



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 02:50 am BST

PDB ID : 1XVP
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

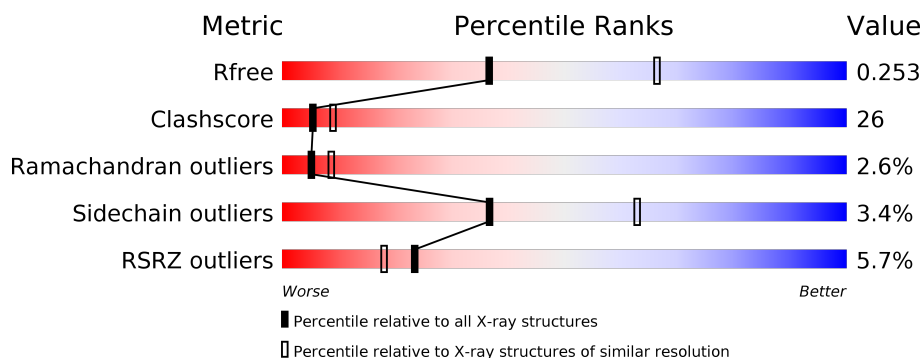
1 Overall quality at a glance

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on 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	<div> <div>6%</div> <div>49%</div> <div>47%</div> <div>• •</div> </div>
1	C	236	<div> <div>5%</div> <div>47%</div> <div>51%</div> <div>•</div> </div>
2	B	246	<div> <div>4%</div> <div>54%</div> <div>42%</div> <div>•</div> </div>
2	D	246	<div> <div>6%</div> <div>57%</div> <div>42%</div> <div>•</div> </div>
3	E	13	<div> <div>15%</div> <div>23%</div> <div>54%</div> <div>23%</div> </div>
3	F	13	<div> <div>15%</div> <div>38%</div> <div>46%</div> <div>8% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	13	<div><div></div><div>8%</div><div>46%</div><div>46%</div><div>8%</div></div>
3	H	13	<div><div></div><div>23%</div><div>54%</div><div>38%</div><div>8%</div></div>

2 Entry composition

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 NR1H3.

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.

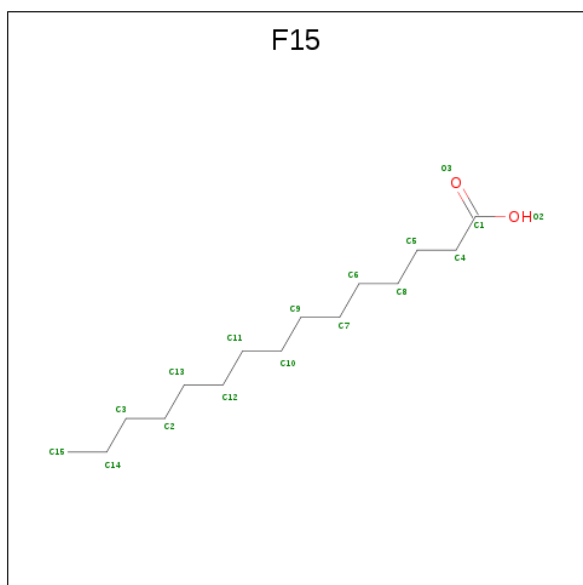
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	10	Total	C	N	O	0	0	0
			86	55	18	13			
3	F	12	Total	C	N	O	0	0	0
			102	63	23	16			

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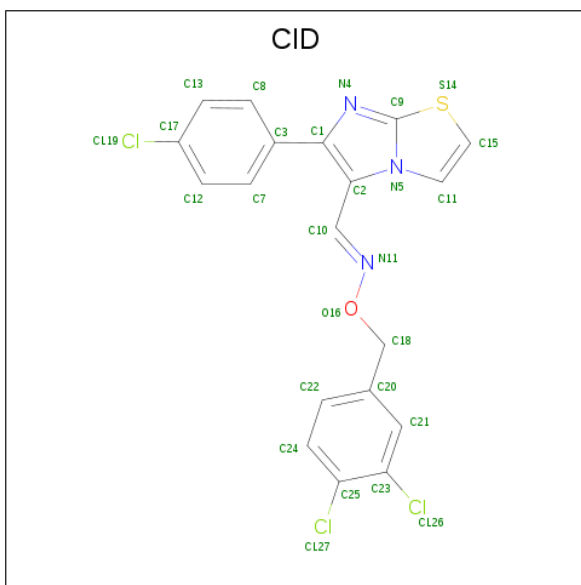
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	12	Total	C	N	O	0	0	0
			106	66	23	17			
3	H	12	Total	C	N	O	0	0	0
			106	66	23	17			

- Molecule 4 is PENTADECANOIC ACID (three-letter code: F15) (formula: C₁₅H₃₀O₂).



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 (three-letter code: CID) (formula: C₁₉H₁₂Cl₃N₃OS).



