GLN:HB3	2.47	0.50
1:A:259:SER:HB3	3:H:685:GLU:CD	2.37	0.50
1:C:252:ALA:HB2	1:C:330:LEU:HD21	1.94	0.50
1:A:282:TRP:O	1:A:286:ILE:HG12	2.12	0.49
1:C:353:LEU:O	1:C:357:MET:HG3	2.12	0.49
2:D:216:ASN:HB3	2:D:224:TYR:O	2.11	0.49
2:B:345:GLU:OE2	3:F:690:LEU:HG	2.12	0.49
2:D:182:PHE:HE1	2:D:267:LEU:HD11	1.77	0.49
2:B:103:PRO:N	2:B:298:GLY:HA2	2.27	0.49
1:C:230:MET:HE1	1:C:392:LEU:HD22	1.93	0.49
1:C:301:LEU:HD12	3:G:633:LEU:HD11	1.95	0.49
1:C:315:HIS:O	1:C:318:ILE:HG13	2.12	0.49
1:C:427:SER:HA	1:C:430:LEU:HD12	1.92	0.49
2:D:233:GLY:C	2:D:333:ILE:HD11	2.37	0.49
1:C:257:ASN:CG	1:C:257:ASN:O	2.56	0.49
1:C:307:GLU:OE2	1:C:426:ARG:HA	2.12	0.49
2:D:199:VAL:HB	2:D:323:ASN:ND2	2.28	0.49
4:A:1002:F15:H6	4:A:1002:F15:H9	1.95	0.49
2:D:186:PRO:HG2	2:D:189:ASP:CB	2.42	0.49
2:B:106:LEU:HA	2:B:110:GLN:OE1	2.13	0.49
2:B:248:THR:HG22	2:B:315:LEU:HD11	1.95	0.49
1:C:258:PRO:HA	1:C:263:ASP:OD2	2.12	0.49
2:B:106:LEU:HD23	2:B:110:GLN:OE1	2.12	0.49
2:B:187:ILE:O	2:B:191:ILE:HG13	2.13	0.49
2:D:315:LEU:O	2:D:318:GLU:HB2	2.13	0.49
1:A:314:SER:O	1:A:354:VAL:HG22	2.12	0.48
1:A:430:LEU:HD11	2:B:321:SER:HA	1.94	0.48
2:D:301:ARG:C	2:D:303:PRO:CD	2.86	0.48
1:A:370:LEU:HD11	1:A:418:LEU:O	2.13	0.48
1:A:397:TYR:HB3	2:B:307:PHE:CE2	2.49	0.48
1:A:407:LYS:O	1:A:407:LYS:HG3	2.13	0.48
2:D:200:GLU:HG2	2:D:319:LEU:O	2.13	0.48
2:D:132:PHE:HE1	2:D:167:PHE:HD2	1.61	0.48
2:D:261:LEU:HD13	2:D:292:LEU:CA	2.42	0.48
1:C:318:ILE:HG23	1:C:358:ARG:CB	2.43	0.48
2:B:252:LEU:HB3	2:B:308:LEU:HD11	1.96	0.48
2:B:292:LEU:HD23	2:B:296:ILE:HG13	1.95	0.48
1:C:294:LEU:O	1:C:297:GLN:HB2	2.14	0.48
2:B:228:ASP:O	2:B:232:VAL:HG23	2.12	0.48
2:D:289:ALA:O	2:D:293:GLN:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:336:LEU:HA	2:D:339:MET:HE3	1.96	0.48
1:A:276:LEU:HD22	1:A:451:LEU:HA	1.95	0.48
1:A:385:ASN:OD1	1:A:388:GLU:HB2	2.14	0.48
2:B:124:HIS:CD2	2:B:174:LYS:HB3	2.49	0.48
1:C:423:PRO:O	1:C:426:ARG:HB3	2.14	0.48
1:A:411:GLN:CG	1:A:414:ARG:HB2	2.35	0.48
1:A:440:LYS:HG3	1:A:452:MET:HE1	1.95	0.48
2:B:278:ARG:O	2:B:278:ARG:HG2	2.13	0.48
1:C:438:PHE:CD1	1:C:442:ILE:HD12	2.48	0.48
1:A:295:ASP:O	1:A:299:ILE:HG13	2.14	0.47
1:A:438:PHE:CG	1:C:442:ILE:HD11	2.49	0.47
1:A:360:MET:HE1	1:A:418:LEU:HG	1.96	0.47
2:B:133:VAL:O	2:B:137:PRO:HD3	2.15	0.47
1:C:236:LEU:CB	1:C:365:THR:HG23	2.33	0.47
2:D:207:ASN:OD1	2:D:249:LEU:HG	2.14	0.47
2:D:228:ASP:O	2:D:232:VAL:HG23	2.14	0.47
1:A:372:ALA:O	1:A:375:LEU:HB3	2.13	0.47
1:C:236:LEU:HD13	1:C:365:THR:HA	1.96	0.47
1:A:263:ASP:O	1:A:264:PRO:C	2.57	0.47
1:C:411:GLN:HA	1:C:412:PRO:HD3	1.53	0.47
2:D:242:LEU:HD12	2:D:242:LEU:O	2.15	0.47
1:C:315:HIS:CD2	1:C:362:MET:HE2	2.49	0.47
2:D:132:PHE:HE1	2:D:167:PHE:CD2	2.33	0.47
2:D:158:VAL:HG12	2:D:339:MET:HE1	1.97	0.47
2:B:151:LEU:N	2:B:151:LEU:HD22	2.30	0.47
1:C:310:ILE:CD1	1:C:429:GLY:HA2	2.44	0.47
2:D:133:VAL:HG12	2:D:222:LEU:HD11	1.97	0.47
1:A:453:GLU:OE2	3:E:630:HIS:HB3	2.15	0.47
1:C:296:ASP:CG	1:C:384:SER:HG	2.23	0.47
2:B:196:GLY:HA3	2:B:272:ARG:HD2	1.96	0.47
1:C:313:PHE:CD1	1:C:313:PHE:C	2.92	0.47
2:D:253:GLN:O	2:D:254:LEU:C	2.57	0.47
2:B:148:LEU:HB3	2:B:231:ARG:NH1	2.30	0.47
1:A:334:ARG:HE	1:C:256:LEU:HD22	1.80	0.46
2:D:256:GLU:O	2:D:260:VAL:HG23	2.15	0.46
1:A:313:PHE:HE2	4:A:1002:F15:H26	1.80	0.46
2:B:128:MET:CE	2:B:168:MET:HG2	2.46	0.46
1:C:272:ALA:HB2	4:C:1001:F15:H26	1.97	0.46
2:D:172:VAL:HG21	2:D:202:CYS:SG	2.56	0.46
2:D:292:LEU:HD22	2:D:309:TYR:CD1	2.50	0.46
2:B:225:THR:O	2:B:228:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:204:ILE:HD12	2:D:263:ALA:HA	1.97	0.46
2:D:296:ILE:CD1	2:D:309:TYR:HB2	2.45	0.46
1:C:459:HIS:NE2	1:C:460:GLN:HG3	2.30	0.46
3:E:638:GLN:O	3:E:639:GLU:O	2.34	0.46
