Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2025 – 04:26 PM JST

PDB ID	:	9J71 / pdb_00009j71
Title	:	Crystal strcuture of Keap1_compound_7
Authors	:	Xu, K.
Deposited on	:	2024-08-17
Resolution	:	2.99 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 (i) 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 (i)) were used in the production of this report:

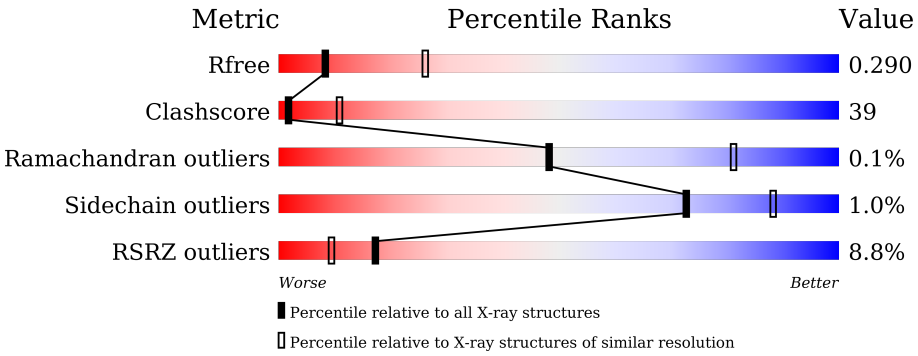
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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 <=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	288	3% 50% 48%
1	B	288	8% 47% 52%
1	C	288	22% 37% 60%
1	X	288	2% 50% 48%

2 Entry composition

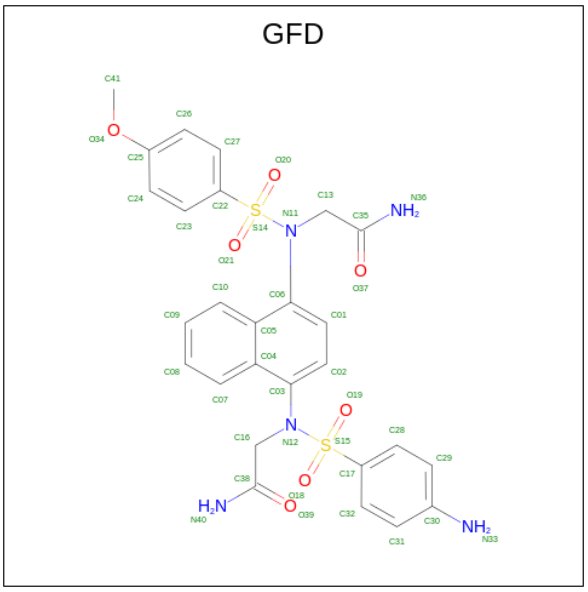
There are 3 unique types of molecules in this entry. The entry contains 9199 atoms, of which 176 are hydrogens and 0 are deuteriums.

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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2201	1368	398	420	15			
1	B	285	Total	C	N	O	S	0	0	0
			2194	1363	397	419	15			
1	C	280	Total	C	N	O	S	0	1	0
			2166	1348	391	412	15			
1	X	286	Total	C	N	O	S	0	0	0
			2201	1368	398	420	15			

- Molecule 2 is 2-[(4-aminophenyl)sulfonyl-[4-[(2-azanyl-2-oxidanylidene-ethyl)-(4-methoxyphenyl)sulfonyl-amino]naphthalen-1-yl]amino]ethanamide (CCD ID: GFD) (formula: $C_{27}H_{27}N_5O_7S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	1
			136	54	54	10	14	4		

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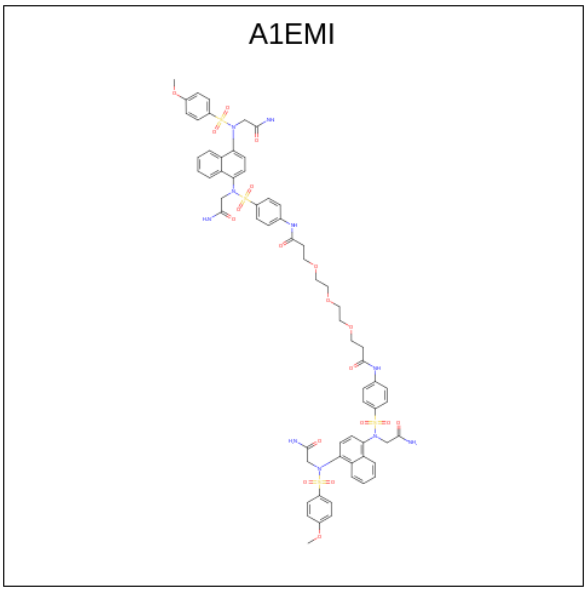
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	S	0	1
			136	54	54	10	14	4		

- Molecule 3 is {N}-[4-[(2-azanyl-2-oxidanylidene-ethyl)-[4-[(2-azanyl-2-oxidanylidene-ethyl)-(4-methoxyphenyl)sulfonyl-amino]naphthalen-1-yl]sulfamoyl]phenyl]-3-[2-[2-[3-[[4-[(2-azanyl-2-oxidanylidene-ethyl)-[4-[(2-azanyl-2-oxidanylidene-ethyl)-(4-methoxyphenyl)sulfonyl-amino]naphthalen-1-yl]sulfamoyl]phenyl]amino]-3-oxidanylidene-propoxy]ethoxy]ethoxy]propanamide (CCD ID: A1EMI) (formula: $C_{64}H_{68}N_{10}O_{19}S_4$) (labeled as "Ligand of Interest" by depositor).



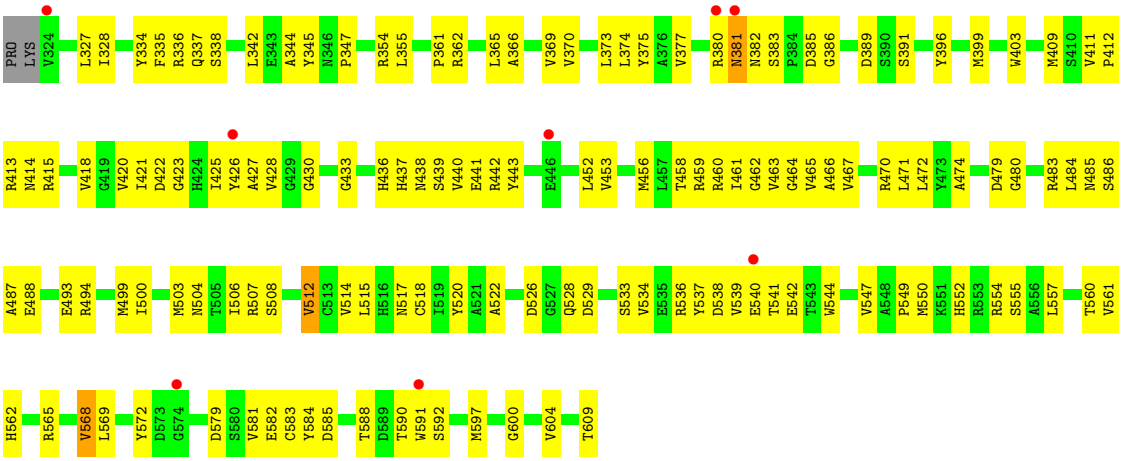
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	X	1	Total	C	H	N	O	S	0	0
			165	64	68	10	19	4		

3 Residue-property plots (i)

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.

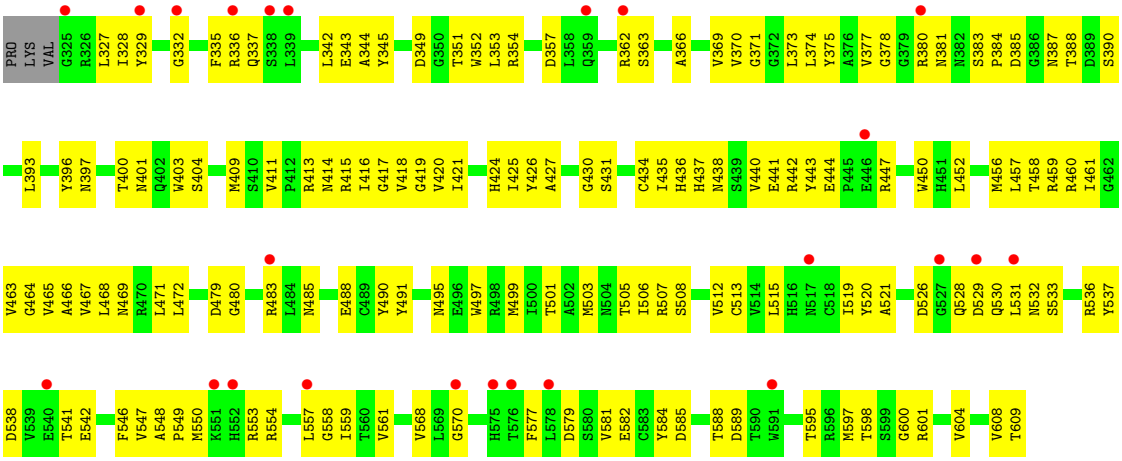
• Molecule 1: Kelch-like ECH-associated protein 1

Chain A:

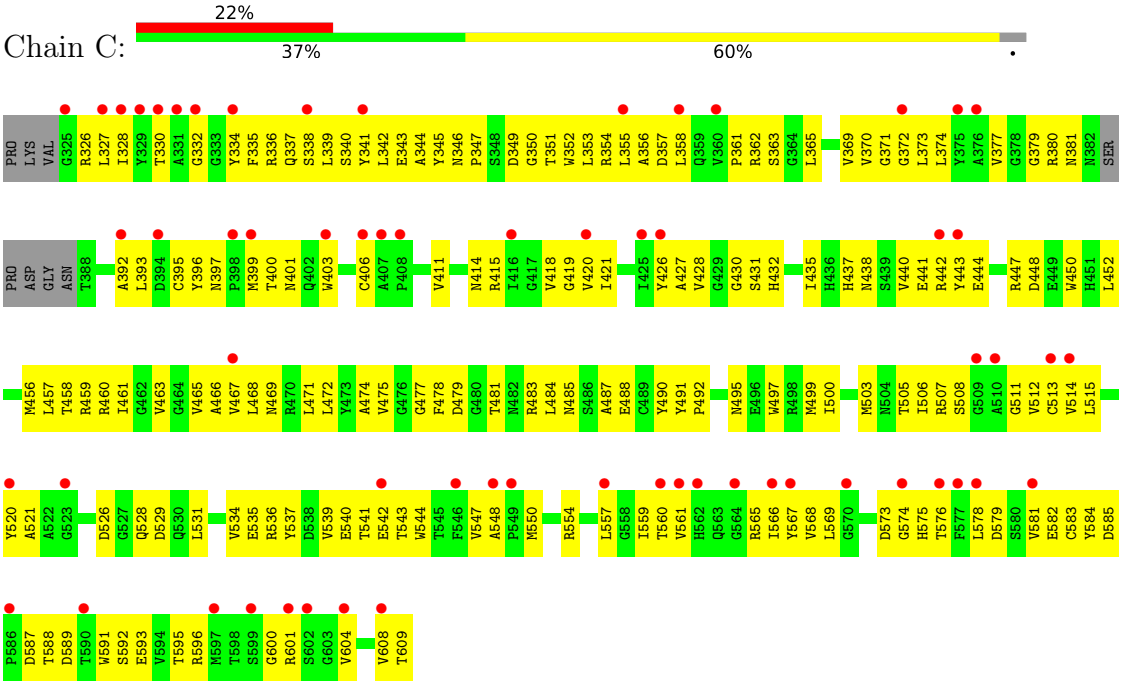


• Molecule 1: Kelch-like ECH-associated protein 1

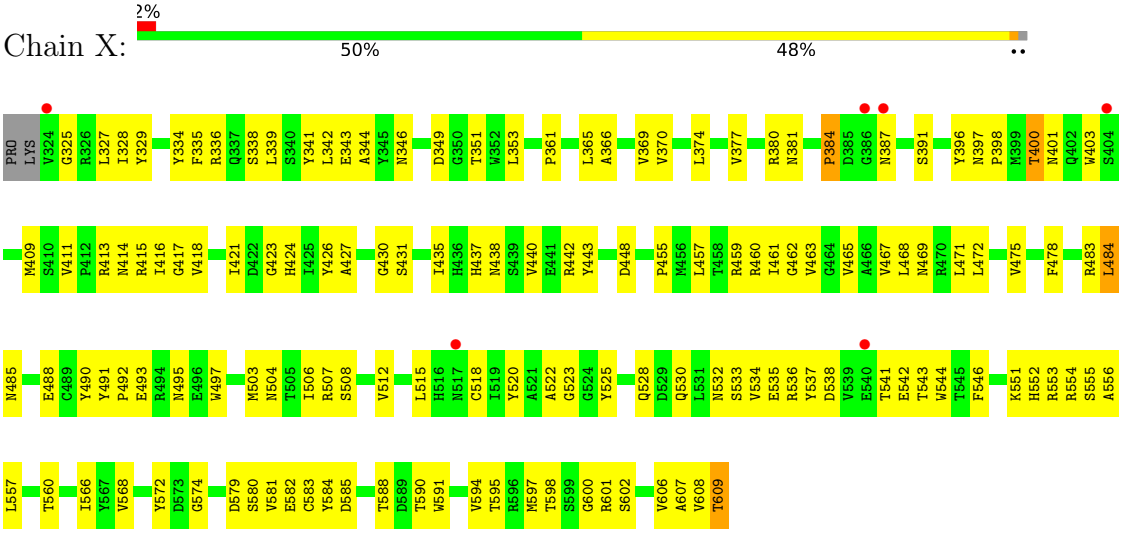
Chain B:



• Molecule 1: Kelch-like ECH-associated protein 1



• Molecule 1: Kelch-like ECH-associated protein 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.47Å 73.87Å 123.08Å 90.00° 100.55° 90.00°	Depositor
Resolution (Å)	44.45 – 2.99 44.45 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.4 (44.45-2.99) 85.2 (44.45-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.57 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.253 , 0.291 0.253 , 0.290	Depositor DCC
R_{free} test set	37220 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	59.3	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	9199	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 7.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GFD, A1EMI

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	0.20	0/2254	0.47	0/3068
1	B	0.17	0/2247	0.43	0/3058
1	C	0.18	0/2220	0.46	0/3019
1	X	0.20	0/2254	0.44	0/3068
All	All	0.19	0/8975	0.45	0/12213

There are no bond length outliers.

There are no bond angle outliers.

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	2201	0	2091	169	0
1	B	2194	0	2083	164	1
1	C	2166	0	2058	207	1
1	X	2201	0	2091	153	0
2	A	82	54	0	11	0
2	C	82	54	0	4	0
3	X	97	68	0	12	0
All	All	9023	176	8323	683	1

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 39.