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

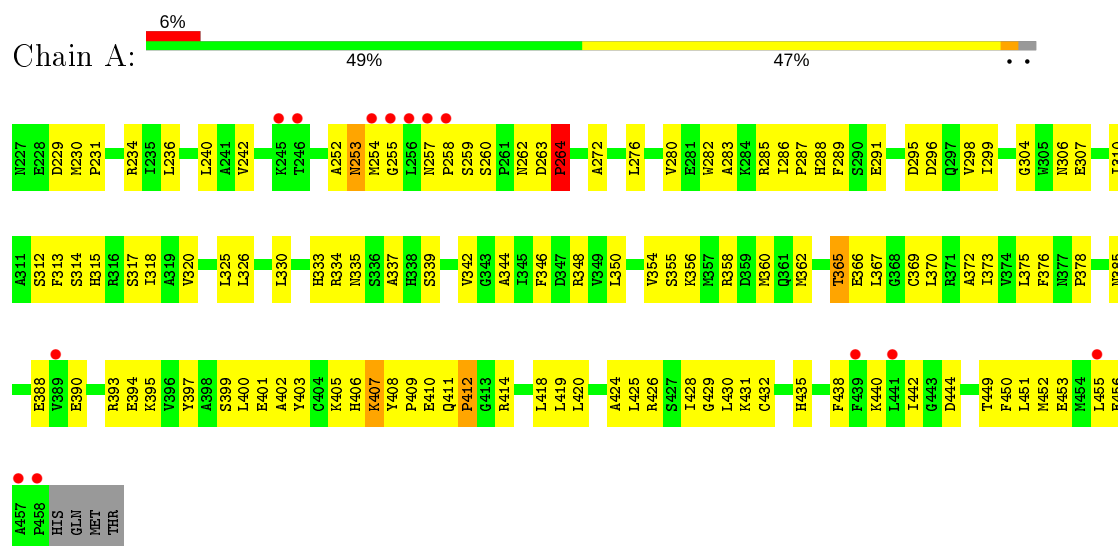
- Molecule 6 is water.

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

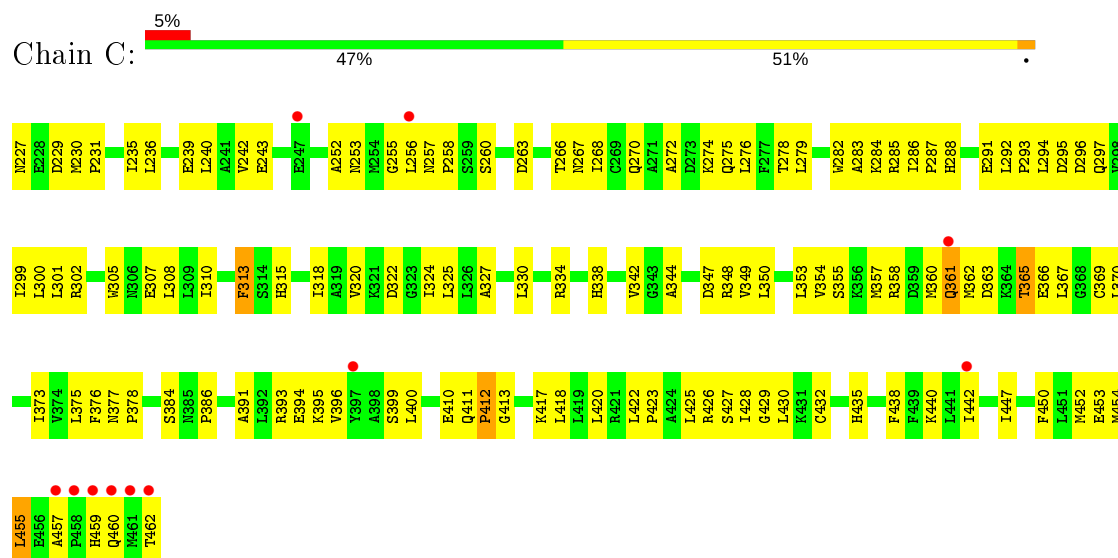
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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