3:G:635:ARG:HH21	3:G:636:LEU:HD11	1.79	0.46
2:B:265:MET:HE1	2:B:313:LEU:HD21	1.97	0.46
1:C:462:THR:HG23	2:D:235:GLN:OE1	2.16	0.46
2:D:204:ILE:CD1	2:D:263:ALA:HA	2.46	0.46
2:B:110:GLN:HB3	2:B:291:THR:HG23	1.97	0.46
2:B:133:VAL:HA	2:B:137:PRO:HG3	1.97	0.46
2:B:150:THR:HB	2:B:151:LEU:HD22	1.97	0.46
2:B:160:HIS:O	2:B:161:PHE:C	2.59	0.46
2:B:200:GLU:HG3	2:B:323:ASN:ND2	2.31	0.46
1:C:348:ARG:HD2	6:C:4:HOH:O	2.15	0.46
2:D:158:VAL:HG22	2:D:232:VAL:HG13	1.98	0.46
2:D:211:CYS:HB3	2:D:214:THR:OG1	2.16	0.46
1:A:394:GLU:OE2	2:B:311:LYS:HE3	2.16	0.45
2:B:119:GLY:O	2:B:123:ARG:HG3	2.16	0.45
2:D:256:GLU:HB3	2:D:257:PRO:CD	2.46	0.45
1:A:365:THR:HG22	1:A:366:GLU:N	2.31	0.45
1:C:257:ASN:HD21	1:C:260:SER:HB3	1.81	0.45
2:D:323:ASN:HB3	6:D:1018:HOH:O	2.17	0.45
1:A:230:MET:HE2	1:A:395:LYS:HB2	1.98	0.45
2:B:252:LEU:O	2:B:253:GLN:C	2.59	0.45
1:C:313:PHE:HE1	1:C:349:VAL:HG11	1.81	0.45
1:C:284:LYS:C	1:C:286:ILE:H	2.25	0.45
1:C:334:ARG:NH2	1:C:350:LEU:HD12	2.32	0.45
2:B:186:PRO:O	2:B:190:GLN:HG3	2.17	0.45
1:C:252:ALA:HA	1:C:330:LEU:HD11	1.98	0.45
1:C:283:ALA:O	1:C:286:ILE:HB	2.16	0.45
1:C:322:ASP:HA	1:C:350:LEU:CD1	2.47	0.45
1:C:440:LYS:HE3	1:C:452:MET:HE1	1.98	0.45
2:D:113:LEU:HD23	2:D:291:THR:CG2	2.40	0.45
1:A:426:ARG:HH11	2:B:321:SER:HB2	1.82	0.44
2:B:124:HIS:HE1	2:B:178:ASP:OD2	1.99	0.44
1:C:412:PRO:HB2	6:C:93:HOH:O	2.15	0.44
2:B:106:LEU:O	2:B:107:SER:O	2.35	0.44
2:B:216:ASN:ND2	2:B:225:THR:HG22	2.32	0.44
1:C:294:LEU:HA	1:C:297:GLN:HE21	1.82	0.44
2:D:125:MET:C	2:D:127:THR:H	2.25	0.44
1:A:432:CYS:HB3	4:A:1002:F15:H5	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:VAL:HG23	6:B:68:HOH:O	2.18	0.44
2:B:307:PHE:O	2:B:311:LYS:HG3	2.17	0.44
2:B:211:CYS:HB2	2:B:218:LEU:HD11	2.00	0.44
1:C:255:GLY:HA2	1:C:263:ASP:OD2	2.17	0.44
1:C:360:MET:HE1	1:C:418:LEU:HD12	1.99	0.44
2:D:326:TYR:CE1	5:D:1003[B]:CID:N4	2.86	0.44
2:B:201:ILE:O	2:B:205:VAL:HG23	2.17	0.44
2:B:290:LEU:HD23	2:B:293:GLN:NE2	2.32	0.44
1:A:337:ALA:HB2	1:A:346:PHE:CD2	2.52	0.44
1:A:414:ARG:HG2	1:A:418:LEU:HD11	2.00	0.44
1:C:252:ALA:CB	1:C:330:LEU:HD21	2.48	0.44
2:D:285:GLN:HE21	2:D:285:GLN:HB3	1.59	0.44
1:A:263:ASP:C	1:A:263:ASP:OD2	2.59	0.44
2:B:286:GLU:O	2:B:290:LEU:HG	2.17	0.44
1:C:460:GLN:HE21	1:C:460:GLN:HB2	1.64	0.44
2:D:133:VAL:HA	2:D:137:PRO:HG3	2.00	0.44
2:B:265:MET:HE3	2:B:289:ALA:HB2	2.00	0.44
2:B:216:ASN:CG	2:B:225:THR:HG22	2.43	0.43
1:C:301:LEU:CD1	3:G:633:LEU:HD11	2.48	0.43
2:B:133:VAL:O	2:B:137:PRO:CD	2.67	0.43
2:B:261:LEU:HD13	2:B:292:LEU:HB2	1.99	0.43
1:C:288:HIS:O	1:C:291:GLU:HB2	2.18	0.43
1:C:422:LEU:HA	1:C:422:LEU:HD23	1.68	0.43
1:C:427:SER:HG	2:D:320:ARG:HD3	1.82	0.43
1:A:362:MET:HE3	1:A:367:LEU:CA	2.48	0.43
2:D:119:GLY:O	2:D:123:ARG:HG3	2.18	0.43
1:C:313:PHE:HD2	4:C:1001:F15:C4	2.32	0.43
2:D:319:LEU:O	2:D:323:ASN:HB2	2.18	0.43
2:B:120:ALA:CB	2:B:178:ASP:HB3	2.49	0.43
1:C:440:LYS:HB2	1:C:447:ILE:HD11	1.99	0.43
1:A:318:ILE:O	1:A:318:ILE:HG22	2.19	0.43
2:B:137:PRO:O	2:B:138:PRO:C	2.61	0.43
2:D:261:LEU:CD1	2:D:292:LEU:HA	2.46	0.43
2:B:145:HIS:O	2:B:146:GLN:CB	2.67	0.42
3:E:632:ILE:H	3:E:632:ILE:HG13	1.60	0.42
1:A:356:LYS:HE2	2:B:278:ARG:HH22	1.84	0.42
2:B:128:MET:HE1	2:B:168:MET:CG	2.49	0.42
1:C:240:LEU:HD22	1:C:243:GLU:OE2	2.19	0.42
1:C:274:LYS:HG2	1:C:275:GLN:HE21	1.83	0.42
1:A:257:ASN:HA	1:A:258:PRO:HD3	1.82	0.42
2:B:314:GLY:O	2:B:318:GLU:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:340:MET:HG3	2:B:343:LEU:HB2	2.01	0.42
1:C:338:HIS:CE1	1:C:347:ASP:OD1	2.73	0.42
1:C:361:GLN:HE21	1:C:361:GLN:HB3	1.69	0.42
1:C:310:ILE:HA	1:C:313:PHE:CE2	2.54	0.42
2:D:117:LEU:CD1	2:D:261:LEU:HD23	2.50	0.42
2:B:161:PHE:O	2:B:162:ALA:C	2.62	0.42