All (683) 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:X:555:SER:OG	3:X:701:A1EMI:O18	1.54	1.21
1:C:585:ASP:OD2	1:C:588:THR:HG23	1.46	1.12
1:C:515:LEU:HD13	1:C:561:VAL:HG21	1.33	1.07
1:A:579:ASP:HB3	1:A:600:GLY:HA2	1.35	1.07
1:A:503:MET:HE1	1:A:507:ARG:HD2	1.35	1.06
1:X:602:SER:OG	3:X:701:A1EMI:O20	1.73	1.04
1:B:377:VAL:HG21	1:B:418:VAL:HG21	1.40	1.02
1:X:414:ASN:OD1	1:X:415:ARG:HG3	1.59	1.02
1:A:537:TYR:OH	1:A:542:GLU:OE1	1.80	0.99
1:B:501:THR:OG1	1:B:542:GLU:OE2	1.79	0.99
1:C:441:GLU:HB3	1:C:452:LEU:HD23	1.40	0.99
1:X:380:ARG:HB2	1:X:414:ASN:HD22	1.30	0.96
1:C:585:ASP:OD1	1:C:587:ASP:N	2.00	0.94
1:A:380:ARG:NE	1:A:389:ASP:OD1	2.01	0.94
1:B:397:ASN:HB3	1:B:400:THR:HG22	1.47	0.94
1:A:538:ASP:OD1	1:A:540:GLU:HG3	1.70	0.91
1:A:557:LEU:HD23	1:A:557:LEU:H	1.36	0.91
1:X:594:VAL:HG23	1:X:595:THR:HG22	1.49	0.90
1:C:513:CYS:SG	1:C:566:ILE:HD11	2.11	0.90
1:A:552:HIS:HB2	1:A:554:ARG:HH21	1.37	0.89
1:X:380:ARG:HB2	1:X:414:ASN:ND2	1.88	0.89
1:C:566:ILE:HG22	1:C:584:TYR:HB3	1.54	0.88
1:A:422:ASP:HB3	1:A:470:ARG:HH22	1.37	0.88
1:C:444:GLU:OE1	1:C:447:ARG:NH2	2.06	0.88
1:C:569:LEU:HD23	1:C:581:VAL:HG22	1.55	0.88
1:C:426:TYR:OH	1:C:442:ARG:NH2	2.07	0.88
1:C:372:GLY:HA2	1:C:609:THR:HG21	1.56	0.87
1:C:508:SER:OG	2:C:701[A]:GFD:O37	1.90	0.87
1:X:537:TYR:OH	1:X:542:GLU:OE1	1.94	0.84
1:C:369:VAL:HG21	1:C:609:THR:OG1	1.77	0.84
1:A:557:LEU:HD12	1:A:568:VAL:HG13	1.59	0.84
1:B:501:THR:HG1	1:B:542:GLU:CD	1.84	0.84
1:C:573:ASP:HB3	1:C:578:LEU:HD21	1.60	0.83
2:C:701[B]:GFD:O19	2:C:701[B]:GFD:N40	2.11	0.83
1:C:465:VAL:HG13	1:C:472:LEU:HD11	1.60	0.83
1:A:522:ALA:HA	1:A:534:VAL:HG22	1.61	0.83
1:B:377:VAL:CG2	1:B:418:VAL:HG21	2.08	0.82
1:C:585:ASP:CG	1:C:588:THR:H	1.87	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:MET:HE1	1:A:507:ARG:CD	2.10	0.81
1:C:534:VAL:HG13	1:C:547:VAL:HG13	1.63	0.81
1:C:377:VAL:HG12	1:C:393:LEU:HD13	1.61	0.81
1:C:328:ILE:HD13	1:C:608:VAL:HB	1.62	0.81
1:A:515:LEU:HD13	1:A:561:VAL:HG21	1.63	0.80
1:X:328:ILE:HG23	1:X:560:THR:HG21	1.64	0.80
1:B:550:MET:HE1	1:B:554:ARG:HD3	1.63	0.80
1:C:421:ILE:HG12	1:C:467:VAL:HG21	1.64	0.80
1:C:339:LEU:HD23	1:C:341:TYR:CE2	2.17	0.79
1:B:464:GLY:HA3	1:B:512:VAL:CG2	2.13	0.79
1:C:327:LEU:HD22	1:C:346:ASN:HA	1.63	0.79
1:A:456:MET:HE1	1:A:460:ARG:HD2	1.63	0.79
1:X:415:ARG:NH1	1:X:415:ARG:HG2	1.98	0.79
1:X:349:ASP:OD1	1:X:351:THR:HG22	1.83	0.77
1:B:426:TYR:CE2	1:B:442:ARG:HB2	2.19	0.76
1:C:566:ILE:CG2	1:C:584:TYR:HB3	2.15	0.76
1:X:415:ARG:HG2	1:X:415:ARG:HH11	1.49	0.76
1:C:327:LEU:HD11	1:C:346:ASN:HB2	1.66	0.76
1:A:370:VAL:HG22	1:A:420:VAL:HG21	1.66	0.75
1:A:409:MET:HE1	1:A:413:ARG:HD2	1.66	0.75
1:B:414:ASN:ND2	1:B:415:ARG:HG3	2.01	0.75
1:X:438:ASN:HB3	1:X:459:ARG:HG2	1.68	0.75
1:B:370:VAL:HG12	1:B:420:VAL:HG21	1.67	0.75
1:X:431:SER:HB3	1:X:461:ILE:HG21	1.69	0.74
1:X:542:GLU:HG3	1:X:542:GLU:O	1.86	0.74
1:X:555:SER:OG	3:X:701:A1EMI:S13	2.45	0.74
1:C:365:LEU:HB2	1:C:377:VAL:O	1.86	0.74
1:B:421:ILE:HD12	1:B:426:TYR:HE1	1.52	0.74
1:A:550:MET:HE1	1:A:554:ARG:CG	2.18	0.73
1:A:550:MET:HE1	1:A:554:ARG:HG2	1.69	0.73
1:A:579:ASP:O	1:A:597:MET:HG3	1.88	0.73
1:B:456:MET:HE1	1:B:460:ARG:HB2	1.68	0.73
1:C:441:GLU:HB3	1:C:452:LEU:CD2	2.16	0.73
1:C:330:THR:HG23	1:C:604:VAL:HG21	1.69	0.73
1:C:528:GLN:HG3	1:C:529[A]:ASP:OD1	1.88	0.73
1:A:542:GLU:HG2	1:X:435:ILE:CD1	2.18	0.73
1:X:334:TYR:HB3	3:X:701:A1EMI:O19	1.88	0.73
1:B:362:ARG:NH2	1:B:378:GLY:O	2.21	0.73
1:A:370:VAL:HG13	1:A:423:GLY:HA2	1.71	0.72
1:A:579:ASP:HB3	1:A:600:GLY:CA	2.17	0.72
1:B:568:VAL:CG2	1:B:582:GLU:HB2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:ALA:HB3	1:B:519:ILE:CD1	2.20	0.72
1:B:342:LEU:HD22	1:B:403:TRP:CZ2	2.25	0.71
1:A:391:SER:O	1:A:409:MET:HG3	1.90	0.71
1:A:337:GLN:OE1	1:A:382:ASN:ND2	2.24	0.71
1:B:430:GLY:C	1:B:461:ILE:HG22	2.16	0.71
1:A:462:GLY:HA3	2:A:701[A]:GFD:O37	1.91	0.70
1:X:556:ALA:HB2	3:X:701:A1EMI:C04	2.20	0.70
1:B:550:MET:HE1	1:B:554:ARG:CD	2.21	0.70
1:B:512:VAL:HG12	1:B:521:ALA:HA	1.72	0.70
1:B:397:ASN:HB3	1:B:400:THR:CG2	2.20	0.70
1:X:537:TYR:HB2	1:X:544:TRP:CD2	2.27	0.70
1:X:421:ILE:HG12	1:X:467:VAL:HG21	1.74	0.70
1:X:369:VAL:HG23	1:X:607:ALA:HB1	1.72	0.70
1:X:557:LEU:HD23	1:X:557:LEU:H	1.57	0.70
1:B:464:GLY:HA3	1:B:512:VAL:HG21	1.74	0.69
1:A:557:LEU:HD12	1:A:568:VAL:CG1	2.22	0.69
2:A:701[B]:GFD:O19	2:A:701[B]:GFD:N40	2.25	0.69
1:C:456:MET:HE1	1:C:460:ARG:HD2	1.74	0.69
1:C:557:LEU:H	1:C:557:LEU:HD23	1.55	0.69
1:A:534:VAL:HG12	1:A:547:VAL:HG22	1.74	0.69
1:C:369:VAL:HG11	1:C:609:THR:OG1	1.92	0.69
1:A:430:GLY:C	1:A:461:ILE:HG22	2.17	0.69
1:A:542:GLU:HG2	1:X:435:ILE:HD11	1.73	0.69
1:X:472:LEU:HB3	1:X:490:TYR:HB3	1.73	0.69
1:B:542:GLU:HG3	1:B:542:GLU:O	1.90	0.68
1:C:565:ARG:HH12	1:C:585:ASP:HB2	1.58	0.68
1:C:438:ASN:HB3	1:C:459:ARG:HG2	1.75	0.68
1:B:426:TYR:HE2	1:B:442:ARG:HB2	1.58	0.68
1:A:572:TYR:HE1	2:A:701[A]:GFD:C41	2.07	0.68
1:B:528:GLN:NE2	1:X:384:PRO:O	2.26	0.68
1:B:538:ASP:HB3	1:B:541:THR:OG1	1.94	0.67
1:A:382:ASN:OD1	1:A:383:SER:N	2.28	0.67
1:B:554:ARG:NH2	1:B:570:GLY:O	2.28	0.67
1:A:409:MET:CE	1:A:413:ARG:HD2	2.25	0.67
1:A:436:HIS:O	1:A:459:ARG:HD3	1.95	0.67
1:C:340:SER:HB2	1:C:361:PRO:HB3	1.77	0.67
1:B:550:MET:HE1	1:B:554:ARG:CG	2.25	0.66
1:A:335:PHE:CD2	1:A:336:ARG:HG3	2.31	0.66
1:C:547:VAL:HG22	1:C:548:ALA:N	2.11	0.66
1:X:507:ARG:NH2	1:X:533:SER:OG	2.29	0.66
1:A:355:LEU:HD23	1:A:396:TYR:OH	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ASN:HB3	1:A:459:ARG:HG2	1.76	0.66
1:B:335:PHE:HA	1:B:577:PHE:CD1	2.31	0.66
1:C:343:GLU:HA	1:C:353:LEU:O	1.96	0.65
1:C:397:ASN:CG	1:C:400:THR:HG22	2.21	0.65
1:C:427:ALA:O	1:C:440:VAL:HG13	1.96	0.65
1:B:370:VAL:HG22	1:B:375:TYR:HE1	1.61	0.65
1:B:547:VAL:HG22	1:B:589:ASP:OD1	1.96	0.65
1:C:465:VAL:CG1	1:C:472:LEU:HD11	2.26	0.65
1:A:493:GLU:HG2	1:A:494:ARG:N	2.12	0.64
1:C:327:LEU:CD1	1:C:346:ASN:HB2	2.26	0.64
1:B:431:SER:HB3	1:B:461:ILE:HG21	1.79	0.64
1:X:503:MET:HE1	1:X:507:ARG:HD2	1.79	0.64
1:X:507:ARG:NH1	1:X:535:GLU:OE2	2.30	0.64
1:C:466:ALA:HB2	1:C:512:VAL:HG12	1.80	0.64
1:A:488:GLU:HG2	1:A:499:MET:SD	2.38	0.64
1:B:414:ASN:OD1	3:X:701:A1EMI:N96	2.31	0.64
1:B:519:ILE:HB	1:B:537:TYR:HB3	1.79	0.64
1:C:585:ASP:OD2	1:C:588:THR:CG2	2.36	0.64
1:X:339:LEU:HD12	1:X:339:LEU:H	1.63	0.64
1:X:485:ASN:HB3	1:X:506:ILE:HG13	1.79	0.64
1:C:569:LEU:HD23	1:C:581:VAL:CG2	2.27	0.63
1:C:573:ASP:OD1	1:C:576:THR:N	2.31	0.63
1:A:370:VAL:CG1	1:A:423:GLY:HA2	2.27	0.63
1:C:487:ALA:HB3	1:C:500:ILE:HD11	1.80	0.63
1:C:550:MET:HE1	1:C:554:ARG:HD2	1.79	0.63
1:A:542:GLU:O	1:A:542:GLU:HG3	1.97	0.63
1:B:421:ILE:HD12	1:B:426:TYR:CE1	2.32	0.63
1:X:483:ARG:NH1	1:X:508:SER:OG	2.32	0.63
1:A:464:GLY:HA3	1:A:512:VAL:CG2	2.27	0.63
1:C:349:ASP:OD1	1:C:351:THR:HG23	1.98	0.63
1:X:416:ILE:HD11	1:X:427:ALA:HB1	1.81	0.63
1:B:378:GLY:HA3	1:B:416:ILE:HG21	1.81	0.62
1:C:362:ARG:HB2	1:C:365:LEU:HD23	1.80	0.62
1:B:370:VAL:HG22	1:B:375:TYR:CE1	2.32	0.62
1:X:397:ASN:HB3	1:X:400:THR:HG23	1.79	0.62
1:B:530:GLN:OE1	1:B:530:GLN:N	2.32	0.62
1:B:568:VAL:HG22	1:B:582:GLU:HB2	1.80	0.62
1:X:431:SER:HB3	1:X:461:ILE:CG2	2.30	0.62
1:X:391:SER:O	1:X:409:MET:HG3	2.00	0.62
1:A:421:ILE:HG12	1:A:467:VAL:HG21	1.82	0.62
1:C:431:SER:HB3	1:C:461:ILE:HG21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:GLU:O	1:B:542:GLU:CG	2.48	0.61
1:C:565:ARG:HH12	1:C:585:ASP:CB	2.12	0.61
1:B:579:ASP:HB3	1:B:600:GLY:HA2	1.81	0.61
1:C:362:ARG:NH1	1:C:392:ALA:HB3	2.14	0.61
1:B:515:LEU:HD13	1:B:561:VAL:HG21	1.82	0.61
1:B:396:TYR:CE1	1:B:401:ASN:HA	2.35	0.61
1:C:584:TYR:HB2	1:C:591:TRP:CE2	2.36	0.61
1:A:374:LEU:HD23	1:A:375:TYR:N	2.15	0.61
1:C:421:ILE:HG12	1:C:467:VAL:CG2	2.30	0.61
1:A:555:SER:OG	2:A:701[B]:GFD:O18	2.18	0.61
1:C:507:ARG:NH1	1:C:535:GLU:OE2	2.33	0.61
1:C:547:VAL:HG22	1:C:548:ALA:H	1.66	0.61
1:C:354:ARG:HH21	1:C:357:ASP:CG	2.09	0.60
1:C:457:LEU:N	1:C:488:GLU:OE1	2.33	0.60
1:A:522:ALA:CA	1:A:534:VAL:HG22	2.30	0.60
1:C:418:VAL:HG22	1:C:427:ALA:HA	1.84	0.60
1:B:342:LEU:HD22	1:B:403:TRP:HZ2	1.62	0.60
1:X:468:LEU:HD12	1:X:469:ASN:N	2.17	0.60
1:B:503:MET:HE2	1:B:507:ARG:HD2	1.84	0.60
1:B:597:MET:HE1	1:B:601:ARG:CD	2.32	0.60
1:C:468:LEU:HD13	1:C:514:VAL:HG21	1.82	0.60
1:B:397:ASN:CB	1:B:400:THR:HG22	2.26	0.60
1:C:330:THR:CG2	1:C:604:VAL:HG21	2.31	0.60
1:C:327:LEU:O	1:C:608:VAL:HG23	2.01	0.60
1:B:547:VAL:HG21	1:B:584:TYR:OH	2.02	0.59
1:C:339:LEU:HD12	1:C:339:LEU:H	1.67	0.59
1:C:539:VAL:O	1:C:542:GLU:HG2	2.02	0.59
1:C:443:TYR:OH	1:C:448:ASP:OD1	2.14	0.59
1:A:385:ASP:OD1	1:A:385:ASP:N	2.35	0.59
1:B:335:PHE:HA	1:B:577:PHE:HD1	1.67	0.59
1:X:554:ARG:NH2	1:X:580:SER:OG	2.26	0.59
1:A:458:THR:HG21	1:A:484:LEU:HD13	1.84	0.59
1:B:426:TYR:CE2	1:B:442:ARG:HD3	2.36	0.59
1:X:365:LEU:HB2	1:X:377:VAL:O	2.02	0.59
1:A:487:ALA:HB3	1:A:500:ILE:HD11	1.84	0.59
1:A:534:VAL:HG12	1:A:547:VAL:CG2	2.32	0.59
1:B:585:ASP:CG	1:B:588:THR:HG23	2.28	0.59
1:C:441:GLU:HA	1:C:452:LEU:HA	1.84	0.59
1:C:466:ALA:HB2	1:C:512:VAL:CG1	2.32	0.59
1:C:515:LEU:HD13	1:C:561:VAL:CG2	2.20	0.59
1:X:468:LEU:HD12	1:X:469:ASN:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:334:TYR:CB	3:X:701:A1EMI:O19	2.51	0.59
1:C:441:GLU:CB	1:C:452:LEU:HD23	2.25	0.58
1:C:444:GLU:OE1	1:C:447:ARG:HD2	2.04	0.58
1:X:597:MET:HE1	1:X:601:ARG:HD2	1.84	0.58
1:C:342:LEU:HD21	1:C:396:TYR:CE1	2.38	0.58
1:B:327:LEU:HD13	1:B:344:ALA:HB1	1.85	0.58
1:X:503:MET:HE2	1:X:535:GLU:OE2	2.04	0.58
1:X:339:LEU:HD23	1:X:341:TYR:CE2	2.38	0.58
1:A:520:TYR:OH	1:A:536:ARG:NH1	2.36	0.58
1:X:430:GLY:O	1:X:437:HIS:HB2	2.04	0.58
1:C:515:LEU:HB3	1:C:520:TYR:CE2	2.39	0.57
1:A:411:VAL:HG23	1:A:412:PRO:HD2	1.86	0.57
1:X:342:LEU:HD22	1:X:403:TRP:CZ2	2.40	0.57
1:B:335:PHE:HD1	1:B:577:PHE:CD1	2.23	0.57
1:B:383:SER:HB3	1:B:384:PRO:HD2	1.87	0.57
1:C:458:THR:HG23	1:C:499:MET:HE1	1.86	0.57
1:X:339:LEU:HD12	1:X:339:LEU:N	2.19	0.57
1:B:427:ALA:O	1:B:440:VAL:HG13	2.04	0.57
1:C:393:LEU:HD22	1:C:450:TRP:HZ2	1.70	0.57
1:C:465:VAL:HG13	1:C:472:LEU:CD1	2.34	0.57
1:C:568:VAL:CG2	1:C:582:GLU:HB2	2.35	0.57
1:X:552:HIS:HB2	1:X:554:ARG:HH21	1.67	0.57
1:A:411:VAL:HG21	1:A:437:HIS:CE1	2.40	0.57