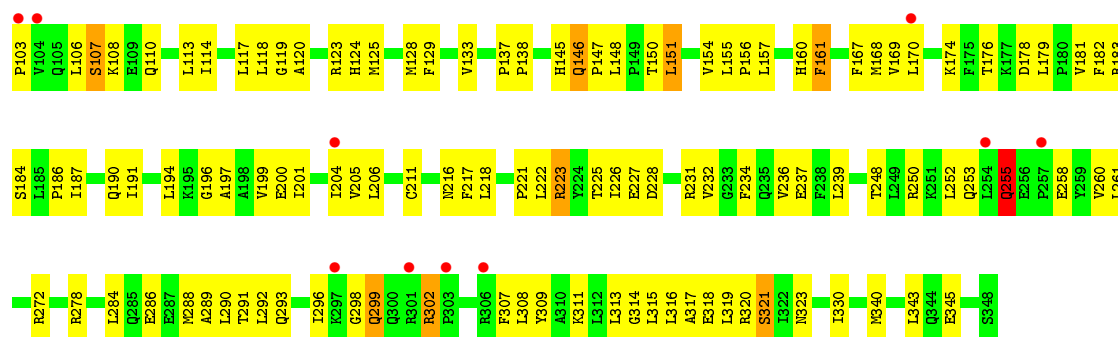


- Molecule 1: Retinoic acid receptor RXR-alpha

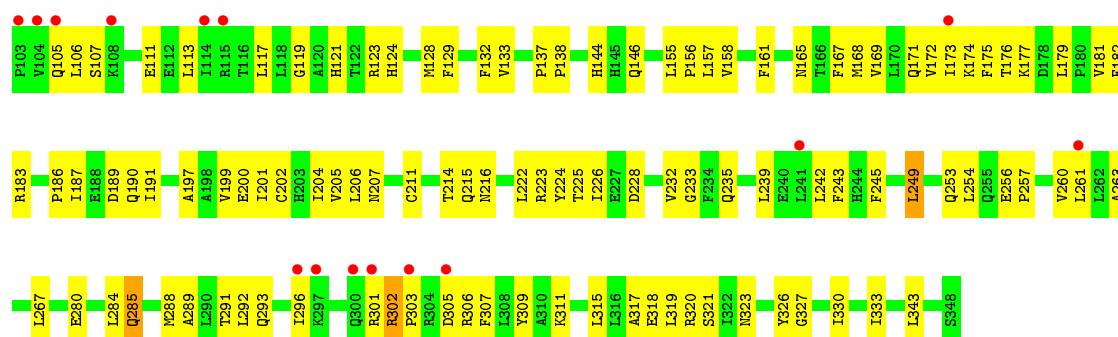


- Molecule 2: Orphan nuclear receptor NR1I3

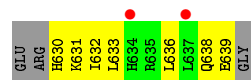




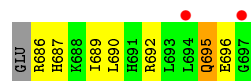
• Molecule 2: Orphan nuclear receptor NR1I3



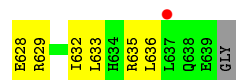
• Molecule 3: nuclear receptor coactivator 1 isoform 1



• Molecule 3: nuclear receptor coactivator 1 isoform 1

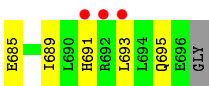


• Molecule 3: nuclear receptor coactivator 1 isoform 1



• Molecule 3: nuclear receptor coactivator 1 isoform 1





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 47.46 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.3 (50.00-2.60) 89.7 (47.46-2.60)	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)	0.31 , 55.6	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	0.95	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 [i](#)

5.1 Standard geometry [i](#)

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	0.38	0/1862	0.66	0/2523
1	C	0.41	0/1898	0.69	1/2570 (0.0%)
2	B	0.38	0/2036	0.64	0/2758
2	D	0.39	0/2036	0.66	0/2758
3	E	0.34	0/87	0.66	0/116
3	F	0.38	0/103	0.73	0/135
3	G	0.33	0/107	0.56	0/142
3	H	0.40	0/107	0.51	0/142
All	All	0.39	0/8236	0.66	1/11144 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	455	LEU	CA-CB-CG	5.30	127.49	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1824	0	1849	102	0
1	C	1859	0	1880	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1990	0	2023	107	0
2	D	1990	0	2023	99	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	428	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 26.