2:B:292:LEU:C	2:B:292:LEU:CD2	2.92	0.42
2:D:187:ILE:HA	2:D:190:GLN:HE21	1.83	0.42
2:D:301:ARG:O	2:D:303:PRO:HD2	2.20	0.42
1:A:402:ALA:O	1:A:406:HIS:HB3	2.20	0.42
2:B:236:VAL:HA	2:B:239:LEU:HD12	2.01	0.42
2:B:261:LEU:CD1	2:B:292:LEU:HA	2.49	0.42
2:B:313:LEU:HD23	2:B:316:LEU:HD12	2.02	0.42
1:C:236:LEU:HD13	1:C:365:THR:CA	2.49	0.42
2:D:176:THR:HA	2:D:179:LEU:HD12	2.02	0.42
2:B:255:GLN:HB2	2:B:258:GLU:OE1	2.20	0.42
2:B:261:LEU:HD13	2:B:292:LEU:CB	2.50	0.42
1:C:286:ILE:HG23	1:C:287:PRO:HD2	2.02	0.42
1:A:350:LEU:O	1:A:355:SER:CB	2.67	0.42
2:B:103:PRO:HA	2:B:298:GLY:CA	2.44	0.42
2:B:133:VAL:HG12	2:B:222:LEU:HG	2.02	0.42
1:C:420:LEU:HD21	2:D:285:GLN:OE1	2.20	0.42
2:D:155:LEU:HB3	2:D:156:PRO:HD3	2.02	0.42
2:D:171:GLN:NE2	2:D:174:LYS:HD2	2.35	0.42
2:B:150:THR:HG22	2:B:151:LEU:HD13	2.02	0.41
2:D:161:PHE:O	2:D:165:ASN:CB	2.66	0.41
2:D:249:LEU:HD12	2:D:249:LEU:C	2.45	0.41
2:B:329:GLN:C	2:B:331:GLN:H	2.28	0.41
2:B:148:LEU:O	2:B:149:PRO:C	2.63	0.41
2:D:121:HIS:HB2	2:D:175:PHE:CE1	2.56	0.41
2:D:214:THR:O	2:D:215:GLN:CB	2.68	0.41
1:A:313:PHE:CD1	1:A:313:PHE:C	2.98	0.41
1:A:378:PRO:CD	1:A:393:ARG:HD3	2.42	0.41
2:B:125:MET:C	2:B:127:THR:H	2.27	0.41
2:B:161:PHE:HE1	2:B:234:PHE:CZ	2.39	0.41
1:C:459:HIS:CE1	1:C:460:GLN:HG3	2.56	0.41
1:C:462:THR:CG2	2:D:235:GLN:OE1	2.68	0.41
1:A:307:GLU:HB3	1:A:425:LEU:CD2	2.48	0.41
1:A:333:HIS:CD2	1:A:335:ASN:H	2.38	0.41
2:B:129:PHE:CE2	2:B:206:LEU:HD12	2.56	0.41
1:C:227:ASN:O	1:C:231:PRO:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:ILE:HG23	1:C:358:ARG:HD3	2.03	0.41
1:A:420:LEU:HG	1:A:420:LEU:O	2.19	0.41
2:B:157:LEU:O	2:B:160:HIS:HB3	2.20	0.41
1:C:239:GLU:HG2	1:C:282:TRP:HE1	1.86	0.41
1:C:342:VAL:HG12	1:C:435:HIS:CD2	2.55	0.41
1:C:343:GLY:O	1:C:344:ALA:C	2.62	0.41
1:A:426:ARG:O	1:A:430:LEU:HG	2.21	0.41
2:B:217:PHE:O	2:B:223:ARG:HA	2.20	0.41
1:C:334:ARG:HH21	1:C:350:LEU:HD12	1.85	0.41
1:C:377:ASN:HA	1:C:378:PRO:HD2	1.92	0.41
1:C:403:TYR:CD1	1:C:403:TYR:C	2.99	0.41
2:D:197:ALA:CB	2:D:267:LEU:HA	2.51	0.41
1:A:392:LEU:C	1:A:394:GLU:H	2.28	0.41
1:A:452:MET:HA	1:A:455:LEU:HD21	2.02	0.41
1:C:360:MET:CE	1:C:418:LEU:HD12	2.51	0.41
2:D:105:GLN:O	2:D:106:LEU:HG	2.20	0.41
2:D:215:GLN:O	2:D:243:PHE:HE2	2.04	0.41
1:A:320:VAL:HG13	1:A:325:LEU:HD11	2.03	0.40
2:B:199:VAL:HB	2:B:323:ASN:OD1	2.20	0.40
1:C:324:ILE:HG13	4:C:1001:F15:H12	2.04	0.40
2:D:242:LEU:O	2:D:245:PHE:HB3	2.20	0.40
1:A:276:LEU:HD12	1:A:276:LEU:HA	1.73	0.40
1:A:431:LYS:HD2	1:A:431:LYS:HA	1.93	0.40
1:C:236:LEU:O	1:C:240:LEU:HG	2.21	0.40
1:C:460:GLN:O	1:C:461:MET:C	2.63	0.40
2:D:235:GLN:O	2:D:239:LEU:HG	2.21	0.40
2:D:302:ARG:HD2	2:D:302:ARG:O	2.20	0.40
1:A:305:TRP:CD1	1:A:454:MET:HE3	2.56	0.40
1:A:313:PHE:CE2	4:A:1002:F15:H26	2.55	0.40
1:C:279:LEU:HD11	1:C:308:LEU:HD13	2.03	0.40
1:C:360:MET:O	1:C:360:MET:HG3	2.21	0.40
2:D:105:GLN:HB3	2:D:106:LEU:H	1.66	0.40
2:D:191:ILE:HD11	3:H:691:HIS:CD2	2.54	0.40
1:A:411:GLN:HA	1:A:412:PRO:HD3	1.64	0.40
1:C:440:LYS:CB	1:C:447:ILE:HD12	2.49	0.40
2:D:306:ARG:HG3	2:D:307:PHE:H	1.86	0.40
3:F:686:ARG:HG2	3:F:687:HIS:ND1	2.36	0.40
1:C:230:MET:HG2	1:C:396:VAL:CG2	2.52	0.40
2:D:271:ASP:O	2:D:272:ARG:C	2.65	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	230/236 (98%)	191 (83%)	31 (14%)	8 (4%)	3	4
1	C	234/236 (99%)	197 (84%)	30 (13%)	7 (3%)	3	6
2	B	244/246 (99%)	208 (85%)	28 (12%)	8 (3%)	3	5
2	D	244/246 (99%)	216 (88%)	27 (11%)	1 (0%)	30	51
3	E	8/13 (62%)	5 (62%)	2 (25%)	1 (12%)	0	0
3	F	10/13 (77%)	7 (70%)	2 (20%)	1 (10%)	0	0
3	G	10/13 (77%)	5 (50%)	5 (50%)	0	100	100
3	H	10/13 (77%)	8 (80%)	2 (20%)	0	100	100
All	All	990/1016 (97%)	837 (84%)	127 (13%)	26 (3%)	4	7