1:C:511:GLY:CA	1:C:559:ILE:HG21	2.35	0.57
1:B:507:ARG:NH2	1:B:533:SER:O	2.38	0.57
1:C:397:ASN:HB3	1:C:400:THR:HG22	1.86	0.57
1:A:414:ASN:OD1	1:A:415:ARG:N	2.38	0.57
1:B:381:ASN:N	1:B:388:THR:O	2.27	0.57
1:X:566:ILE:HB	1:X:584:TYR:HB3	1.87	0.57
1:A:436:HIS:CD2	1:A:480:GLY:HA2	2.40	0.56
1:C:574:GLY:C	1:C:575:HIS:HD1	2.12	0.56
1:B:426:TYR:CD1	1:B:472:LEU:HD12	2.40	0.56
1:C:573:ASP:CG	1:C:576:THR:H	2.13	0.56
1:C:344:ALA:O	1:C:352:TRP:HA	2.04	0.56
1:C:377:VAL:CG1	1:C:393:LEU:HD13	2.35	0.56
1:B:349:ASP:OD1	1:B:351:THR:HG22	2.05	0.56
1:B:515:LEU:CD1	1:B:561:VAL:HG21	2.35	0.56
1:B:581:VAL:HB	1:B:595:THR:HG22	1.87	0.56
1:C:371:GLY:O	1:C:373:LEU:HD12	2.06	0.56
1:A:422:ASP:HB3	1:A:470:ARG:NH2	2.13	0.56
1:A:588:THR:OG1	1:A:590:THR:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:LEU:HD22	1:C:403:TRP:CZ2	2.41	0.56
1:C:458:THR:CG2	1:C:499:MET:HE1	2.35	0.56
1:A:383:SER:HB2	1:A:386:GLY:O	2.06	0.56
1:X:397:ASN:HB3	1:X:400:THR:CG2	2.35	0.56
1:A:515:LEU:HD13	1:A:561:VAL:CG2	2.35	0.56
1:C:332:GLY:O	1:C:604:VAL:HG23	2.06	0.56
1:A:456:MET:CE	1:A:460:ARG:HD2	2.33	0.55
1:A:537:TYR:HB2	1:A:544:TRP:CD2	2.41	0.55
1:C:583:CYS:N	1:C:592:SER:O	2.35	0.55
1:X:414:ASN:O	1:X:415:ARG:HB2	2.06	0.55
1:B:369:VAL:HA	1:B:373:LEU:O	2.05	0.55
1:B:426:TYR:HD1	1:B:472:LEU:HD12	1.72	0.55
1:B:490:TYR:HB2	1:B:497:TRP:CH2	2.41	0.55
1:B:547:VAL:HG22	1:B:548:ALA:H	1.69	0.55
1:B:579:ASP:HB3	1:B:600:GLY:CA	2.37	0.55
1:A:487:ALA:CB	1:A:500:ILE:HD11	2.37	0.55
1:B:585:ASP:OD2	1:B:588:THR:HG23	2.05	0.55
1:X:349:ASP:CG	1:X:351:THR:HG22	2.31	0.55
1:A:409:MET:HE1	1:A:427:ALA:HB1	1.88	0.55
1:C:345:TYR:HE2	1:C:350:GLY:HA2	1.71	0.55
1:C:396:TYR:HB2	1:C:403:TRP:CD2	2.42	0.55
1:X:579:ASP:HB3	1:X:600:GLY:HA2	1.87	0.55
1:A:422:ASP:CB	1:A:470:ARG:HH22	2.15	0.55
1:A:479:ASP:HB3	1:A:484:LEU:HD11	1.89	0.55
1:C:369:VAL:HG21	1:C:609:THR:CB	2.36	0.55
1:A:517:ASN:O	1:A:539:VAL:HG12	2.06	0.54
1:X:335:PHE:O	1:X:336:ARG:HB2	2.07	0.54
1:X:468:LEU:HG	1:X:469:ASN:OD1	2.08	0.54
1:C:419:GLY:N	1:C:465:VAL:HG11	2.22	0.54
1:B:533:SER:HA	1:B:549:PRO:HB3	1.89	0.54
1:A:421:ILE:HD12	1:A:426:TYR:CE2	2.42	0.54
1:A:456:MET:CE	1:A:474:ALA:HB3	2.36	0.54
1:A:522:ALA:CB	1:A:534:VAL:HG22	2.37	0.54
1:B:550:MET:HE1	1:B:554:ARG:HG2	1.88	0.54
1:X:461:ILE:HG12	1:X:478:PHE:O	2.08	0.54
1:A:537:TYR:HB2	1:A:544:TRP:CE3	2.42	0.54
1:B:532:ASN:HB3	1:B:553:ARG:HA	1.90	0.54
1:A:362:ARG:HG2	1:A:381:ASN:HB3	1.89	0.54
1:A:464:GLY:HA3	1:A:512:VAL:HG21	1.90	0.54
1:C:456:MET:CE	1:C:460:ARG:HD2	2.38	0.54
1:C:547:VAL:CG2	1:C:548:ALA:H	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:TYR:HE1	1:C:583:CYS:HG	1.55	0.54
1:A:540:GLU:O	1:B:434:CYS:HB2	2.09	0.53
1:X:537:TYR:HB2	1:X:544:TRP:CE3	2.43	0.53
1:A:493:GLU:HG2	1:A:494:ARG:H	1.73	0.53
1:B:519:ILE:O	1:B:537:TYR:N	2.33	0.53
1:X:414:ASN:OD1	1:X:415:ARG:CG	2.47	0.53
1:C:414:ASN:OD1	1:C:415:ARG:N	2.41	0.53
1:C:421:ILE:HB	1:C:426:TYR:HE2	1.70	0.53
1:X:568:VAL:CG2	1:X:582:GLU:HB2	2.39	0.53
1:X:415:ARG:HB3	1:X:462:GLY:H	1.73	0.53
1:X:490:TYR:HB2	1:X:497:TRP:CH2	2.43	0.53
1:A:354:ARG:C	1:A:355:LEU:HD12	2.33	0.53
1:A:399:MET:HE2	1:A:399:MET:HA	1.91	0.53
1:A:464:GLY:HA3	1:A:512:VAL:HG23	1.89	0.53
1:B:335:PHE:O	1:B:336:ARG:HB2	2.08	0.53
1:B:426:TYR:CD2	1:B:442:ARG:HB2	2.43	0.53
1:C:395:CYS:HB2	1:C:406:CYS:SG	2.49	0.53
1:X:430:GLY:C	1:X:461:ILE:HG22	2.33	0.53
1:A:335:PHE:O	1:A:336:ARG:HB2	2.09	0.53
1:C:349:ASP:CG	1:C:351:THR:HG23	2.33	0.53
1:C:490:TYR:HB2	1:C:497:TRP:CH2	2.44	0.53
1:C:411:VAL:HG21	1:C:437:HIS:CE1	2.44	0.53
1:X:334:TYR:HA	1:X:339:LEU:HD12	1.91	0.53
1:X:537:TYR:HB2	1:X:544:TRP:CE2	2.44	0.53
1:A:504:ASN:HD21	1:X:455:PRO:HB3	1.74	0.53
1:B:550:MET:CE	1:B:554:ARG:HD3	2.34	0.53
1:X:493:GLU:HA	1:X:493:GLU:OE1	2.09	0.53
1:C:397:ASN:O	1:C:401:ASN:N	2.41	0.53
1:A:428:VAL:HB	1:A:465:VAL:HG21	1.90	0.52
1:A:506:ILE:HG22	1:A:526:ASP:HA	1.89	0.52
1:C:414:ASN:OD1	2:C:701[A]:GFD:N40	2.42	0.52
1:X:553:ARG:NH1	1:X:553:ARG:HG3	2.24	0.52
1:C:396:TYR:HB2	1:C:403:TRP:CE3	2.45	0.52
1:X:415:ARG:HH12	3:X:701:A1EMI:C04	2.22	0.52
1:C:393:LEU:HD22	1:C:450:TRP:CZ2	2.44	0.52
1:C:547:VAL:CG2	1:C:548:ALA:N	2.73	0.52
1:A:557:LEU:H	1:A:557:LEU:CD2	2.17	0.52
1:A:383:SER:HB3	1:A:385:ASP:OD1	2.09	0.52
1:A:441:GLU:HB3	1:A:452:LEU:HG	1.91	0.52
1:C:397:ASN:CB	1:C:400:THR:HG22	2.40	0.52
1:A:584:TYR:HB2	1:A:591:TRP:CZ3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:LEU:HD22	1:C:491:TYR:HD2	1.74	0.52
1:B:366:ALA:HB3	1:B:377:VAL:HG23	1.92	0.51
1:C:335:PHE:O	1:C:336:ARG:HB2	2.09	0.51
1:B:336:ARG:NH2	1:X:528:GLN:O	2.30	0.51
1:B:416:ILE:HD11	1:B:427:ALA:HB1	1.93	0.51
1:X:374:LEU:HD23	1:X:374:LEU:C	2.35	0.51
1:B:417:GLY:HA3	1:B:465:VAL:HG23	1.91	0.51
1:B:464:GLY:CA	1:B:512:VAL:CG2	2.87	0.51
1:C:345:TYR:HB2	1:C:352:TRP:CZ2	2.46	0.51
1:A:483:ARG:HG3	1:A:483:ARG:HH11	1.75	0.51
1:C:595:THR:HG22	1:C:596:ARG:N	2.26	0.51
1:A:458:THR:HB	1:A:488:GLU:OE1	2.11	0.51
1:A:518:CYS:SG	1:A:536:ARG:HD2	2.50	0.51
1:C:369:VAL:HG11	1:C:609:THR:HG1	1.75	0.51
1:C:370:VAL:CG2	1:C:420:VAL:HG21	2.41	0.51
1:C:327:LEU:CD2	1:C:346:ASN:HA	2.37	0.51
1:A:438:ASN:HB3	1:A:459:ARG:CG	2.40	0.51
1:B:332:GLY:O	1:B:604:VAL:HG12	2.10	0.51
1:C:579:ASP:HB3	1:C:600:GLY:HA2	1.93	0.51
1:X:506:ILE:N	1:X:506:ILE:HD12	2.25	0.51
1:A:366:ALA:HB3	1:A:418:VAL:HG13	1.93	0.51
1:B:464:GLY:HA3	1:B:512:VAL:HG22	1.92	0.51
1:C:550:MET:HG2	1:C:591:TRP:CE2	2.45	0.51
1:X:538:ASP:O	1:X:542:GLU:N	2.37	0.51
1:A:335:PHE:HD2	1:A:336:ARG:HG3	1.76	0.51
1:B:381:ASN:O	1:B:387:ASN:HA	2.11	0.51
1:C:345:TYR:HB2	1:C:352:TRP:CH2	2.46	0.51
1:C:550:MET:CE	1:C:554:ARG:HD2	2.39	0.51
1:B:369:VAL:HG11	1:B:609:THR:HB	1.92	0.50
1:B:335:PHE:HD1	1:B:577:PHE:HD1	1.59	0.50
1:X:504:ASN:CB	1:X:546:PHE:HE2	2.24	0.50
1:A:472:LEU:C	1:A:472:LEU:HD23	2.36	0.50
1:X:366:ALA:HB3	1:X:418:VAL:HG13	1.93	0.50
1:C:581:VAL:O	1:C:593:GLU:HA	2.11	0.50
1:C:584:TYR:HB2	1:C:591:TRP:CZ2	2.45	0.50
1:X:460:ARG:HB3	1:X:463:VAL:HB	1.94	0.50
1:X:503:MET:HE2	1:X:507:ARG:HH11	1.76	0.50
1:X:541:THR:OG1	1:X:543:THR:HG22	2.11	0.50
1:B:465:VAL:HG13	1:B:472:LEU:HD21	1.94	0.50
1:C:342:LEU:HD22	1:C:403:TRP:HZ2	1.76	0.50
1:C:365:LEU:HB3	1:C:379:GLY:HA3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ARG:HG3	1:A:483:ARG:NH1	2.26	0.50
1:A:494:ARG:HH21	1:B:479:ASP:CG	2.20	0.50
1:B:335:PHE:C	1:B:337:GLN:H	2.18	0.50
1:C:456:MET:CE	1:C:474:ALA:CB	2.90	0.50
1:C:326:ARG:HB2	1:C:609:THR:C	2.35	0.50
1:A:345:TYR:CE2	1:A:347:PRO:HA	2.47	0.49
1:B:532:ASN:HB3	1:B:553:ARG:CA	2.41	0.49
1:B:438:ASN:HB3	1:B:459:ARG:HG2	1.94	0.49
1:C:584:TYR:HB2	1:C:591:TRP:CD2	2.47	0.49
1:X:329:TYR:CE1	1:X:609:THR:HG22	2.47	0.49
1:X:418:VAL:HA	1:X:426:TYR:O	2.12	0.49
1:A:456:MET:HB3	1:A:488:GLU:OE2	2.12	0.49
1:C:515:LEU:CD1	1:C:561:VAL:HG21	2.23	0.49
1:B:501:THR:CG2	1:B:542:GLU:OE2	2.60	0.49
1:B:501:THR:CB	1:B:542:GLU:OE2	2.60	0.49
1:C:576:THR:O	1:C:578:LEU:HD22	2.13	0.49
1:X:409:MET:HE1	1:X:427:ALA:HB1	1.95	0.49
1:A:456:MET:HE3	1:A:474:ALA:HB3	1.95	0.49
1:B:503:MET:HE3	1:B:521:ALA:CB	2.43	0.49
1:X:530:GLN:OE1	1:X:574:GLY:CA	2.61	0.49
1:A:456:MET:CE	1:A:474:ALA:CB	2.91	0.49
1:A:515:LEU:CD1	1:A:561:VAL:HG21	2.39	0.49
1:C:397:ASN:OD1	1:C:399:MET:N	2.45	0.49
1:C:584:TYR:CZ	1:C:585:ASP:O	2.66	0.49
1:A:413:ARG:NH1	1:A:439:SER:O	2.46	0.49
1:A:503:MET:CE	1:A:507:ARG:HD2	2.24	0.49
1:A:512:VAL:HA	1:A:520:TYR:O	2.13	0.49
1:B:468:LEU:HG	1:B:469:ASN:OD1	2.12	0.49
1:B:505:THR:HG23	1:B:546:PHE:HZ	1.78	0.49
1:B:520:TYR:OH	1:B:536:ARG:NH1	2.46	0.48
1:B:532:ASN:HB3	1:B:553:ARG:HG2	1.94	0.48
1:C:582:GLU:HA	1:C:592:SER:O	2.12	0.48
1:X:583:CYS:HB2	1:X:594:VAL:HG11	1.95	0.48
1:C:487:ALA:CB	1:C:500:ILE:HD11	2.41	0.48
1:A:381:ASN:C	1:A:381:ASN:HD22	2.21	0.48
1:C:505:THR:OG1	1:C:507:ARG:NH1	2.46	0.48
1:X:525:TYR:HB2	3:X:701:A1EMI:O17	2.12	0.48
1:X:581:VAL:HB	1:X:595:THR:HG23	1.95	0.48
1:C:511:GLY:C	1:C:559:ILE:HG21	2.39	0.48
1:X:484:LEU:N	1:X:484:LEU:HD22	2.29	0.48
1:X:572:TYR:CE2	1:X:574:GLY:HA2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:VAL:HA	1:A:373:LEU:O	2.13	0.48
1:A:369:VAL:HG23	1:A:373:LEU:O	2.13	0.48
1:A:555:SER:OG	2:A:701[A]:GFD:O21	2.31	0.48
1:B:466:ALA:HB3	1:B:519:ILE:HD11	1.95	0.48
1:C:484:LEU:N	1:C:484:LEU:HD12	2.29	0.48
1:A:327:LEU:HD13	1:A:344:ALA:HB1	1.95	0.48
1:A:460:ARG:HH21	1:A:488:GLU:HG3	1.77	0.48
1:C:468:LEU:HD23	1:C:539:VAL:CG1	2.43	0.48
1:C:487:ALA:HB3	1:C:500:ILE:CG1	2.43	0.48
1:X:463:VAL:HG23	1:X:475:VAL:O	2.14	0.48
1:X:409:MET:HE1	1:X:416:ILE:CD1	2.44	0.48
1:X:415:ARG:HH12	3:X:701:A1EMI:C05	2.27	0.48
1:C:372:GLY:HA2	1:C:609:THR:CG2	2.36	0.48
1:C:430:GLY:O	1:C:437:HIS:HB2	2.13	0.48
1:B:411:VAL:HG21	1:B:437:HIS:CE1	2.49	0.48
1:A:504:ASN:OD1	1:X:455:PRO:HG3	2.14	0.48
1:B:409:MET:HE1	1:B:413:ARG:HB2	1.96	0.48
1:C:354:ARG:NH2	1:C:357:ASP:OD1	2.46	0.47
1:B:457:LEU:N	1:B:488:GLU:OE1	2.37	0.47
1:X:344:ALA:HB3	1:X:353:LEU:HB2	1.95	0.47
1:C:340:SER:OG	1:C:358:LEU:HB2	2.14	0.47
1:C:503:MET:HB3	1:C:535:GLU:OE2	2.14	0.47
1:C:565:ARG:HH12	1:C:585:ASP:CG	2.22	0.47
1:A:409:MET:CE	1:A:427:ALA:CB	2.93	0.47
1:A:467:VAL:O	1:A:514:VAL:HG11	2.14	0.47
1:A:456:MET:HE3	1:A:474:ALA:CB	2.44	0.47
1:A:584:TYR:HB2	1:A:591:TRP:CE3	2.50	0.47
1:B:468:LEU:O	1:B:471:LEU:HB2	2.14	0.47
1:C:330:THR:HG22	1:C:601:ARG:NH1	2.30	0.47
1:X:553:ARG:HG3	1:X:553:ARG:HH11	1.80	0.47
1:A:409:MET:CE	1:A:427:ALA:HB1	2.45	0.47
1:B:327:LEU:HB2	1:B:329:TYR:CE1	2.50	0.47
1:B:371:GLY:O	1:B:373:LEU:HD12	2.15	0.47
1:B:490:TYR:HB2	1:B:497:TRP:CZ3	2.49	0.47
1:X:431:SER:CB	1:X:461:ILE:HG21	2.42	0.47
1:A:335:PHE:CD2	1:A:335:PHE:C	2.93	0.47
1:B:515:LEU:HD13	1:B:561:VAL:CG2	2.43	0.47
1:C:335:PHE:C	1:C:337:GLN:H	2.23	0.47
1:C:397:ASN:HB3	1:C:400:THR:CG2	2.45	0.47
1:A:462:GLY:HA3	2:A:701[A]:GFD:C35	2.45	0.47
1:C:334:TYR:HA	1:C:338:SER:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:327:LEU:O	1:X:608:VAL:HA	2.14	0.47
1:X:588:THR:OG1	1:X:590:THR:HG23	2.15	0.47
1:A:430:GLY:O	1:A:437:HIS:HB2	2.15	0.47
1:B:436:HIS:CD2	1:B:480:GLY:HA2	2.49	0.47
1:A:504:ASN:ND2	1:X:455:PRO:HB3	2.29	0.46
1:A:334:TYR:HB3	2:A:701[B]:GFD:O21	2.15	0.46