All (428) 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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:345:GLU:CD	3:F:689:ILE:HG22	2.10	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:362:MET:CE	1:C:367:LEU:HB2	2.21	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
2:B:155:LEU:HB3	2:B:156:PRO:HD3	1.76	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
1:C:362:MET:HE3	1:C:367:LEU:HB2	1.75	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	1:A:360:MET:O	1.99	0.61
2:D:169:VAL:O	2:D:173:ILE:HG13	2.00	0.61
2:B:179:LEU:HB2	2:B:182:PHE:HB3	1.82	0.60
2:B:117:LEU:HB3	2:B:260:VAL:HG11	1.81	0.60
1:A:360:MET:HE2	1:A:362:MET:HB2	1.82	0.60
2:D:182:PHE:CE1	2:D:267:LEU:HD11	2.36	0.60
2:B:176:THR:HA	2:B:179:LEU:HG	1.83	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
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:385:ASN:HB3	1:A:388:GLU:OE2	2.02	0.60
1:A:365:THR:HG21	1:A:403:TYR:CD2	2.36	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: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:348:ARG:HD2	6:A:100:HOH:O	2.02	0.59
1:A:307:GLU:HB3	1:A:425:LEU:HD21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:313:PHE:CD2	4:C:1001:F15:H22	2.38	0.58
1:C:230:MET:HG2	1:C:396:VAL:HG22	1.85	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
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:HG	1:A:425:LEU:O	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
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:D:307:PHE:O	2:D:311:LYS:HG3	2.07	0.55
1:C:360:MET:O	1:C:361:GLN:C	2.45	0.55
2:D:124:HIS:CD2	2:D:174:LYS:HB3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	2:D:249:LEU:HD12	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
1:C:384:SER:C	1:C:386:PRO:HD3	2.27	0.54
2:D:186:PRO:HG2	2:D:189:ASP:CG	2.27	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: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:298:VAL:HG13	3:E:633:LEU:HD23	1.90	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:O	2:B:292:LEU:HD23	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:O	2:B:302:ARG:HD2	2.09	0.53
1:A:440:LYS:HE3	1:A:452:MET:HE1	1.91	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: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
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:345:GLU:OE1	3:F:689:ILE:HG22	2.10	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:216:ASN:CG	2:D:225:THR:HG22	2.31	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
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:261:LEU:HD13	2:B:292:LEU:CA	2.40	0.51
2:B:292:LEU:C	2:B:292:LEU:HD23	2.30	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:A:306:ASN:HD21	1:A:429:GLY:C	2.15	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
1:A:360:MET:CE	1:A:362:MET:HB2	2.41	0.50
1:A:385:ASN:CG	1:A:388:GLU:HB2	2.31	0.50
2:B:236:VAL:HG13	2:B:237:GLU:HG3	1.92	0.50
2:D:226:ILE:HG22	6:D:1016:HOH:O	2.11	0.50
3:H:685:GLU:HG3	3:H:685:GLU:O	2.11	0.50
2:D:173:ILE:HD13	3:H:693:LEU:HD12	1.93	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
1:C:362:MET:HE1	1:C:367:LEU:HB2	1.94	0.50
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: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:HE2	1:C:395:LYS:HB2	1.94	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
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
1:A:362:MET:HE3	1:A:367:LEU:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:407:LYS:HG3	1:A:407:LYS:O	2.13	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
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:292:LEU:HD23	2:B:296:ILE:HG13	1.95	0.48
2:B:252:LEU:HB3	2:B:308:LEU:HD11	1.96	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
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
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
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:228:ASP:O	2:D:232:VAL:HG23	2.14	0.47
2:D:207:ASN:OD1	2:D:249:LEU:HG	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:455:LEU:C	1:A:456:GLU:HG2	2.34	0.47
1:C:240:LEU:C	1:C:242:VAL:H	2.18	0.47
1:C:302:ARG:HA	1:C:454:MET:HE3	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:132:PHE:HE1	2:D:167:PHE:CD2	2.33	0.47
2:B:151:LEU:HD22	2:B:151:LEU:N	2.30	0.47
2:D:133:VAL:HG12	2:D:222:LEU:HD11	1.97	0.47
1:C:310:ILE:CD1	1:C:429:GLY:HA2	2.44	0.47
1:A:453:GLU:OE2	3:E:630:HIS:HB3	2.15	0.47
2:B:196:GLY:HA3	2:B:272:ARG:HD2	1.96	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
1:C:315:HIS:HB2	1:C:357:MET:HE2	1.98	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:106:LEU:HB3	2:D:111:GLU:CD	2.35	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
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
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:133:VAL:HA	2:B:137:PRO:HG3	1.97	0.46
2:B:110:GLN:HB3	2:B:291:THR:HG23	1.97	0.46
2:B:150:THR:HB	2:B:151:LEU:HD22	1.97	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
1:C:462:THR:HG23	2:D:235:GLN:CD	2.36	0.45
2:D:211:CYS:HB3	2:D:214:THR:HG1	1.80	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:C:313:PHE:HE1	1:C:349:VAL:HG11	1.81	0.45
1:A:259:SER:HB3	3:H:685:GLU:CD	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:113:LEU:HD23	2:D:291:THR:CG2	2.40	0.45
2:D:233:GLY:C	2:D:333:ILE:HD11	2.37	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
1:C:257:ASN:O	1:C:257:ASN:CG	2.56	0.44
1:A:432:CYS:HB3	4:A:1002:F15:H5	1.99	0.44
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
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
2:D:301:ARG:C	2:D:303:PRO:CD	2.86	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
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
2:D:119:GLY:O	2:D:123:ARG:HG3	2.18	0.43
1:A:263:ASP:O	1:A:264:PRO:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ILE:O	1:A:318:ILE:HG22	2.19	0.43
1:C:313:PHE:CD1	1:C:313:PHE:C	2.92	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:HG13	3:E:632:ILE:H	1.60	0.42
1:A:356:LYS:HE2	2:B:278:ARG:HH22	1.84	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
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: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:D:253:GLN:O	2:D:254:LEU:C	2.57	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: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:378:PRO:CD	1:A:393:ARG:HD3	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:318:ILE:HG23	1:C:358:ARG:HD3	2.03	0.41
1:A:420:LEU:O	1:A:420:LEU:HG	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:A:426:ARG:O	1:A:430:LEU:HG	2.21	0.41
2:B:160:HIS:O	2:B:161:PHE:C	2.59	0.41
1:C:440:LYS:HE3	1:C:452:MET:HE3	2.03	0.41
2:D:197:ALA:CB	2:D:267:LEU:HA	2.51	0.41
2:B:217:PHE:O	2:B:223:ARG:HA	2.20	0.41
1:C:296:ASP:OD2	1:C:384:SER:OG	2.37	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:A:452:MET:HA	1:A:455:LEU:HD21	2.02	0.41
1:C:305:TRP:CD1	1:C:454:MET:HE3	2.56	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:HA	1:A:276:LEU:HD12	1.73	0.40
1:A:431:LYS:HD2	1:A:431:LYS:HA	1.93	0.40
2:B:252:LEU:O	2:B:253:GLN:C	2.59	0.40
1:C:236:LEU:O	1:C:240:LEU:HG	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:MET:HG2	1:C:396:VAL:CG2	2.52	0.40
1:C:284:LYS:C	1:C:286:ILE:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/236 (98%)	191 (83%)	31 (14%)	8 (4%)	3	5
1	C	234/236 (99%)	197 (84%)	30 (13%)	7 (3%)	4	7
2	B	244/246 (99%)	208 (85%)	28 (12%)	8 (3%)	4	6
2	D	244/246 (99%)	216 (88%)	27 (11%)	1 (0%)	34	57
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%)	5	9