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	PRO
1	A	449	THR
2	B	107	SER
2	B	146	GLN
1	C	361	GLN
1	A	442	ILE
1	C	253	ASN
1	C	285	ARG
1	C	412	PRO
3	F	695	GLN
1	A	242	VAL
1	A	254	MET
1	A	304	GLY
2	B	255	GLN
1	C	327	ALA
3	E	631	LYS
1	A	285	ARG

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Mol	Chain	Res	Type
2	B	147	PRO
1	C	292	LEU
2	D	302	ARG
2	B	299	GLN
1	C	457	ALA
1	A	412	PRO
2	B	161	PHE
2	B	302	ARG
2	B	330	ILE

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	200/204 (98%)	190 (95%)	10 (5%)	22	46
1	C	204/204 (100%)	196 (96%)	8 (4%)	28	55
2	B	219/219 (100%)	207 (94%)	12 (6%)	19	41
2	D	219/219 (100%)	212 (97%)	7 (3%)	34	62
3	E	9/12 (75%)	9 (100%)	0	100	100
3	F	10/12 (83%)	10 (100%)	0	100	100
3	G	11/12 (92%)	10 (91%)	1 (9%)	9	19
3	H	11/12 (92%)	10 (91%)	1 (9%)	9	19
All	All	883/894 (99%)	844 (96%)	39 (4%)	25	50