1:B:414:ASN:HD21	1:B:415:ARG:HG3	1.78	0.46
1:C:328:ILE:CD1	1:C:608:VAL:HB	2.38	0.46
1:C:560:THR:HG22	1:C:561:VAL:N	2.30	0.46
1:B:459:ARG:O	1:B:479:ASP:HA	2.15	0.46
1:C:477:GLY:C	1:C:484:LEU:HD13	2.40	0.46
1:X:418:VAL:C	1:X:465:VAL:HG21	2.40	0.46
1:X:566:ILE:O	1:X:583:CYS:HA	2.14	0.46
1:B:353:LEU:HD23	1:B:353:LEU:HA	1.74	0.46
1:B:550:MET:HB3	1:B:582:GLU:OE1	2.14	0.46
1:C:595:THR:CG2	1:C:596:ARG:N	2.78	0.46
1:X:424:HIS:HB3	1:X:442:ARG:HD2	1.97	0.46
1:X:532:ASN:HB3	1:X:553:ARG:HG2	1.96	0.46
1:C:568:VAL:HG22	1:C:582:GLU:O	2.16	0.46
1:C:585:ASP:OD1	1:C:585:ASP:C	2.58	0.46
1:X:414:ASN:O	1:X:415:ARG:CB	2.64	0.46
1:C:561:VAL:HG23	1:C:566:ILE:HD12	1.97	0.46
1:A:537:TYR:HB2	1:A:544:TRP:CE2	2.51	0.46
1:A:557:LEU:CD1	1:A:568:VAL:CG1	2.93	0.46
1:B:362:ARG:HH21	1:B:378:GLY:C	2.20	0.46
1:B:421:ILE:HG12	1:B:467:VAL:HG21	1.98	0.46
1:B:420:VAL:HA	1:B:424:HIS:O	2.16	0.46
1:B:597:MET:HE1	1:B:601:ARG:HG2	1.98	0.46
1:A:528:GLN:O	1:A:529:ASP:HB2	2.16	0.46
1:B:418:VAL:HA	1:B:426:TYR:O	2.16	0.46
1:B:513:CYS:SG	1:B:559:ILE:HD11	2.55	0.46
1:X:457:LEU:N	1:X:488:GLU:OE1	2.41	0.46
1:B:458:THR:HG23	1:B:499:MET:HE1	1.96	0.46
1:X:512:VAL:HA	1:X:520:TYR:O	2.16	0.46
1:X:538:ASP:HB3	1:X:541:THR:OG1	2.16	0.46
1:B:505:THR:OG1	1:B:507:ARG:NH1	2.48	0.45
1:C:327:LEU:C	1:C:608:VAL:HG23	2.41	0.45
1:C:490:TYR:CE1	1:C:495:ASN:HA	2.51	0.45
1:X:329:TYR:O	1:X:606:VAL:HA	2.16	0.45
1:A:508:SER:OG	2:A:701[A]:GFD:O20	2.33	0.45
1:B:378:GLY:O	1:B:390:SER:OG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:LEU:HD23	1:C:539:VAL:HG11	1.97	0.45
1:C:561:VAL:HG23	1:C:566:ILE:HA	1.99	0.45
1:B:354:ARG:NH1	1:B:357:ASP:OD1	2.47	0.45
1:C:547:VAL:CG2	1:C:584:TYR:OH	2.63	0.45
1:A:539:VAL:HG22	1:B:435:ILE:HG12	1.98	0.45
1:A:550:MET:CE	1:A:554:ARG:HG2	2.44	0.45
1:C:487:ALA:HB3	1:C:500:ILE:CD1	2.45	0.45
1:C:503:MET:HE1	1:C:507:ARG:HB2	1.98	0.45
1:C:547:VAL:HG21	1:C:584:TYR:OH	2.16	0.45
1:A:503:MET:HA	1:A:544:TRP:CD1	2.52	0.45
1:C:520:TYR:CZ	1:C:536:ARG:HD3	2.52	0.45
1:B:472:LEU:HD23	1:B:472:LEU:C	2.42	0.45
1:B:597:MET:HE1	1:B:601:ARG:HD2	1.99	0.45
1:X:560:THR:HB	1:X:606:VAL:HG12	1.98	0.45
1:B:464:GLY:CA	1:B:512:VAL:HG21	2.45	0.45
1:X:381:ASN:O	1:X:387:ASN:HA	2.17	0.45
1:A:537:TYR:HB2	1:A:544:TRP:CZ3	2.52	0.45
1:A:557:LEU:HD23	1:A:557:LEU:N	2.19	0.45
1:A:335:PHE:C	1:A:337:GLN:H	2.24	0.45
1:A:466:ALA:HB1	1:A:514:VAL:CG1	2.46	0.45
1:B:460:ARG:HB3	1:B:463:VAL:HB	1.99	0.45
1:X:585:ASP:CG	1:X:588:THR:HG23	2.42	0.45
1:C:491:TYR:O	1:C:495:ASN:N	2.50	0.44
1:X:325:GLY:O	1:X:327:LEU:HD22	2.18	0.44
1:A:415:ARG:NH1	2:A:701[A]:GFD:O39	2.50	0.44
1:A:334:TYR:HB3	2:A:701[A]:GFD:O18	2.18	0.44
1:A:342:LEU:HD22	1:A:403:TRP:CZ2	2.52	0.44
1:X:409:MET:CE	1:X:413:ARG:HD2	2.47	0.44
1:X:490:TYR:CZ	1:X:492:PRO:HA	2.52	0.44
1:A:465:VAL:HG13	1:A:472:LEU:HD21	1.99	0.44
1:B:380:ARG:HH12	1:B:415:ARG:NH2	2.14	0.44
1:B:441:GLU:HA	1:B:452:LEU:HA	2.00	0.44
1:C:490:TYR:O	1:C:492:PRO:HD3	2.17	0.44
1:X:411:VAL:HG21	1:X:437:HIS:NE2	2.33	0.44
1:C:339:LEU:HD12	1:C:339:LEU:N	2.31	0.44
1:X:491:TYR:O	1:X:495:ASN:N	2.48	0.44
1:X:507:ARG:HD3	1:X:523:GLY:O	2.16	0.44
1:B:419:GLY:O	1:B:426:TYR:HB2	2.18	0.44
1:C:347:PRO:HB3	1:C:567:TYR:OH	2.17	0.44
1:X:409:MET:CE	1:X:427:ALA:CB	2.96	0.44
1:B:328:ILE:O	1:B:344:ALA:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:MET:CE	1:B:507:ARG:HD2	2.48	0.44
1:C:526:ASP:HB3	1:C:531:LEU:HD21	2.00	0.44
1:X:503:MET:HB3	1:X:535:GLU:OE2	2.18	0.44
1:A:337:GLN:CG	1:A:382:ASN:HD22	2.31	0.44
1:B:377:VAL:HG12	1:B:393:LEU:HD13	2.00	0.44
1:B:515:LEU:HB3	1:B:520:TYR:CE1	2.52	0.44
1:B:568:VAL:HG21	1:B:582:GLU:HB2	1.98	0.44
1:X:442:ARG:HG2	1:X:443:TYR:N	2.33	0.44
1:X:488:GLU:HG3	1:X:497:TRP:CE3	2.53	0.44
1:C:490:TYR:CE2	1:C:492:PRO:HA	2.53	0.43
1:A:338:SER:OG	1:A:382:ASN:HB2	2.18	0.43
1:B:554:ARG:HH21	1:B:570:GLY:N	2.16	0.43
1:C:346:ASN:HB3	1:C:349:ASP:OD1	2.18	0.43
1:X:427:ALA:O	1:X:440:VAL:HG13	2.17	0.43
1:A:460:ARG:HB3	1:A:463:VAL:HB	2.01	0.43
1:A:582:GLU:HA	1:A:592:SER:O	2.18	0.43
1:B:366:ALA:O	1:B:377:VAL:HG22	2.18	0.43
1:C:397:ASN:OD1	1:C:397:ASN:C	2.60	0.43
1:X:503:MET:CE	1:X:507:ARG:HH11	2.31	0.43
1:A:347:PRO:HG2	1:A:562:HIS:CE1	2.54	0.43
1:C:363:SER:O	1:C:380:ARG:N	2.43	0.43
2:C:701[B]:GFD:O19	2:C:701[B]:GFD:C38	2.67	0.43
1:X:490:TYR:CE2	1:X:492:PRO:HA	2.54	0.43
1:X:490:TYR:O	1:X:492:PRO:HD3	2.17	0.43
1:B:327:LEU:O	1:B:608:VAL:HA	2.19	0.43
1:B:425:ILE:HB	1:B:443:TYR:HB3	2.00	0.43
1:A:328:ILE:O	1:A:344:ALA:HA	2.19	0.43
1:B:430:GLY:O	1:B:437:HIS:HB2	2.18	0.43
1:C:356:ALA:O	1:C:403:TRP:NE1	2.44	0.43
1:B:335:PHE:HA	1:B:577:PHE:CE1	2.53	0.43
1:B:343:GLU:OE2	1:B:598:THR:HG21	2.19	0.43
1:C:374:LEU:C	1:C:374:LEU:HD23	2.43	0.43
1:X:328:ILE:CG2	1:X:560:THR:HG21	2.39	0.43
1:X:515:LEU:HB3	1:X:520:TYR:CE1	2.54	0.43
1:X:551:LYS:HD2	1:X:551:LYS:HA	1.69	0.43
1:X:334:TYR:CA	1:X:339:LEU:CD1	2.97	0.43
1:A:380:ARG:CZ	1:A:414:ASN:HD22	2.32	0.43
1:A:503:MET:HG2	1:A:544:TRP:CE2	2.54	0.43
1:C:330:THR:HG23	1:C:604:VAL:CG2	2.46	0.43
1:C:537:TYR:OH	1:C:542:GLU:OE2	2.35	0.43
1:X:508:SER:OG	3:X:701:A1EMI:N56	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:THR:HG21	1:A:484:LEU:CD1	2.47	0.42
1:A:550:MET:HE1	1:A:554:ARG:CD	2.49	0.42
1:C:328:ILE:HD13	1:C:608:VAL:CB	2.39	0.42
1:X:579:ASP:HB3	1:X:600:GLY:CA	2.49	0.42
1:A:370:VAL:HG22	1:A:420:VAL:CG2	2.44	0.42
1:B:557:LEU:HD12	1:B:558:GLY:O	2.18	0.42
1:C:355:LEU:N	1:C:355:LEU:HD22	2.34	0.42
1:C:548:ALA:HB2	1:C:589:ASP:OD1	2.20	0.42
1:X:554:ARG:HH22	1:X:580:SER:HG	1.59	0.42
1:X:338:SER:O	1:X:361:PRO:HB3	2.20	0.42
1:X:343:GLU:OE2	1:X:598:THR:HG21	2.20	0.42
1:A:425:ILE:HB	1:A:443:TYR:HB3	2.01	0.42
1:A:436:HIS:O	1:A:459:ARG:CD	2.67	0.42
1:B:501:THR:HG23	1:B:542:GLU:OE2	2.18	0.42
1:C:365:LEU:C	1:C:365:LEU:HD12	2.44	0.42
1:X:396:TYR:CE2	1:X:398:PRO:HA	2.54	0.42
1:A:486:SER:HB2	1:A:499:MET:HE3	2.01	0.42
1:B:393:LEU:HD22	1:B:450:TRP:CZ2	2.55	0.42
1:B:557:LEU:HD12	1:B:558:GLY:C	2.44	0.42
1:C:490:TYR:HB2	1:C:497:TRP:CZ3	2.54	0.42
1:X:525:TYR:CD1	1:X:530:GLN:NE2	2.87	0.42
1:A:504:ASN:CG	1:X:455:PRO:HG3	2.44	0.42
1:C:471:LEU:CD2	1:C:491:TYR:HD2	2.32	0.42
1:C:583:CYS:O	1:C:591:TRP:HA	2.20	0.42
1:A:440:VAL:HG23	1:A:453:VAL:CG2	2.50	0.42
1:B:483:ARG:HD3	1:B:508:SER:HB3	2.02	0.42
1:B:526:ASP:N	1:B:531:LEU:HD21	2.35	0.42
1:A:355:LEU:HD12	1:A:355:LEU:N	2.34	0.42
1:C:468:LEU:HG	1:C:469:ASN:OD1	2.19	0.42
1:A:365:LEU:HB2	1:A:377:VAL:O	2.19	0.42
1:B:327:LEU:HD13	1:B:344:ALA:CB	2.48	0.42
1:B:370:VAL:O	1:B:370:VAL:HG23	2.20	0.42
1:C:520:TYR:CD1	1:C:536:ARG:HB3	2.54	0.42
1:C:547:VAL:HG21	1:C:584:TYR:CZ	2.55	0.42
1:X:334:TYR:HA	1:X:339:LEU:CD1	2.50	0.42
1:X:396:TYR:CZ	1:X:401:ASN:HA	2.54	0.42
1:X:421:ILE:HD13	1:X:492:PRO:HG2	2.01	0.42
1:B:421:ILE:HD11	1:B:472:LEU:HB2	2.02	0.42
1:B:444:GLU:OE1	1:B:447:ARG:NH1	2.53	0.42
1:B:519:ILE:O	1:B:536:ARG:HA	2.20	0.42
1:B:597:MET:HE1	1:B:601:ARG:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:ILE:HB	1:C:426:TYR:CE2	2.53	0.42
1:C:483:ARG:HD3	1:C:508:SER:HB3	2.02	0.42
1:B:374:LEU:HD23	1:B:374:LEU:C	2.44	0.41
1:C:520:TYR:CE1	1:C:536:ARG:HD3	2.55	0.41
1:C:521:ALA:O	1:C:534:VAL:HG23	2.20	0.41
1:B:491:TYR:O	1:B:495:ASN:N	2.52	0.41
1:C:456:MET:HE1	1:C:474:ALA:HB1	2.01	0.41
1:B:345:TYR:HB2	1:B:352:TRP:CH2	2.55	0.41
1:C:345:TYR:CD2	1:C:346:ASN:N	2.88	0.41
1:X:369:VAL:CG2	1:X:607:ALA:HB1	2.46	0.41
1:X:490:TYR:HB2	1:X:497:TRP:CZ3	2.55	0.41
1:X:518:CYS:SG	1:X:536:ARG:HD2	2.60	0.41
1:B:471:LEU:HD21	1:B:491:TYR:CD2	2.55	0.41
1:X:370:VAL:HG13	1:X:423:GLY:HA2	2.03	0.41
1:X:556:ALA:HB2	3:X:701:A1EMI:C05	2.49	0.41
1:X:568:VAL:HG22	1:X:582:GLU:HB2	2.03	0.41
1:A:337:GLN:HG2	1:A:382:ASN:HD22	1.85	0.41
1:B:370:VAL:O	1:B:370:VAL:CG2	2.68	0.41
1:C:349:ASP:OD2	1:C:351:THR:CG2	2.68	0.41
1:X:504:ASN:HB2	1:X:546:PHE:CE2	2.56	0.41
1:A:389:ASP:OD2	1:A:433:GLY:N	2.46	0.41
1:A:467:VAL:HA	1:A:471:LEU:O	2.20	0.41
1:A:584:TYR:HB2	1:A:591:TRP:CH2	2.55	0.41
1:C:327:LEU:HD23	1:C:327:LEU:HA	1.82	0.41
1:C:485:ASN:HB3	1:C:506:ILE:HA	2.03	0.41
1:C:537:TYR:HB2	1:C:544:TRP:CD2	2.55	0.41
1:X:522:ALA:HA	1:X:534:VAL:HG22	2.03	0.41
1:A:361:PRO:C	1:A:362:ARG:HG3	2.46	0.41
1:A:415:ARG:HH12	2:A:701[A]:GFD:C02	2.33	0.41
1:A:585:ASP:CG	1:A:588:THR:HG23	2.45	0.41
1:C:432:HIS:HB3	1:C:435:ILE:HB	2.03	0.41
1:C:463:VAL:HG23	1:C:475:VAL:O	2.21	0.41
1:A:386:GLY:HA2	1:C:481:THR:O	2.20	0.41
1:B:363:SER:O	1:B:380:ARG:N	2.53	0.41
1:B:503:MET:CE	1:B:521:ALA:CB	2.98	0.41
1:C:362:ARG:HG2	1:C:381:ASN:HB3	2.02	0.41
1:C:369:VAL:HG11	1:C:608:VAL:O	2.20	0.41
1:A:485:ASN:HB3	1:A:506:ILE:HG13	2.03	0.41
1:A:487:ALA:HB3	1:A:500:ILE:CD1	2.50	0.41
1:X:584:TYR:HB2	1:X:591:TRP:CZ3	2.55	0.41
1:A:533:SER:HA	1:A:549:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:GLU:CG	1:X:435:ILE:HD13	2.51	0.41
1:A:565:ARG:HD2	1:A:583:CYS:SG	2.61	0.41
1:B:532:ASN:HB3	1:B:553:ARG:CG	2.50	0.41
1:C:346:ASN:OD1	1:C:346:ASN:C	2.64	0.41
1:C:479:ASP:N	1:C:484:LEU:HD11	2.36	0.41
1:C:513:CYS:HG	1:C:566:ILE:HD11	1.82	0.41
1:X:335:PHE:N	1:X:339:LEU:HD11	2.36	0.41
1:A:411:VAL:CG2	1:A:412:PRO:HD2	2.51	0.40
1:A:426:TYR:CE1	1:A:442:ARG:HB2	2.56	0.40
1:A:459:ARG:O	1:A:479:ASP:HA	2.21	0.40
1:B:485:ASN:HB3	1:B:506:ILE:HA	2.03	0.40
1:C:475:VAL:HG13	1:C:503:MET:HE2	2.03	0.40
1:A:541:THR:O	1:A:542:GLU:HB3	2.22	0.40
1:B:529:ASP:N	1:B:529:ASP:OD1	2.52	0.40
1:B:537:TYR:HE2	1:B:542:GLU:OE1	2.05	0.40
1:C:477:GLY:O	1:C:484:LEU:HD13	2.22	0.40
1:C:541:THR:HG22	1:C:543:THR:OG1	2.20	0.40
1:C:490:TYR:HB2	1:C:497:TRP:CZ2	2.56	0.40
1:X:396:TYR:CE1	1:X:401:ASN:HA	2.57	0.40
1:A:425:ILE:O	1:A:442:ARG:HA	2.21	0.40
1:X:346:ASN:HB3	1:X:351:THR:CG2	2.52	0.40
1:A:569:LEU:HG	1:A:581:VAL:HG22	2.03	0.40
1:B:385:ASP:OD2	1:B:385:ASP:N	2.40	0.40
1:C:428:VAL:HA	1:C:440:VAL:HG22	2.04	0.40
1:C:461:ILE:HG13	1:C:478:PHE:HB3	2.01	0.40
1:C:566:ILE:HG22	1:C:584:TYR:CB	2.39	0.40
1:X:415:ARG:CB	1:X:462:GLY:H	2.34	0.40
1:X:417:GLY:HA3	1:X:465:VAL:HG13	2.03	0.40
1:X:443:TYR:OH	1:X:448:ASP:OD1	2.33	0.40
1:X:468:LEU:O	1:X:471:LEU:HB2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:SER:OG	1:C:540:GLU:OE2[1_455]	1.75	0.45