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

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Mol	Chain	Res	Type
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
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%)	24	47
1	C	204/204 (100%)	198 (97%)	6 (3%)	42	68
2	B	219/219 (100%)	213 (97%)	6 (3%)	44	71
2	D	219/219 (100%)	214 (98%)	5 (2%)	50	75
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%)	9 (82%)	2 (18%)	1	2
3	H	11/12 (92%)	10 (91%)	1 (9%)	9	18
All	All	883/894 (99%)	853 (97%)	30 (3%)	37	63

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	264	PRO
1	A	296	ASP
1	A	312	SER
1	A	326	LEU
1	A	365	THR
1	A	407	LYS
1	A	410	GLU
1	A	444	ASP
1	A	450	PHE
2	B	108	LYS
2	B	151	LEU
2	B	223	ARG
2	B	250	ARG
2	B	255	GLN
2	B	321	SER
1	C	229	ASP
1	C	313	PHE
1	C	355	SER
1	C	365	THR
1	C	410	GLU
1	C	455	LEU
2	D	146	GLN
2	D	249	LEU
2	D	285	GLN
2	D	305	ASP
2	D	321	SER
3	G	628	GLU
3	G	629	ARG
3	H	689	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	ASN
1	A	270	GLN
1	A	306	ASN
1	A	333	HIS
2	B	121	HIS
2	B	124	HIS
2	B	171	GLN
2	B	215	GLN
2	B	216	ASN

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Mol	Chain	Res	Type
2	B	235	GLN
2	B	244	HIS
2	B	255	GLN
2	B	299	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	460	GLN
2	D	124	HIS
2	D	145	HIS
2	D	171	GLN
2	D	190	GLN
2	D	244	HIS
2	D	285	GLN
2	D	323	ASN
2	D	331	GLN
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 carbohydrates 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[A]	-	25,30,30	2.69	16 (64%)	27,42,42	2.56	4 (14%)
4	F15	A	1002	-	13,16,16	1.11	1 (7%)	12,16,16	0.81	0
4	F15	C	1001	-	13,16,16	0.88	0	12,16,16	0.60	0
5	CID	D	1003[B]	-	25,30,30	2.57	15 (60%)	27,42,42	2.75	3 (11%)

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[A]	-	-	0/9/11/11	0/4/4/4
4	F15	A	1002	-	-	9/12/14/14	-
4	F15	C	1001	-	-	5/12/14/14	-
5	CID	D	1003[B]	-	-	1/9/11/11	0/4/4/4

All (32) 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
5	D	1003[A]	CID	C2-C10	4.58	1.51	1.45
5	D	1003[A]	CID	C21-C23	3.69	1.44	1.38
5	D	1003[B]	CID	C21-C23	3.62	1.44	1.38
5	D	1003[B]	CID	C12-C17	3.20	1.44	1.38
5	D	1003[A]	CID	C12-C17	3.17	1.44	1.38
5	D	1003[A]	CID	C13-C17	3.13	1.44	1.38
5	D	1003[B]	CID	C13-C17	3.09	1.43	1.38
5	D	1003[B]	CID	C7-C12	3.09	1.44	1.38
5	D	1003[A]	CID	C21-C20	3.08	1.44	1.39
5	D	1003[A]	CID	C13-C8	3.08	1.44	1.38
5	D	1003[A]	CID	C3-C1	-3.05	1.45	1.49
5	D	1003[B]	CID	C21-C20	3.02	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1003[B]	CID	C2-C10	3.00	1.49	1.45
5	D	1003[A]	CID	C7-C12	2.99	1.44	1.38
5	D	1003[B]	CID	C3-C1	-2.98	1.45	1.49
5	D	1003[B]	CID	C13-C8	2.87	1.44	1.38
5	D	1003[A]	CID	C8-C3	2.76	1.45	1.39
5	D	1003[B]	CID	C22-C24	2.74	1.43	1.38
5	D	1003[A]	CID	C22-C24	2.72	1.43	1.38
5	D	1003[B]	CID	C8-C3	2.71	1.45	1.39
5	D	1003[B]	CID	C7-C3	2.67	1.45	1.39
5	D	1003[A]	CID	C22-C20	2.64	1.44	1.38
5	D	1003[A]	CID	C7-C3	2.62	1.44	1.39
5	D	1003[B]	CID	C22-C20	2.52	1.44	1.38
5	D	1003[A]	CID	C25-C23	2.48	1.44	1.39
5	D	1003[B]	CID	C24-C25	2.46	1.44	1.38
5	D	1003[A]	CID	C24-C25	2.44	1.43	1.38
5	D	1003[B]	CID	C25-C23	2.40	1.44	1.39
4	A	1002	F15	C5-C4	2.23	1.62	1.52
5	D	1003[A]	CID	C15-S14	2.00	1.81	1.71

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1003[B]	CID	C18-O16-N11	12.77	125.40	108.13
5	D	1003[A]	CID	C18-O16-N11	10.41	122.21	108.13
5	D	1003[A]	CID	O16-N11-C10	6.83	121.29	110.80
5	D	1003[B]	CID	O16-N11-C10	4.71	118.04	110.80
5	D	1003[B]	CID	C2-C10-N11	2.85	124.04	118.07
5	D	1003[A]	CID	C2-C10-N11	2.57	123.45	118.07
5	D	1003[A]	CID	C7-C3-C1	2.08	123.90	120.61

There are no chirality outliers.