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	264	PRO
1	A	276	LEU
1	A	296	ASP
1	A	309	LEU
1	A	312	SER

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Mol	Chain	Res	Type
1	A	326	LEU
1	A	365	THR
1	A	407	LYS
1	A	444	ASP
2	B	111	GLU
2	B	128	MET
2	B	151	LEU
2	B	155	LEU
2	B	166	THR
2	B	194	LEU
2	B	205	VAL
2	B	236	VAL
2	B	250	ARG
2	B	255	GLN
2	B	292	LEU
2	B	321	SER
1	C	229	ASP
1	C	342	VAL
1	C	355	SER
1	C	365	THR
1	C	410	GLU
1	C	418	LEU
1	C	431	LYS
1	C	455	LEU
2	D	146	GLN
2	D	154	VAL
2	D	236	VAL
2	D	249	LEU
2	D	285	GLN
2	D	321	SER
2	D	322	ILE
3	G	629	ARG
3	H	689	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	GLN
1	A	306	ASN
1	A	333	HIS
2	B	121	HIS
2	B	124	HIS

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Mol	Chain	Res	Type
2	B	171	GLN
2	B	215	GLN
2	B	216	ASN
2	B	244	HIS
2	B	255	GLN
2	B	277	GLN
2	B	285	GLN
2	B	344	GLN
1	C	267	ASN
1	C	270	GLN
1	C	275	GLN
1	C	297	GLN
1	C	361	GLN
1	C	377	ASN
1	C	460	GLN
2	D	121	HIS
2	D	124	HIS
2	D	145	HIS
2	D	171	GLN
2	D	190	GLN
2	D	215	GLN
2	D	244	HIS
2	D	323	ASN
2	D	331	GLN
3	E	630	HIS
3	E	634	HIS
3	F	691	HIS
3	H	691	HIS
3	H	695	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	CID	D	1003[B]	-	30,30,30	2.60	17 (56%)	37,42,42	2.38	3 (8%)
4	F15	C	1001	-	16,16,16	1.05	1 (6%)	16,16,16	0.85	0
4	F15	A	1002	-	16,16,16	1.73	3 (18%)	16,16,16	1.15	2 (12%)
5	CID	D	1003[A]	-	30,30,30	2.69	17 (56%)	37,42,42	2.42	4 (10%)

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
5	CID	D	1003[B]	-	-	3/11/11/11	0/4/4/4
4	F15	C	1001	-	-	7/14/14/14	-
4	F15	A	1002	-	-	9/14/14/14	-
5	CID	D	1003[A]	-	-	2/11/11/11	0/4/4/4

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1003[A]	CID	O16-N11	-6.04	1.31	1.41
5	D	1003[B]	CID	O16-N11	-5.90	1.31	1.41
4	A	1002	F15	C4-C1	4.66	1.61	1.50
5	D	1003[A]	CID	C2-C1	4.45	1.45	1.39
5	D	1003[A]	CID	C8-C3	3.82	1.45	1.39
5	D	1003[B]	CID	C8-C3	3.75	1.45	1.39
5	D	1003[B]	CID	C7-C3	3.70	1.45	1.39
5	D	1003[A]	CID	C21-C23	3.66	1.44	1.38
5	D	1003[A]	CID	C7-C3	3.62	1.44	1.39
5	D	1003[B]	CID	C21-C23	3.60	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1003[B]	CID	C7-C12	3.44	1.44	1.38
5	D	1003[A]	CID	C13-C8	3.43	1.44	1.38
5	D	1003[A]	CID	C7-C12	3.33	1.44	1.38
5	D	1003[B]	CID	C12-C17	3.29	1.44	1.38
5	D	1003[B]	CID	C2-C1	3.27	1.44	1.39
5	D	1003[A]	CID	C12-C17	3.25	1.44	1.38
5	D	1003[A]	CID	C13-C17	3.21	1.44	1.38
5	D	1003[B]	CID	C13-C8	3.20	1.44	1.38
5	D	1003[B]	CID	C13-C17	3.17	1.43	1.38
5	D	1003[A]	CID	C21-C20	3.10	1.44	1.39
5	D	1003[B]	CID	C22-C24	3.05	1.43	1.38
5	D	1003[B]	CID	C21-C20	3.04	1.44	1.39
5	D	1003[A]	CID	C22-C24	3.02	1.43	1.38
4	A	1002	F15	C5-C4	2.85	1.62	1.52
5	D	1003[A]	CID	C22-C20	2.84	1.44	1.38
5	D	1003[B]	CID	C22-C20	2.72	1.44	1.38
5	D	1003[A]	CID	C10-C2	2.65	1.51	1.44
5	D	1003[B]	CID	C24-C25	2.53	1.44	1.38
5	D	1003[A]	CID	C25-C23	2.52	1.44	1.39
5	D	1003[A]	CID	C24-C25	2.51	1.43	1.38
5	D	1003[B]	CID	C25-C23	2.44	1.44	1.39
5	D	1003[B]	CID	C2-N5	-2.41	1.37	1.40
5	D	1003[A]	CID	C15-S14	2.37	1.81	1.70
5	D	1003[B]	CID	C15-S14	2.34	1.80	1.70
4	C	1001	F15	O2-C1	-2.21	1.23	1.30
4	A	1002	F15	O2-C1	-2.10	1.23	1.30
5	D	1003[B]	CID	C9-N4	2.09	1.36	1.31
5	D	1003[A]	CID	C2-N5	-2.04	1.37	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1003[B]	CID	C18-O16-N11	11.70	125.40	108.08
5	D	1003[A]	CID	C18-O16-N11	9.54	122.21	108.08
5	D	1003[A]	CID	O16-N11-C10	8.67	121.29	110.23
5	D	1003[B]	CID	O16-N11-C10	6.12	118.04	110.23
5	D	1003[A]	CID	S14-C9-N5	4.55	114.19	110.55
5	D	1003[B]	CID	S14-C9-N5	3.63	113.46	110.55
4	A	1002	F15	O2-C1-C4	2.44	121.72	114.00
4	A	1002	F15	O2-C1-O3	-2.14	117.82	123.33
5	D	1003[A]	CID	C3-C1-C2	2.04	133.53	129.49