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	284/288 (99%)	273 (96%)	11 (4%)	0	100	100
1	B	283/288 (98%)	273 (96%)	10 (4%)	0	100	100
1	C	277/288 (96%)	269 (97%)	8 (3%)	0	100	100
1	X	284/288 (99%)	272 (96%)	11 (4%)	1 (0%)	30	66
All	All	1128/1152 (98%)	1087 (96%)	40 (4%)	1 (0%)	48	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	384	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/234 (99%)	226 (97%)	6 (3%)	41	72
1	B	231/234 (99%)	231 (100%)	0	100	100
1	C	228/234 (97%)	228 (100%)	0	100	100
1	X	232/234 (99%)	229 (99%)	3 (1%)	65	85
All	All	923/936 (99%)	914 (99%)	9 (1%)	73	88

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

Mol	Chain	Res	Type
1	A	381	ASN
1	A	512	VAL
1	A	560	THR
1	A	568	VAL
1	A	604	VAL
1	A	609	THR
1	X	400	THR
1	X	484	LEU
1	X	609	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	337	GLN
1	A	382	ASN
1	A	432	HIS
1	A	504	ASN
1	B	424	HIS
1	B	528	GLN
1	B	563	GLN
1	C	381	ASN
1	C	517	ASN
1	X	359	GLN
1	X	402	GLN
1	X	517	ASN
1	X	552	HIS
1	X	575	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	GFD	A	701[A]	-	44,44,44	1.06	2 (4%)	59,65,65	1.27	6 (10
2	GFD	C	701[B]	-	44,44,44	1.23	4 (9%)	59,65,65	1.25	8 (13
2	GFD	C	701[A]	-	44,44,44	1.13	3 (6%)	59,65,65	1.41	11 (18
2	GFD	A	701[B]	-	44,44,44	1.12	2 (4%)	59,65,65	1.25	6 (10
3	A1EMI	X	701	-	104,104,104	2.85	46 (44%)	135,149,149	2.85	46 (34

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GFD	A	701[A]	-	-	13/42/42/42	0/4/4/4
2	GFD	C	701[B]	-	-	15/42/42/42	0/4/4/4
2	GFD	C	701[A]	-	-	9/42/42/42	0/4/4/4
2	GFD	A	701[B]	-	-	11/42/42/42	0/4/4/4
3	A1EMI	X	701	-	-	30/106/106/106	0/8/8/8

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	701	A1EMI	S14-N11	8.91	1.77	1.65
3	X	701	A1EMI	C16-S13	7.87	1.87	1.76
3	X	701	A1EMI	C61-S64	7.54	1.87	1.76
3	X	701	A1EMI	S64-N65	7.03	1.75	1.65
3	X	701	A1EMI	C68-N65	6.90	1.50	1.44
3	X	701	A1EMI	C07-N12	6.79	1.50	1.44
3	X	701	A1EMI	C15-S14	6.43	1.85	1.76
3	X	701	A1EMI	S79-N78	5.74	1.73	1.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	701	A1EMI	C47-N48	5.41	1.47	1.35
3	X	701	A1EMI	C34-N33	5.31	1.47	1.35
3	X	701	A1EMI	C95-N96	4.62	1.47	1.32
2	C	701[B]	GFD	S15-N12	4.60	1.71	1.65
2	C	701[A]	GFD	S15-N12	4.46	1.71	1.65
3	X	701	A1EMI	C91-N92	4.42	1.47	1.32
3	X	701	A1EMI	O20-S14	4.09	1.48	1.43
3	X	701	A1EMI	C55-N56	3.99	1.45	1.32
2	C	701[B]	GFD	S14-N11	3.97	1.70	1.65
2	A	701[A]	GFD	S15-N12	3.90	1.70	1.65
2	A	701[B]	GFD	S15-N12	3.82	1.70	1.65
2	A	701[B]	GFD	S14-N11	3.70	1.70	1.65
3	X	701	A1EMI	O17-S13	3.63	1.47	1.43
3	X	701	A1EMI	S13-N12	3.63	1.70	1.65
3	X	701	A1EMI	C80-S79	3.52	1.81	1.76
3	X	701	A1EMI	C51-N52	3.48	1.44	1.32
3	X	701	A1EMI	O82-S79	3.35	1.47	1.43
3	X	701	A1EMI	C90-C91	3.21	1.56	1.52
3	X	701	A1EMI	C05-C04	-3.13	1.37	1.43
3	X	701	A1EMI	O66-S64	3.07	1.47	1.43
3	X	701	A1EMI	C72-C71	3.02	1.44	1.38
3	X	701	A1EMI	C25-C15	2.88	1.43	1.38
3	X	701	A1EMI	C75-C74	2.75	1.43	1.36
3	X	701	A1EMI	O81-S79	2.72	1.46	1.43
2	C	701[A]	GFD	S14-N11	2.69	1.68	1.65
3	X	701	A1EMI	C70-C69	-2.60	1.38	1.43
3	X	701	A1EMI	C10-N11	2.57	1.46	1.44
3	X	701	A1EMI	O57-C55	-2.51	1.16	1.24
3	X	701	A1EMI	C30-C16	2.46	1.42	1.38
3	X	701	A1EMI	C01-C06	2.44	1.42	1.36
3	X	701	A1EMI	O18-S13	2.41	1.46	1.43
3	X	701	A1EMI	C02-C03	2.37	1.42	1.36
2	A	701[A]	GFD	S14-N11	2.31	1.68	1.65
3	X	701	A1EMI	O58-C47	-2.31	1.18	1.23
3	X	701	A1EMI	C29-C30	2.31	1.43	1.38
3	X	701	A1EMI	C94-C95	2.30	1.55	1.52
3	X	701	A1EMI	C60-C61	2.28	1.42	1.38
3	X	701	A1EMI	C71-N78	2.21	1.46	1.44
3	X	701	A1EMI	C01-C02	2.16	1.43	1.38
3	X	701	A1EMI	C46-C47	2.09	1.55	1.51
3	X	701	A1EMI	O53-C51	-2.09	1.17	1.24
2	C	701[A]	GFD	O19-S15	2.09	1.45	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	701	A1EMI	O36-C34	-2.06	1.19	1.23
2	C	701[B]	GFD	O20-S14	2.06	1.45	1.43
3	X	701	A1EMI	C73-C72	2.06	1.42	1.38
3	X	701	A1EMI	C94-N65	2.04	1.52	1.48
2	C	701[B]	GFD	O21-S14	2.04	1.45	1.43
3	X	701	A1EMI	O97-C95	-2.03	1.17	1.24
3	X	701	A1EMI	C68-C69	2.02	1.47	1.42