All (15) torsion outliers are listed below:

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

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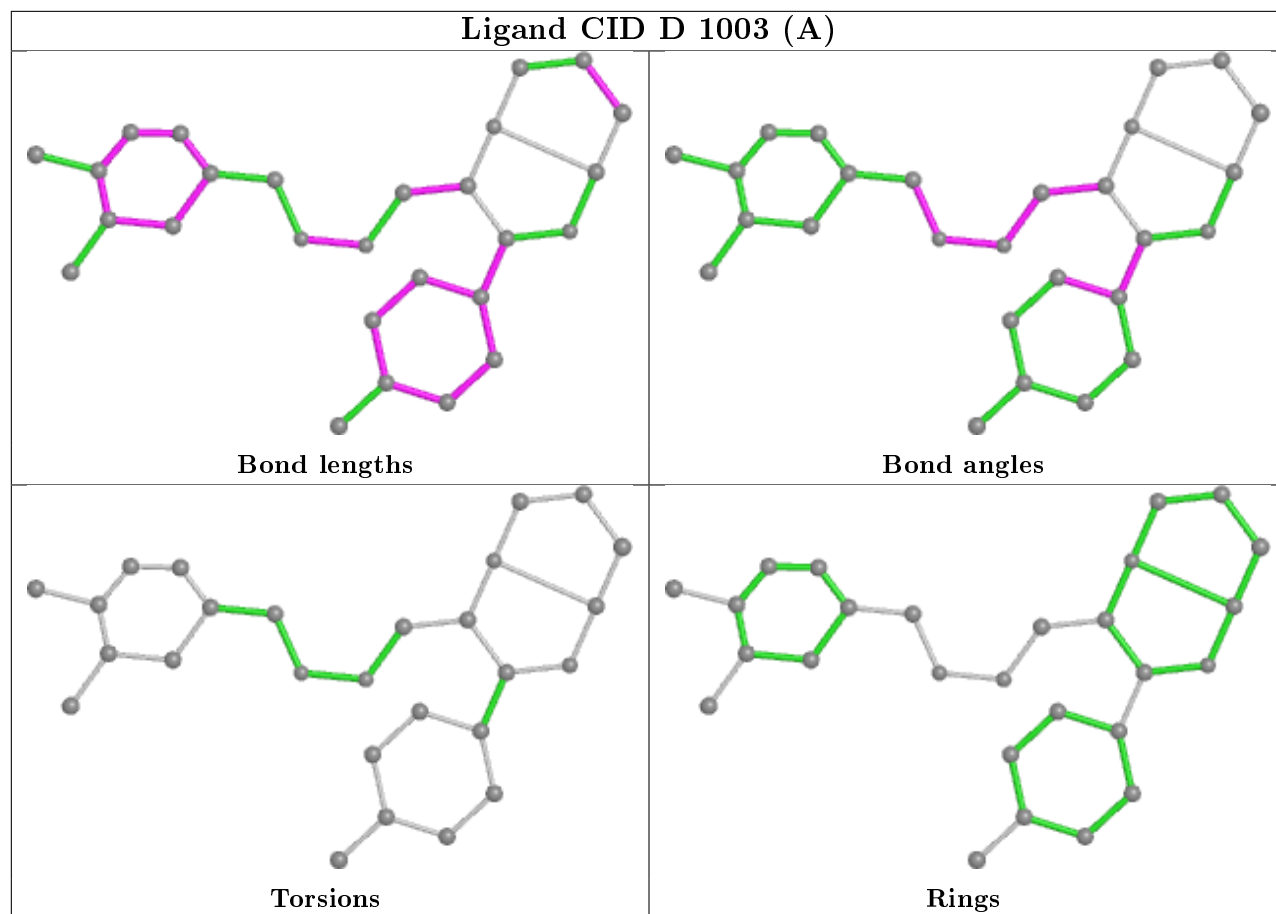
Mol	Chain	Res	Type	Atoms
4	C	1001	F15	C11-C12-C13-C2
4	A	1002	F15	C7-C6-C8-C5
4	A	1002	F15	C6-C7-C9-C10
4	A	1002	F15	C11-C12-C13-C2
4	A	1002	F15	C12-C13-C2-C3
4	C	1001	F15	C13-C2-C3-C14
4	A	1002	F15	C4-C5-C8-C6