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1003[B]	CID	C20-C18-O16-N11
5	D	1003[B]	CID	N11-C10-C2-C1
4	A	1002	F15	C13-C2-C3-C14
4	A	1002	F15	C9-C10-C11-C12
4	A	1002	F15	C11-C10-C9-C7
4	A	1002	F15	C8-C6-C7-C9
4	C	1001	F15	C8-C6-C7-C9
4	C	1001	F15	C10-C11-C12-C13
4	C	1001	F15	C6-C7-C9-C10
4	C	1001	F15	C11-C12-C13-C2
4	A	1002	F15	C7-C6-C8-C5
4	A	1002	F15	C6-C7-C9-C10
5	D	1003[B]	CID	N11-C10-C2-N5
4	A	1002	F15	C11-C12-C13-C2
5	D	1003[A]	CID	N11-C10-C2-C1
4	A	1002	F15	C12-C13-C2-C3
4	C	1001	F15	O3-C1-C4-C5
4	C	1001	F15	C13-C2-C3-C14
4	C	1001	F15	O2-C1-C4-C5
4	A	1002	F15	C4-C5-C8-C6
5	D	1003[A]	CID	N11-C10-C2-N5

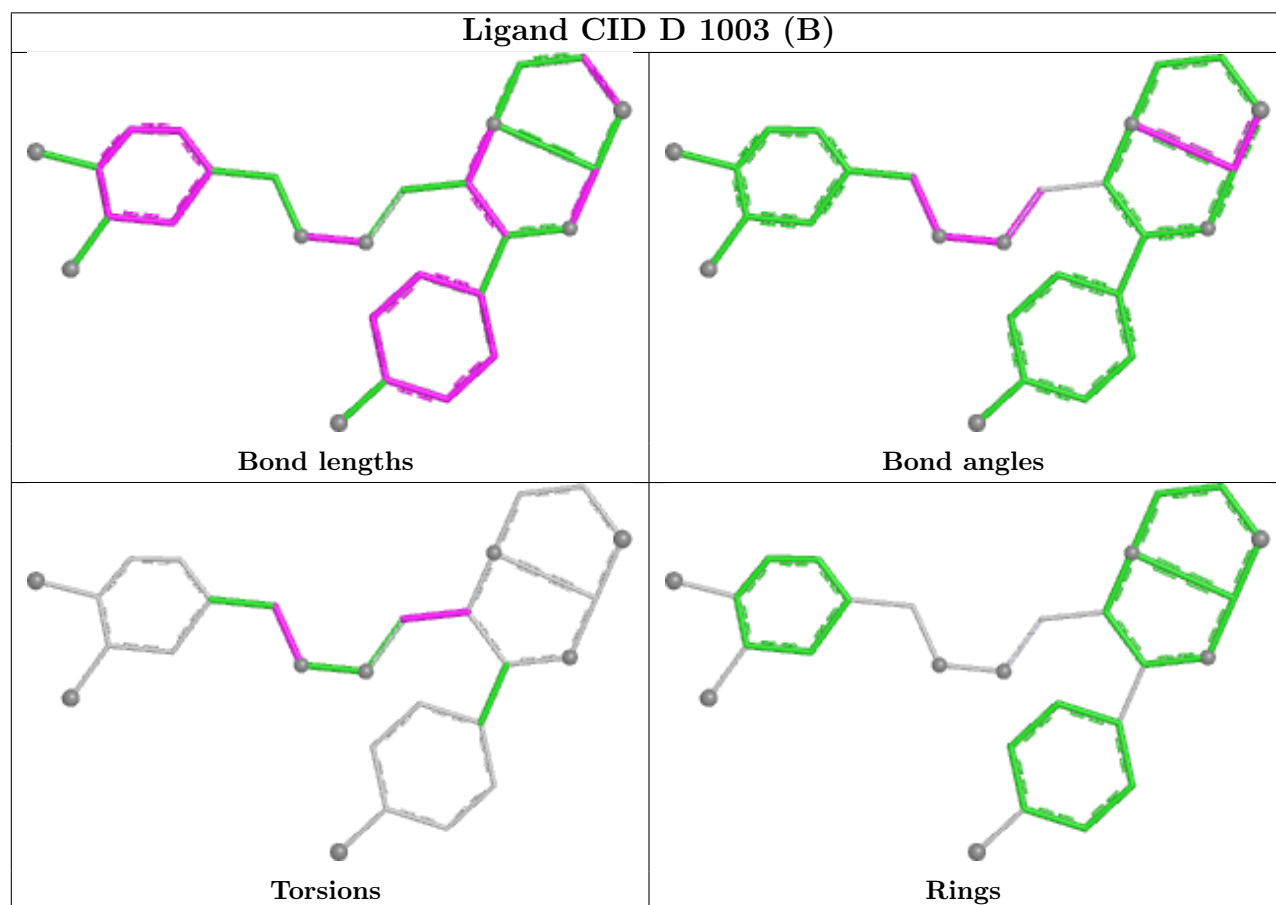
There are no ring outliers.