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	X	701	A1EMI	O67-S64-O66	-11.46	100.95	119.52
3	X	701	A1EMI	O82-S79-O81	-11.37	101.09	119.52
3	X	701	A1EMI	O19-S14-O20	-10.62	102.31	119.52
3	X	701	A1EMI	C50-C51-N52	7.19	127.21	115.86
3	X	701	A1EMI	O17-S13-O18	-6.75	108.58	119.52
3	X	701	A1EMI	C28-N33-C34	-6.31	116.45	127.50
3	X	701	A1EMI	O19-S14-C15	6.03	115.68	108.05
3	X	701	A1EMI	C07-N12-S13	5.89	125.57	117.24
3	X	701	A1EMI	C54-C55-N56	5.56	124.63	115.86
2	A	701[B]	GFD	C16-N12-S15	5.45	126.51	117.23
3	X	701	A1EMI	O20-S14-C15	4.75	114.06	108.05
3	X	701	A1EMI	O17-S13-C16	4.73	114.03	108.05
3	X	701	A1EMI	O18-S13-C16	4.58	113.84	108.05
3	X	701	A1EMI	C03-C04-C05	4.57	124.12	118.45
3	X	701	A1EMI	O57-C55-C54	-4.30	113.74	120.56
3	X	701	A1EMI	O81-S79-N78	4.21	111.69	106.71
2	C	701[B]	GFD	C17-S15-N12	4.05	112.44	106.92
3	X	701	A1EMI	C50-N11-S14	4.02	124.08	117.23
2	A	701[A]	GFD	C22-S14-N11	-4.01	101.45	106.92
3	X	701	A1EMI	C02-C03-C04	-3.94	115.42	120.89
3	X	701	A1EMI	O67-S64-N65	3.88	111.30	106.71
3	X	701	A1EMI	C32-O31-C23	-3.87	109.10	117.51
3	X	701	A1EMI	O82-S79-N78	3.78	111.18	106.71
2	C	701[B]	GFD	C16-N12-S15	3.78	123.67	117.23
3	X	701	A1EMI	O17-S13-N12	3.64	111.02	106.71
3	X	701	A1EMI	C61-S64-N65	3.55	111.76	106.92
2	A	701[A]	GFD	C17-S15-N12	3.53	111.73	106.92
2	C	701[A]	GFD	C13-C35-N36	-3.51	110.33	115.86
3	X	701	A1EMI	O67-S64-C61	3.47	112.44	108.05
2	C	701[A]	GFD	C22-S14-N11	-3.47	102.19	106.92
3	X	701	A1EMI	C03-C04-C07	-3.32	117.01	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	X	701	A1EMI	C30-C16-S13	3.25	123.18	119.76
2	C	701[A]	GFD	C41-O34-C25	3.23	124.53	117.51
3	X	701	A1EMI	O19-S14-N11	3.21	110.51	106.71
2	A	701[B]	GFD	O18-S15-N12	-3.17	102.95	106.71
2	C	701[A]	GFD	C16-N12-S15	3.17	122.63	117.23
3	X	701	A1EMI	C35-C34-N33	3.16	120.16	114.59
2	A	701[A]	GFD	O19-S15-N12	-3.08	103.06	106.71
3	X	701	A1EMI	C54-N12-S13	3.02	122.39	117.23
3	X	701	A1EMI	O82-S79-C80	2.96	111.79	108.05
2	C	701[A]	GFD	O20-S14-N11	2.94	110.19	106.71
2	A	701[A]	GFD	C41-O34-C25	2.94	123.89	117.51
2	A	701[B]	GFD	C17-S15-N12	2.90	110.88	106.92
3	X	701	A1EMI	O81-S79-C80	2.87	111.67	108.05
3	X	701	A1EMI	O53-C51-C50	-2.87	116.01	120.56
3	X	701	A1EMI	C16-S13-N12	-2.85	103.03	106.92
2	A	701[B]	GFD	C16-C38-N40	2.84	120.34	115.86
3	X	701	A1EMI	C01-C06-C05	-2.81	117.00	120.89
2	C	701[B]	GFD	O21-S14-C22	2.75	111.52	108.05
2	C	701[A]	GFD	C13-N11-S14	2.70	121.83	117.23
2	C	701[A]	GFD	C01-C06-N11	-2.70	116.60	119.75
3	X	701	A1EMI	C25-C15-S14	2.70	122.60	119.76
3	X	701	A1EMI	C89-O88-C85	-2.67	111.71	117.51
2	A	701[A]	GFD	C16-N12-S15	2.67	121.78	117.23
2	A	701[A]	GFD	O21-S14-C22	2.66	111.41	108.05
3	X	701	A1EMI	C90-N78-S79	2.61	121.68	117.23
2	C	701[A]	GFD	O37-C35-C13	2.51	124.54	120.56
2	C	701[B]	GFD	C06-N11-S14	2.50	120.78	117.24
3	X	701	A1EMI	O66-S64-C61	2.43	111.12	108.05
3	X	701	A1EMI	C06-C05-C10	-2.38	118.64	122.74
2	C	701[B]	GFD	C41-O34-C25	-2.35	112.41	117.51
2	C	701[A]	GFD	O19-S15-N12	-2.33	103.95	106.71
3	X	701	A1EMI	C90-C91-N92	2.33	119.54	115.86
3	X	701	A1EMI	C21-C15-S14	-2.30	117.34	119.76
2	A	701[B]	GFD	C13-N11-S14	2.29	121.13	117.23
2	A	701[B]	GFD	O39-C38-C16	-2.24	117.00	120.56
3	X	701	A1EMI	C94-N65-S64	2.18	120.94	117.23
2	C	701[B]	GFD	C22-S14-N11	-2.17	103.95	106.92
3	X	701	A1EMI	O20-S14-N11	2.16	109.26	106.71
3	X	701	A1EMI	C08-C07-N12	-2.14	117.26	119.75
3	X	701	A1EMI	C46-C47-N48	2.14	118.36	114.59
2	C	701[B]	GFD	C23-C22-S14	2.14	122.00	119.76
2	C	701[A]	GFD	C27-C22-S14	2.13	122.00	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	701[A]	GFD	C17-S15-N12	2.12	109.80	106.92
3	X	701	A1EMI	O53-C51-N52	-2.11	116.73	122.50
3	X	701	A1EMI	C60-C61-S64	2.10	121.97	119.76
2	C	701[B]	GFD	C01-C06-N11	2.02	122.09	119.75

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701[B]	GFD	C38-C16-N12-S15
2	C	701[A]	GFD	C03-N12-S15-C17
2	C	701[A]	GFD	C35-C13-N11-S14
2	C	701[B]	GFD	C38-C16-N12-C03
2	C	701[B]	GFD	C38-C16-N12-S15
2	C	701[B]	GFD	N11-C13-C35-N36
2	C	701[B]	GFD	N11-C13-C35-O37
2	C	701[B]	GFD	C35-C13-N11-C06
3	X	701	A1EMI	C34-C35-C37-O38
3	X	701	A1EMI	C68-N65-S64-O66
2	C	701[B]	GFD	C26-C25-O34-C41
2	C	701[B]	GFD	C24-C25-O34-C41
2	A	701[B]	GFD	C26-C25-O34-C41
3	X	701	A1EMI	C86-C85-O88-C89
2	A	701[B]	GFD	C24-C25-O34-C41
3	X	701	A1EMI	C84-C85-O88-C89
3	X	701	A1EMI	C24-C23-O31-C32
3	X	701	A1EMI	C22-C23-O31-C32
3	X	701	A1EMI	O41-C42-C43-O44
2	A	701[B]	GFD	C13-N11-S14-O20
2	C	701[B]	GFD	C16-N12-S15-O19
3	X	701	A1EMI	C50-N11-S14-O19
2	C	701[A]	GFD	C03-N12-S15-O19
2	A	701[A]	GFD	C13-N11-S14-O21
2	A	701[B]	GFD	C13-N11-S14-C22
2	C	701[A]	GFD	C16-N12-S15-O19
2	C	701[B]	GFD	C13-N11-S14-O20
3	X	701	A1EMI	C50-N11-S14-O20
3	X	701	A1EMI	C68-N65-S64-C61
3	X	701	A1EMI	C87-C80-S79-O82
2	A	701[A]	GFD	C16-N12-S15-O19
2	A	701[B]	GFD	C13-N11-S14-O21
2	C	701[B]	GFD	C16-N12-S15-O18

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Mol	Chain	Res	Type	Atoms
3	X	701	A1EMI	C94-N65-S64-O66
3	X	701	A1EMI	C83-C80-S79-O82
3	X	701	A1EMI	C10-N11-S14-O20
2	A	701[A]	GFD	C38-C16-N12-C03
2	C	701[A]	GFD	C35-C13-N11-C06
3	X	701	A1EMI	C95-C94-N65-C68
2	A	701[B]	GFD	C16-N12-S15-O18
2	C	701[A]	GFD	C16-N12-S15-C17
2	C	701[B]	GFD	C16-N12-S15-C17
2	C	701[B]	GFD	C13-N11-S14-C22
3	X	701	A1EMI	C50-N11-S14-C15
3	X	701	A1EMI	C94-N65-S64-C61
3	X	701	A1EMI	C87-C80-S79-N78
2	A	701[A]	GFD	C13-N11-S14-O20
2	A	701[B]	GFD	C16-N12-S15-O19
3	X	701	A1EMI	C71-N78-S79-O81
3	X	701	A1EMI	C83-C80-S79-N78
2	A	701[A]	GFD	C16-N12-S15-C17
2	A	701[A]	GFD	C16-N12-S15-O18
2	A	701[A]	GFD	C13-N11-S14-C22
2	C	701[B]	GFD	C13-N11-S14-O21
3	X	701	A1EMI	C94-N65-S64-O67
2	A	701[A]	GFD	C26-C25-O34-C41
2	A	701[A]	GFD	C35-C13-N11-S14
3	X	701	A1EMI	C55-C54-N12-S13
2	A	701[B]	GFD	C38-C16-N12-C03
2	A	701[B]	GFD	C05-C06-N11-C13
3	X	701	A1EMI	C05-C10-N11-C50
3	X	701	A1EMI	C39-C40-O41-C42
2	C	701[A]	GFD	C16-N12-S15-O18
2	A	701[A]	GFD	C24-C25-O34-C41
2	A	701[B]	GFD	C16-N12-S15-C17
3	X	701	A1EMI	C07-N12-S13-O17
3	X	701	A1EMI	C40-C39-O38-C37
2	C	701[B]	GFD	C06-N11-S14-O20
3	X	701	A1EMI	O38-C39-C40-O41
2	A	701[A]	GFD	N12-C16-C38-N40
2	C	701[B]	GFD	C06-N11-S14-C22
3	X	701	A1EMI	C29-C28-N33-C34
3	X	701	A1EMI	C35-C37-O38-C39
3	X	701	A1EMI	C91-C90-N78-S79
2	C	701[A]	GFD	C38-C16-N12-C03

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Mol	Chain	Res	Type	Atoms
2	A	701[A]	GFD	C04-C03-N12-C16
2	A	701[A]	GFD	C05-C06-N11-C13
2	C	701[A]	GFD	C04-C03-N12-C16

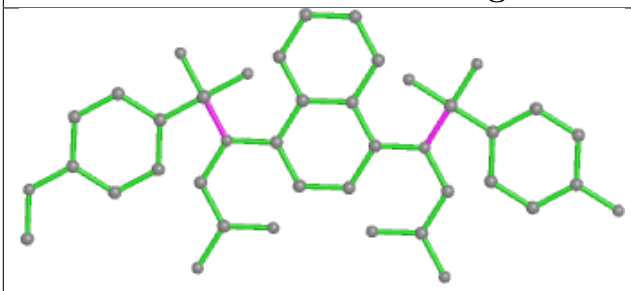
There are no ring outliers.

5 monomers are involved in 27 short contacts:

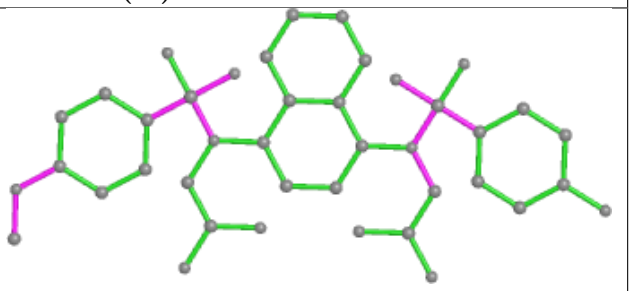
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701[A]	GFD	8	0
2	C	701[B]	GFD	2	0
2	C	701[A]	GFD	2	0
2	A	701[B]	GFD	3	0
3	X	701	A1EMI	12	0

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 then 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.