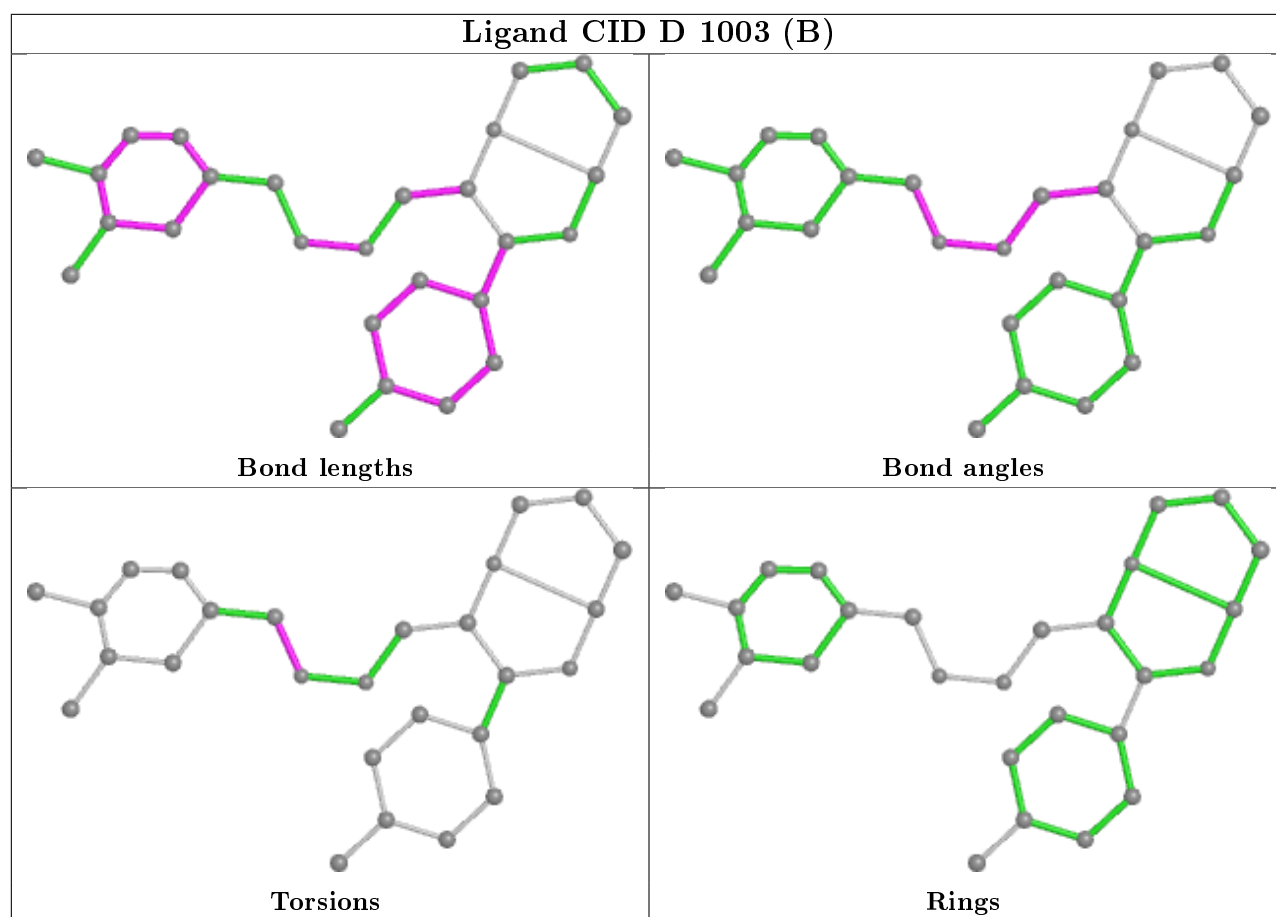
There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	F15	6	0
4	C	1001	F15	7	0
5	D	1003[B]	CID	2	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	232/236 (98%)	0.48	13 (5%)	24	19	43, 77, 131, 157	0
1	C	236/236 (100%)	0.49	11 (4%)	31	25	42, 76, 108, 152	0
2	B	246/246 (100%)	0.47	10 (4%)	37	30	51, 76, 134, 169	0
2	D	246/246 (100%)	0.58	15 (6%)	21	16	48, 77, 133, 176	0
3	E	10/13 (76%)	1.18	2 (20%)	1	0	113, 118, 123, 126	0
3	F	12/13 (92%)	1.17	2 (16%)	1	1	99, 109, 125, 127	0
3	G	12/13 (92%)	0.93	1 (8%)	11	8	111, 119, 122, 129	0
3	H	12/13 (92%)	1.20	3 (25%)	0	0	128, 131, 138, 140	0
All	All	1006/1016 (99%)	0.53	57 (5%)	23	18	42, 78, 133, 176	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	103	PRO	9.4
1	A	256	LEU	8.9
1	A	457	ALA	8.9
1	C	459	HIS	7.3
2	B	103	PRO	6.6
2	D	104	VAL	5.8
1	C	462	THR	5.8
2	B	104	VAL	5.7
3	F	697	GLY	5.3
1	A	458	PRO	5.1
1	C	457	ALA	4.9
1	A	455	LEU	4.1
2	B	301	ARG	4.0
1	C	458	PRO	3.9
1	A	255	GLY	3.8
3	E	634	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	173	ILE	3.6
1	A	246	THR	3.5
2	D	297	LYS	3.3
2	B	306	ARG	3.3
1	A	441	LEU	3.3
2	D	303	PRO	3.2
1	A	254	MET	3.0
2	D	301	ARG	2.9
2	D	300	GLN	2.9
3	G	637	LEU	2.9
1	A	245	LYS	2.9
1	A	257	ASN	2.8
2	B	303	PRO	2.8
2	D	241	LEU	2.7
2	D	261	LEU	2.7
1	C	442	ILE	2.7
1	C	460	GLN	2.7
2	D	105	GLN	2.7
1	C	397	TYR	2.7
1	C	461	MET	2.6
2	B	297	LYS	2.6
1	A	389	VAL	2.6
2	D	305	ASP	2.5
2	D	114	ILE	2.5
2	D	108	LYS	2.5
3	H	692	ARG	2.4
2	D	115	ARG	2.4
3	F	694	LEU	2.4
2	D	296	ILE	2.4
2	B	204	ILE	2.3
1	C	247	GLU	2.2
3	H	691	HIS	2.2
1	A	439	PHE	2.2
2	B	254	LEU	2.2
2	B	257	PRO	2.2
3	E	637	LEU	2.2
1	C	361	GLN	2.1
1	A	258	PRO	2.1
2	B	170	LEU	2.1
3	H	693	LEU	2.1
1	C	256	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