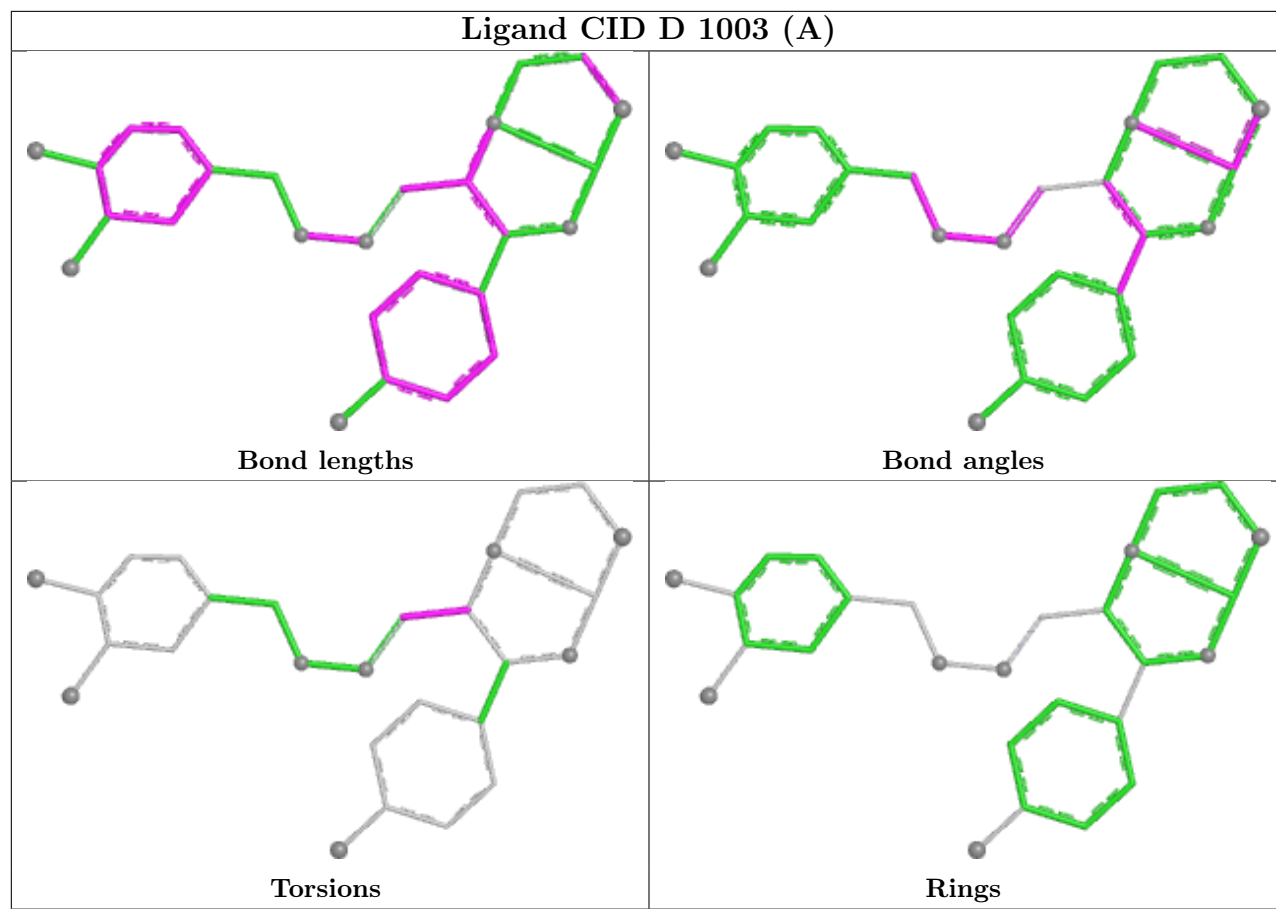
3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1003[B]	CID	2	0
4	C	1001	F15	7	0
4	A	1002	F15	6	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	232/236 (98%)	-1.07	0 100 100	43, 77, 131, 157	0
1	C	236/236 (100%)	-1.15	0 100 100	42, 76, 108, 152	0
2	B	246/246 (100%)	-1.12	0 100 100	51, 76, 134, 169	0
2	D	246/246 (100%)	-1.05	0 100 100	48, 77, 133, 176	0
3	E	10/13 (76%)	-0.84	0 100 100	113, 118, 123, 126	0
3	F	12/13 (92%)	-0.94	0 100 100	99, 109, 125, 127	0
3	G	12/13 (92%)	-0.89	0 100 100	111, 119, 122, 129	0
3	H	12/13 (92%)	-0.46	0 100 100	128, 131, 138, 140	0
All	All	1006/1016 (99%)	-1.08	0 100 100	42, 78, 133, 176	0

There are no RSRZ outliers to report.