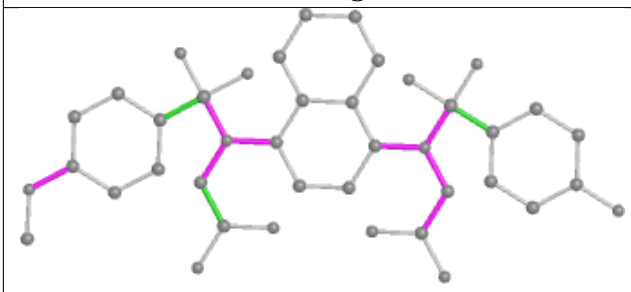
Ligand GFD A 701 (A)



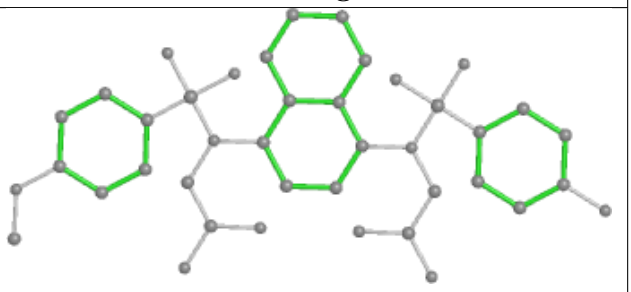
Bond lengths



Bond angles

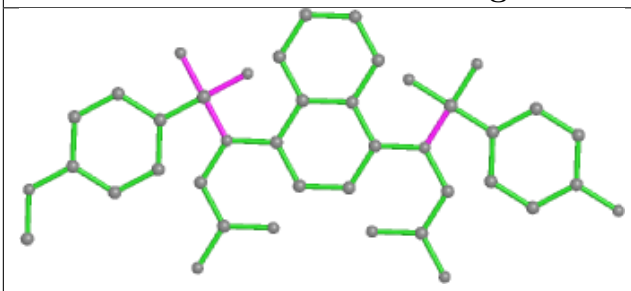


Torsions

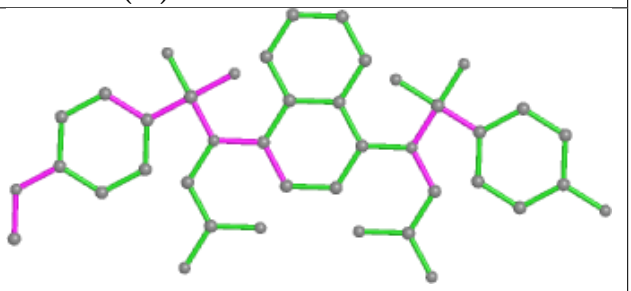


Rings

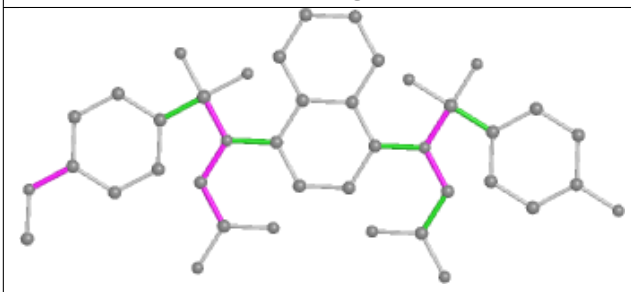
Ligand GFD C 701 (B)



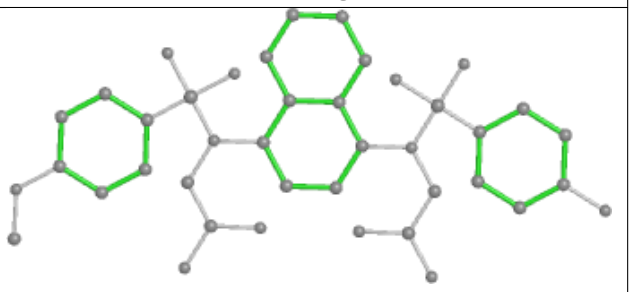
Bond lengths



Bond angles

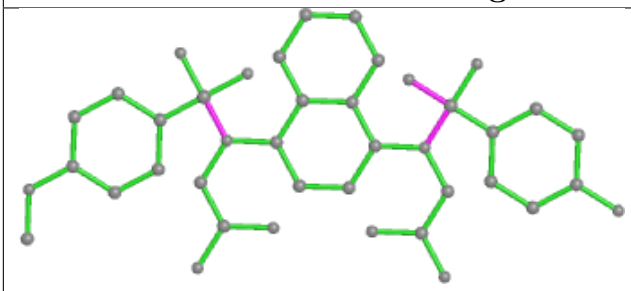


Torsions

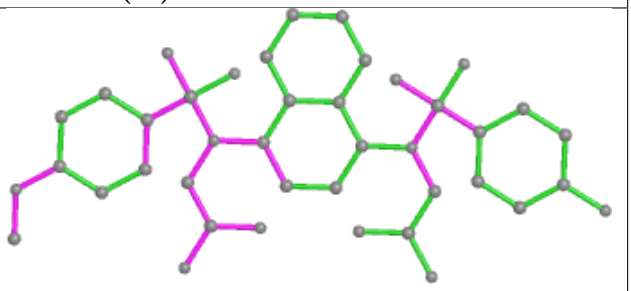


Rings

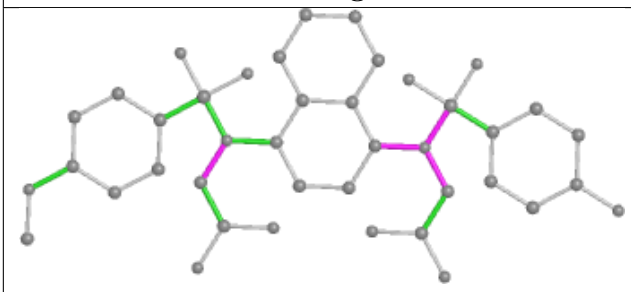
Ligand GFD C 701 (A)



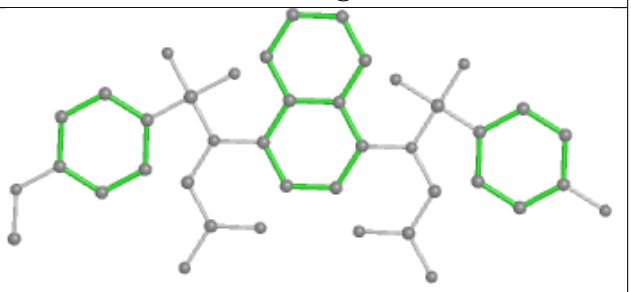
Bond lengths



Bond angles

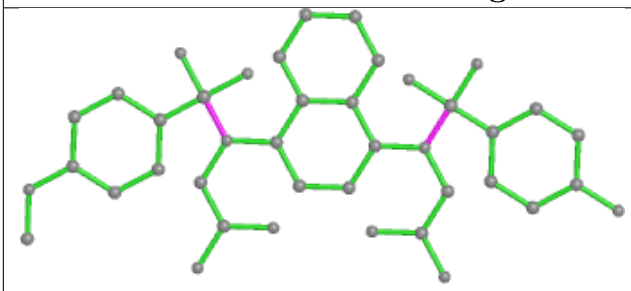


Torsions

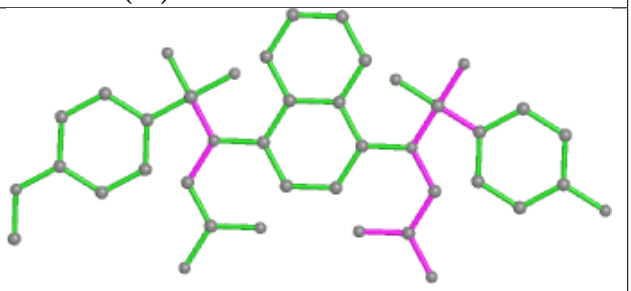


Rings

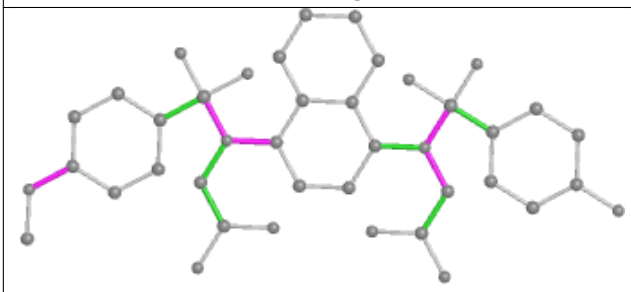
Ligand GFD A 701 (B)



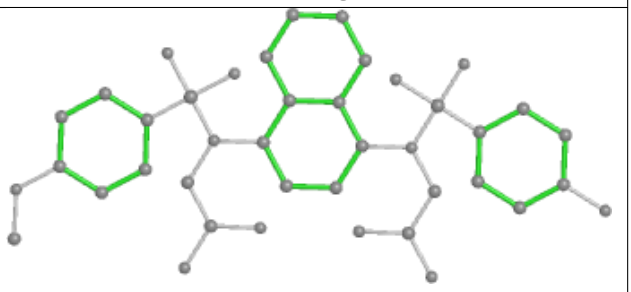
Bond lengths



Bond angles

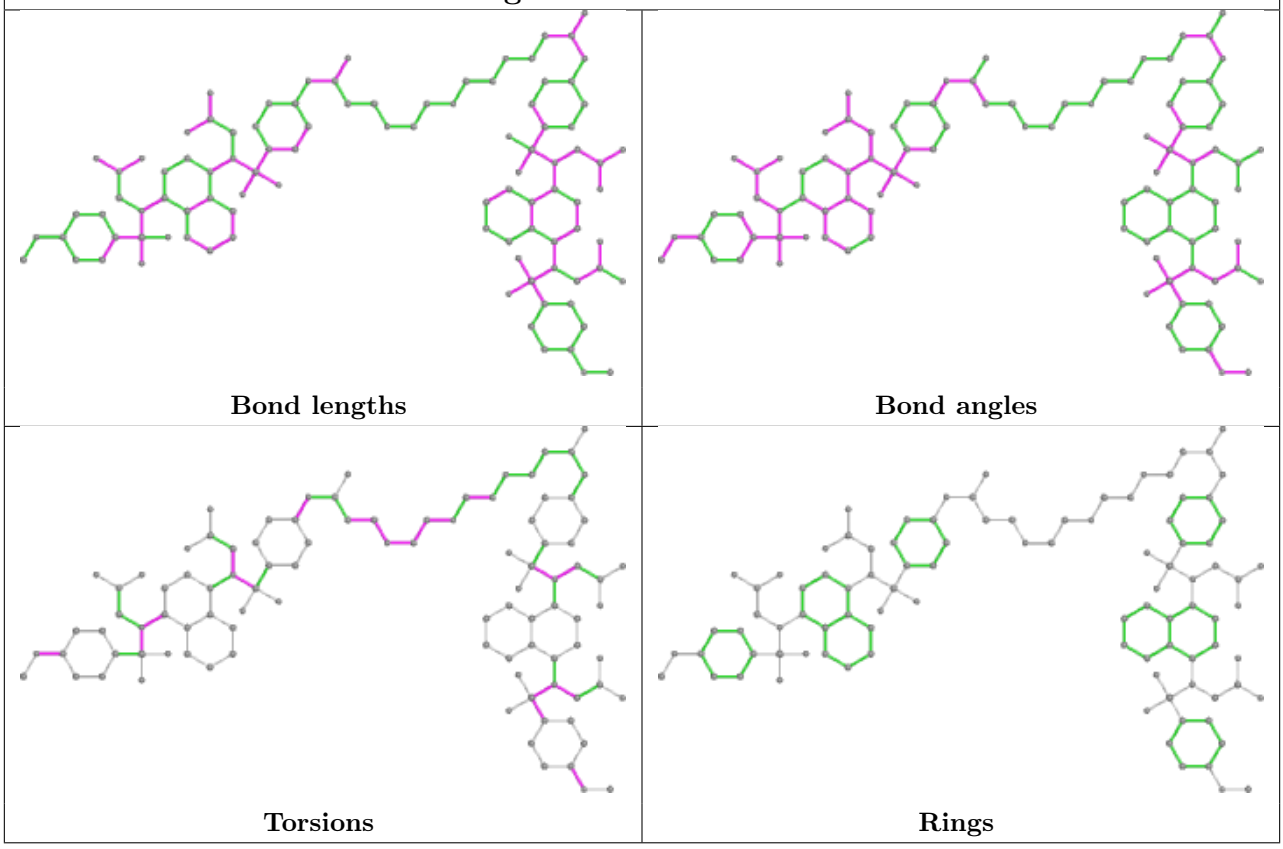


Torsions



Rings

Ligand A1EMI X 701



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, 95^{th} 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	286/288 (99%)	0.56	8 (2%) 55 33	50, 68, 88, 108	0
1	B	285/288 (98%)	0.88	24 (8%) 18 10	51, 79, 101, 110	0
1	C	280/288 (97%)	1.37	62 (22%) 3 2	72, 112, 135, 148	1 (0%)
1	X	286/288 (99%)	0.53	6 (2%) 63 41	45, 63, 85, 129	0
All	All	1137/1152 (98%)	0.83	100 (8%) 17 9	45, 75, 126, 148	1 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	332	GLY	4.2
1	B	380	ARG	3.7
1	C	394	ASP	3.6
1	X	540	GLU	3.6
1	C	329	TYR	3.5
1	X	324	VAL	3.5
1	A	324	VAL	3.4
1	A	574	GLY	3.4
1	C	578	LEU	3.4
1	B	359	GLN	3.4
1	B	540	GLU	3.4
1	C	358	LEU	3.3
1	C	392	ALA	3.3
1	C	327	LEU	3.3
1	C	420	VAL	3.2
1	B	527	GLY	3.2
1	C	602	SER	3.2
1	C	567	TYR	3.1
1	C	542	GLU	3.1
1	C	523	GLY	3.1
1	C	331	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	570	GLY	3.0
1	B	517	ASN	3.0
1	C	426	TYR	3.0
1	C	425	ILE	3.0
1	C	560	THR	3.0
1	C	407	ALA	3.0
1	A	540	GLU	2.9
1	C	514	VAL	2.9
1	C	574	GLY	2.9
1	C	443	TYR	2.8
1	B	446	GLU	2.8
1	A	426	TYR	2.8
1	B	483	ARG	2.8
1	C	334	TYR	2.8
1	B	338	SER	2.7
1	C	608	VAL	2.6
1	B	339	LEU	2.6
1	C	590	THR	2.6
1	C	581	VAL	2.6
1	C	328	ILE	2.6
1	C	513	CYS	2.5
1	C	341	TYR	2.5
1	C	398	PRO	2.5
1	C	330	THR	2.5
1	C	570	GLY	2.5
1	C	338	SER	2.4
1	C	601	ARG	2.4
1	C	372	GLY	2.4
1	C	599	SER	2.4
1	C	403	TRP	2.4
1	C	562	HIS	2.4
1	C	597	MET	2.4
1	C	577	PHE	2.4
1	B	336	ARG	2.4
1	X	387	ASN	2.4
1	C	325	GLY	2.3
1	C	467	VAL	2.3
1	X	386	GLY	2.3
1	A	446	GLU	2.3
1	B	591	TRP	2.3
1	A	381	ASN	2.3
1	B	551	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	575	HIS	2.3
1	X	404	SER	2.3
1	C	399	MET	2.2
1	C	557	LEU	2.2
1	C	549	PRO	2.2
1	C	360	VAL	2.2
1	B	529	ASP	2.2
1	B	329	TYR	2.2
1	C	520	TYR	2.2
1	C	376	ALA	2.2
1	C	355	LEU	2.2
1	C	561	VAL	2.2
1	C	566	ILE	2.2
1	B	325	GLY	2.2
1	B	332	GLY	2.2
1	A	380	ARG	2.2
1	B	362	ARG	2.2
1	C	604	VAL	2.2
1	C	564	GLY	2.1
1	C	576	THR	2.1
1	X	517	ASN	2.1
1	B	552	HIS	2.1
1	B	531	LEU	2.1
1	B	576	THR	2.1
1	B	578	LEU	2.1
1	C	510	ALA	2.1
1	C	416	ILE	2.1
1	A	591	TRP	2.1
1	C	548	ALA	2.0
1	C	375	TYR	2.0
1	C	408	PRO	2.0
1	C	586	PRO	2.0
1	C	442	ARG	2.0
1	C	406	CYS	2.0
1	C	509	GLY	2.0
1	B	557	LEU	2.0
1	C	546	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

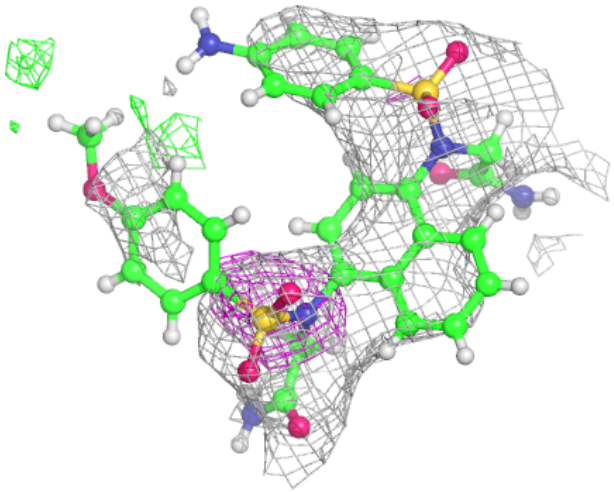
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