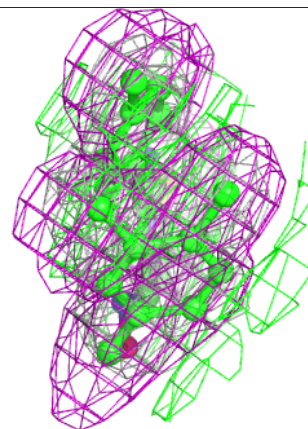
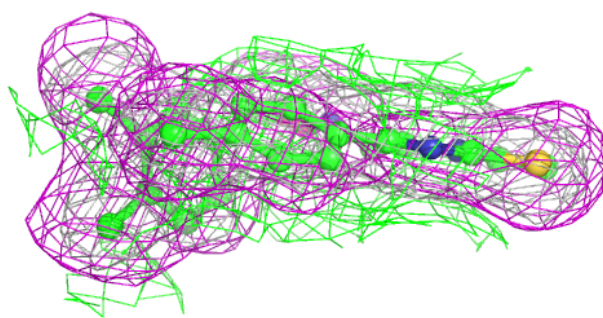
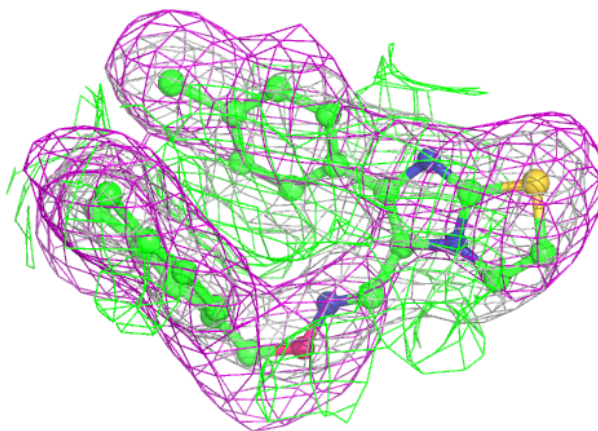
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CID	D	1003[A]	27/27	0.87	0.33	0,0,0,0	27
5	CID	D	1003[B]	27/27	0.87	0.33	0,0,0,0	27
4	F15	C	1001	17/17	0.89	0.43	53,61,91,93	0
4	F15	A	1002	17/17	0.90	0.29	43,63,67,67	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.

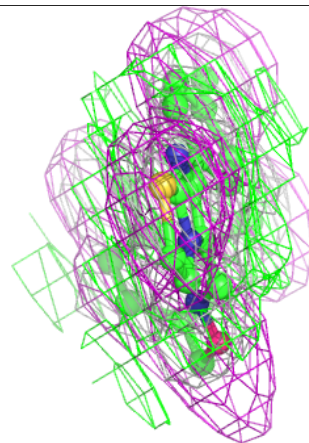
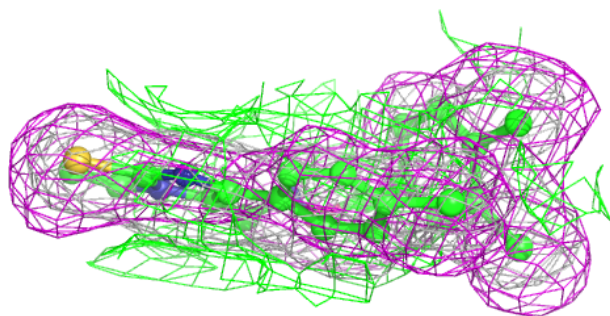
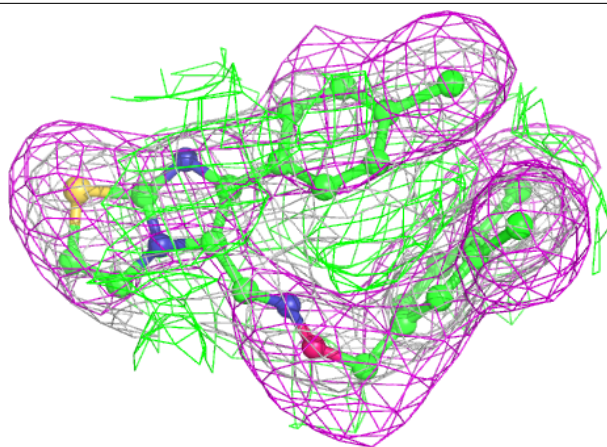
Electron density around CID D 1003 (A):

$2mF_o-DF_c$ (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.