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](#)

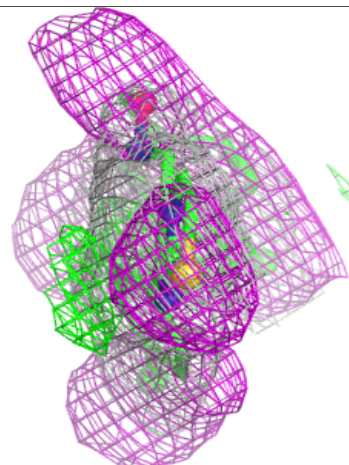
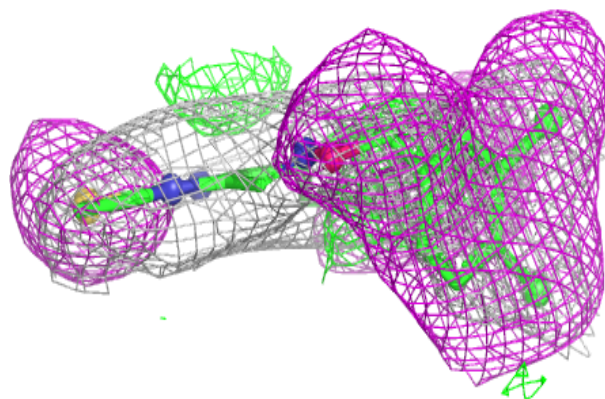
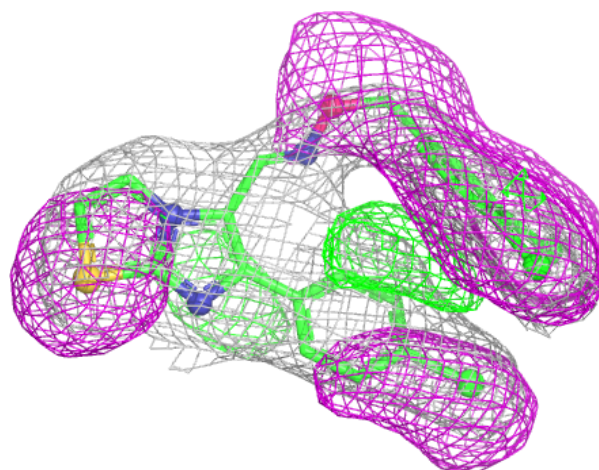
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
5	CID	D	1003[A]	27/27	0.94	0.09	0,0,0,0	27
5	CID	D	1003[B]	27/27	0.94	0.09	0,0,0,0	27
4	F15	A	1002	17/17	0.99	0.04	43,63,67,67	0
4	F15	C	1001	17/17	0.99	0.07	53,61,91,93	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.

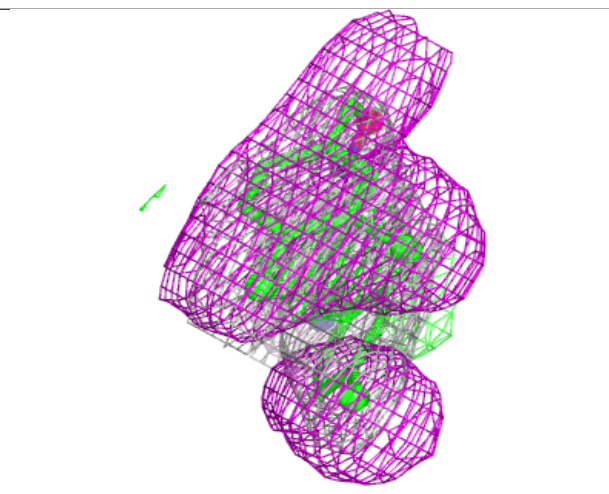
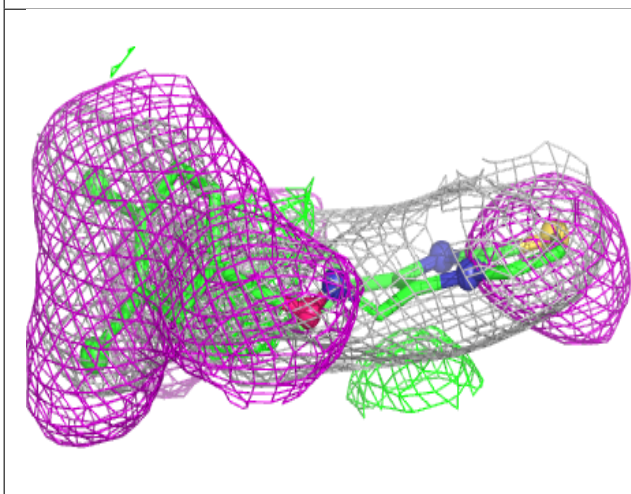
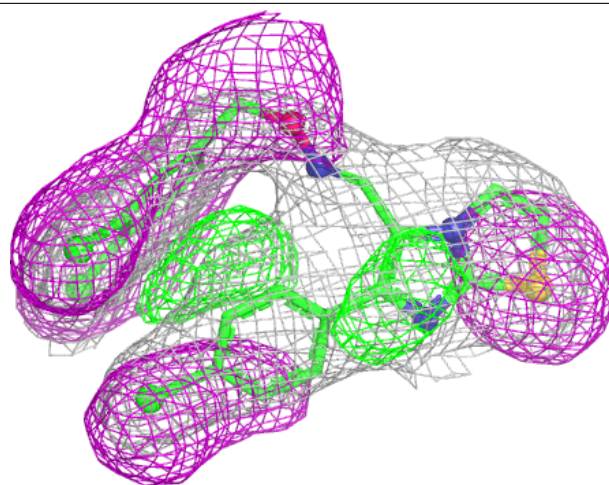
Electron density around CID D 1003 (A):

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



Electron density around CID D 1003 (B):

$2mF_o-DF_c$ (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.