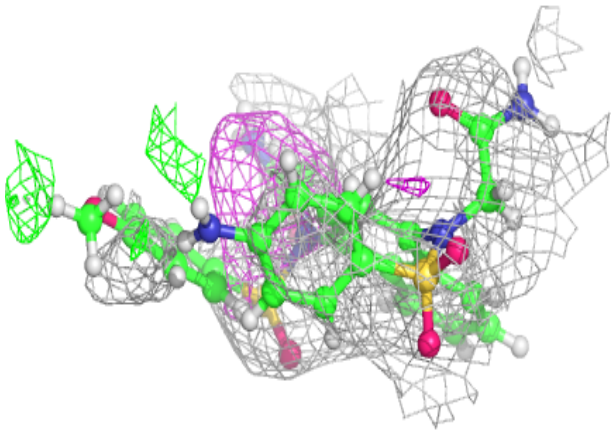
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GFD	C	701[A]	41/41	0.74	0.21	114,128,154,156	68
2	GFD	C	701[B]	41/41	0.74	0.21	113,127,153,154	68
2	GFD	A	701[A]	41/41	0.82	0.23	78,86,105,110	68
2	GFD	A	701[B]	41/41	0.82	0.23	77,88,107,110	68
3	A1EMI	X	701	97/97	0.82	0.19	69,95,118,133	0

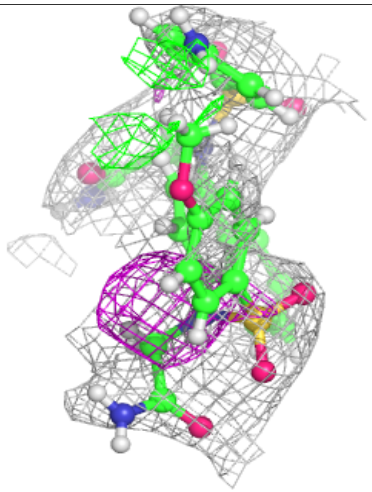
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GFD C 701 (A):

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

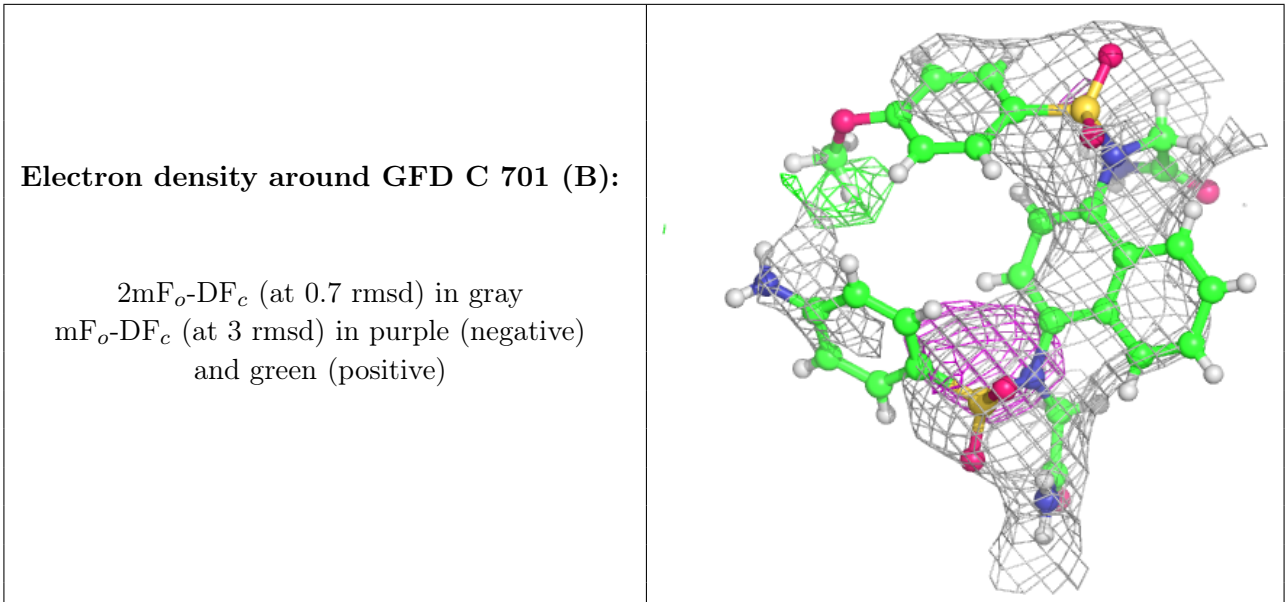


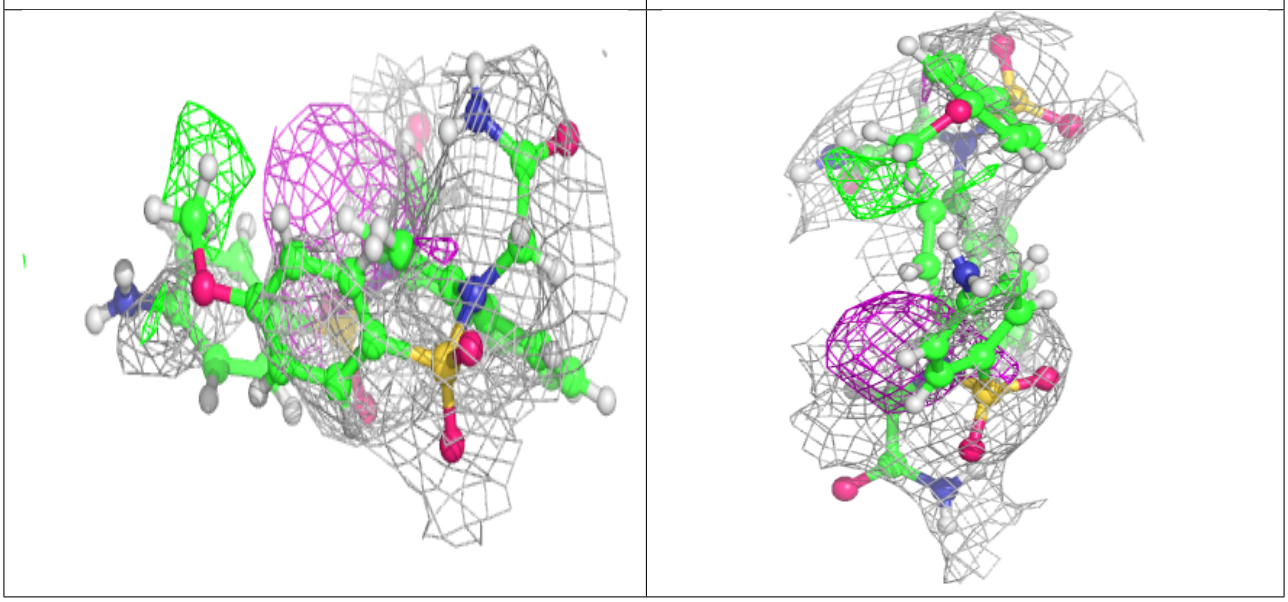




Electron density around GFD C 701 (B):

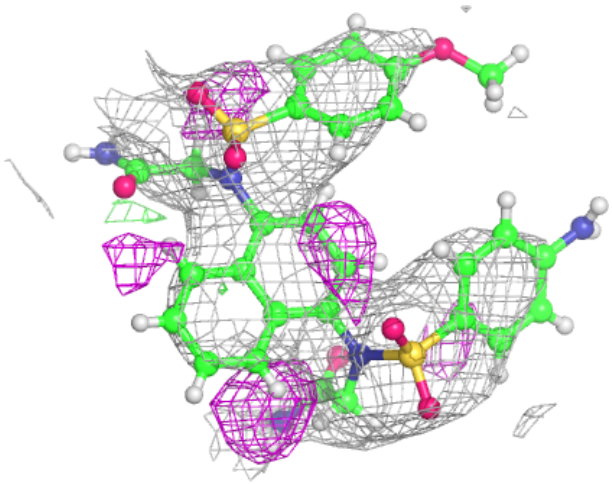
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

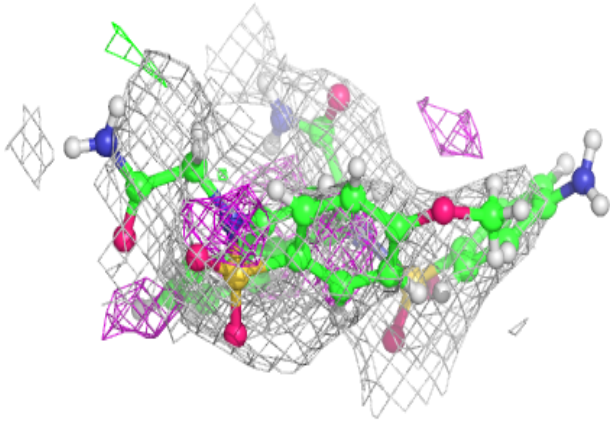


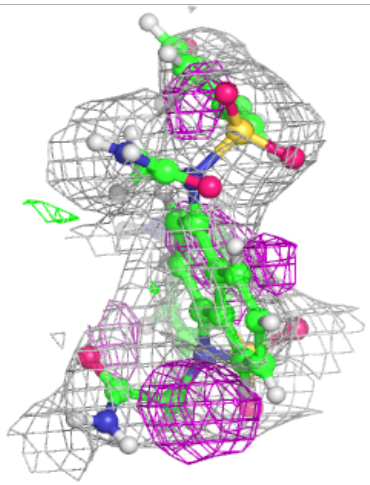


Electron density around GFD A 701 (A):

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

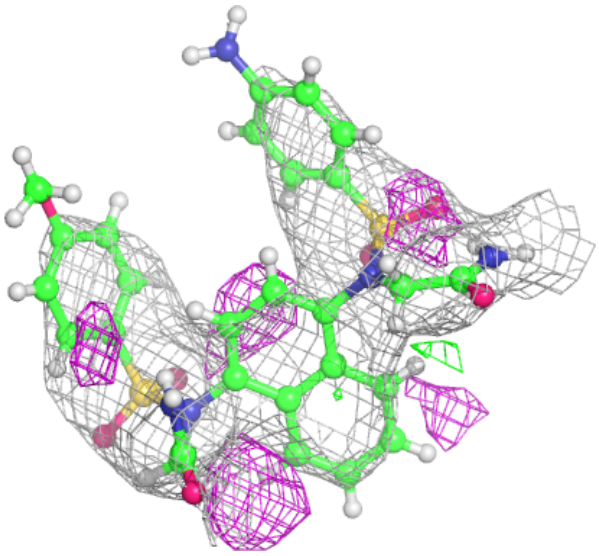


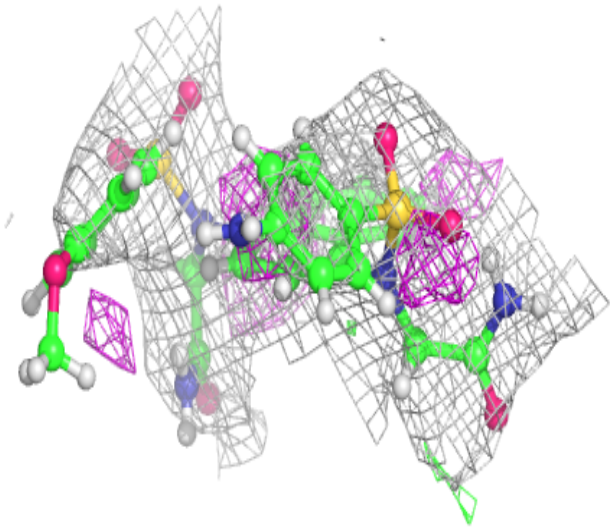


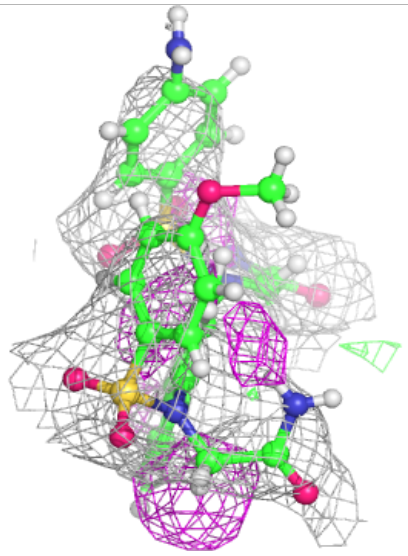


Electron density around GFD A 701 (B):

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

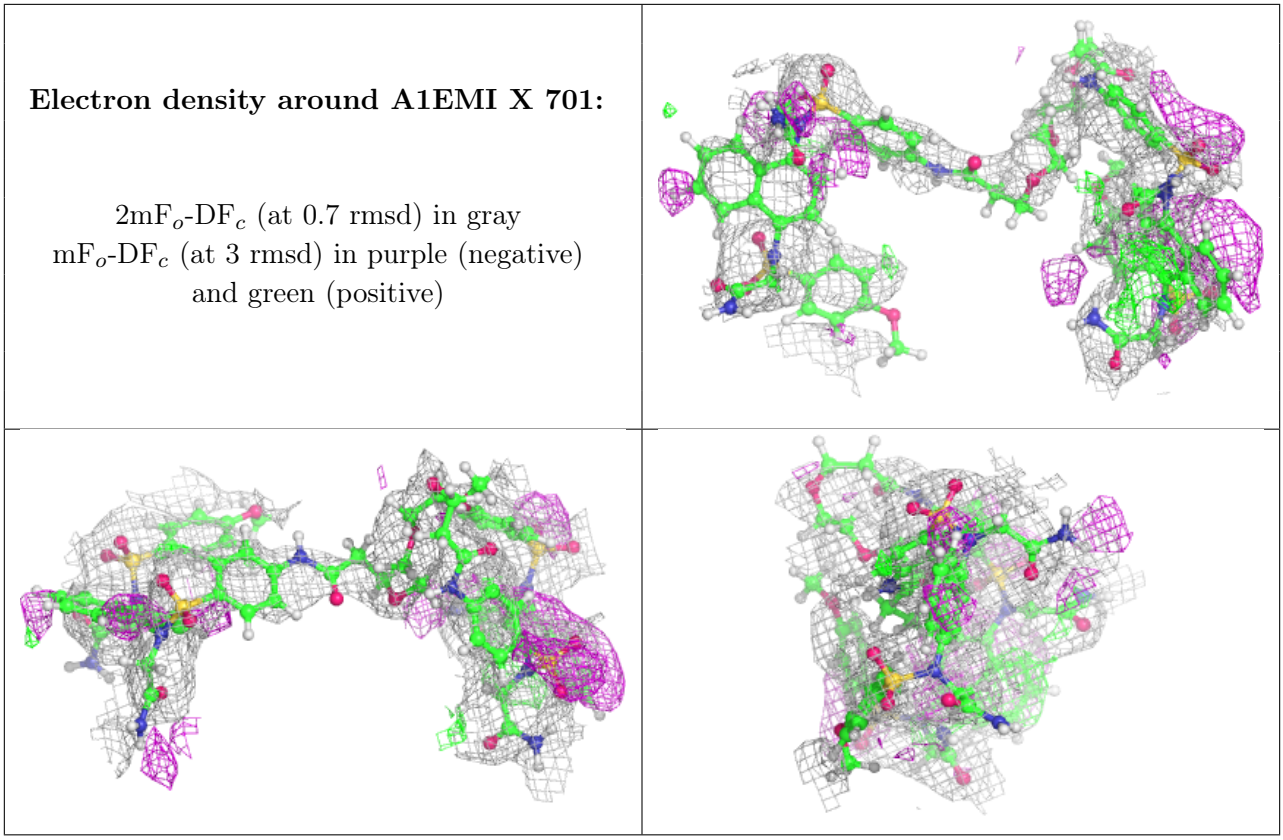






Electron density around A1EMI X 701:

$2mF_o$-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.