Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 02:55 AM EDT

PDB ID	:	2Q6J
Title	:	Crystal Structure of Estrogen Receptor alpha Complexed to a B-N Substituted Ligand
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Deposited on	:	2007-06-05
Resolution	:	2.70 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:

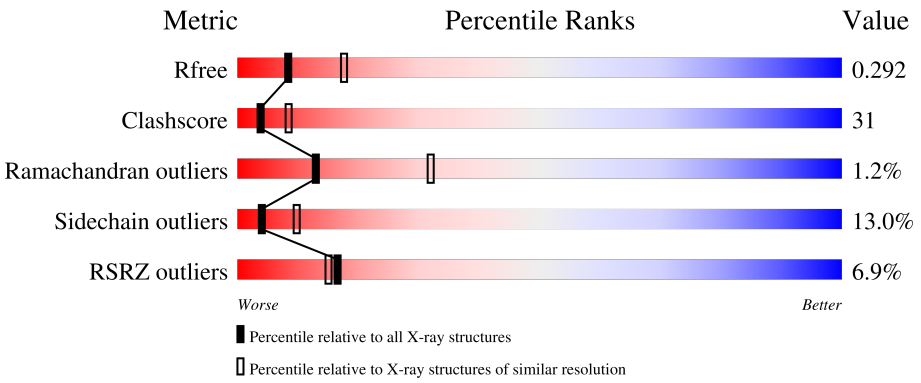
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	258	3% 59% 28% 6% 6%
1	B	258	8% 51% 32% 7% 10%
2	C	13	8% 46% 23% 8% 23%
2	D	13	23% 23% 38% 15% 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	A48	A	700	-	-	X	-
3	A48	B	800	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4042 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	242	1932	1235	331	347	19	0	2	0
1	B	233	1871	1193	325	334	19	0	4	0

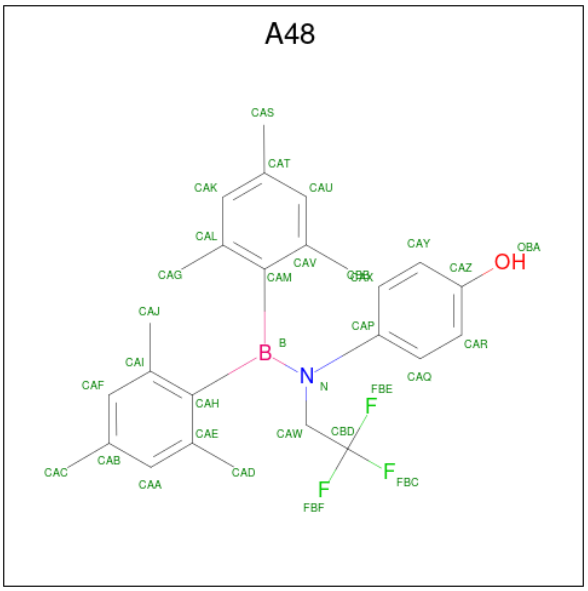
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	SER	-	cloning artifact	UNP P03372
A	537	SER	TYR	engineered mutation	UNP P03372
B	297	SER	-	cloning artifact	UNP P03372
B	537	SER	TYR	engineered mutation	UNP P03372

- Molecule 2 is a protein called GRIP peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	10	85	54	17	14	0	0	0
2	D	10	89	57	19	13	0	0	0

- Molecule 3 is 4-[(DIMESITYLBORYL)(2,2,2-TRIFLUOROETHYL)AMINO]PHENOL (three-letter code: A48) (formula: $C_{26}H_{29}BF_3NO$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	B	C	F	N	O		
3	A	1	32	1	26	3	1	1	0	0
			Total	B	C	F	N	O		
3	B	1	32	1	26	3	1	1	0	0

- Molecule 4 is water.

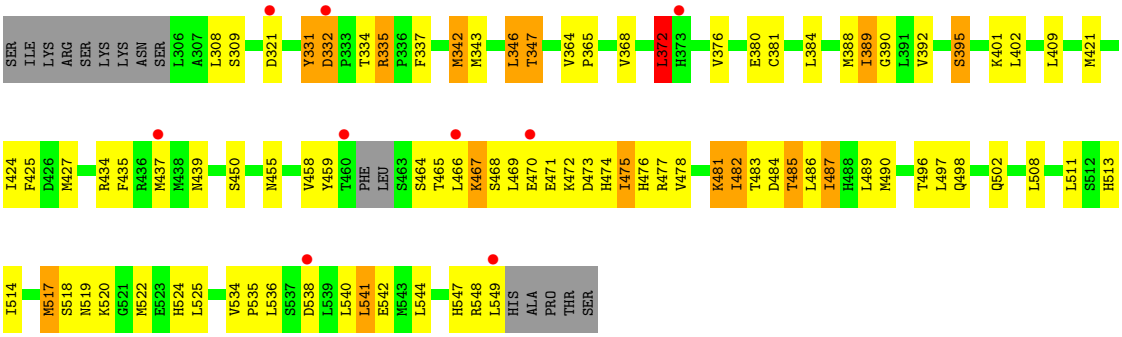
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	1	1	1	0	0

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.

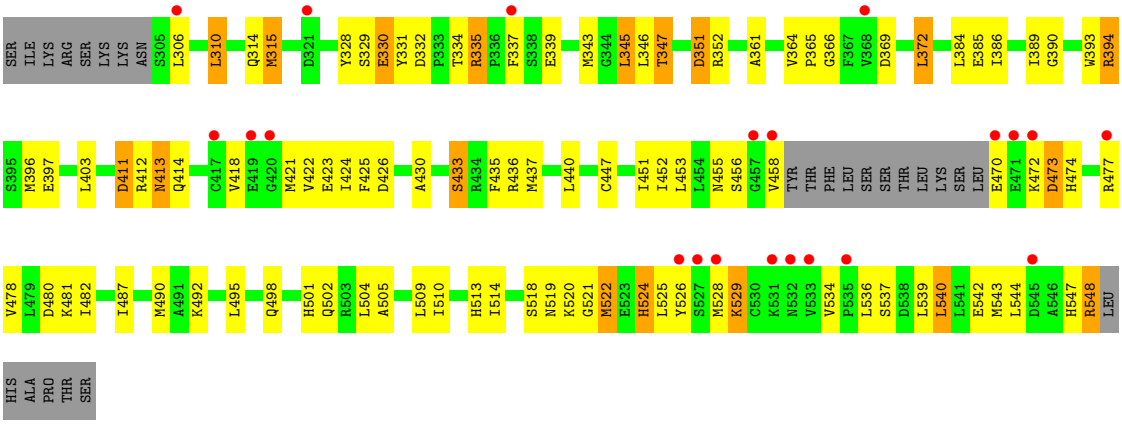
• Molecule 1: Estrogen receptor

Chain A:



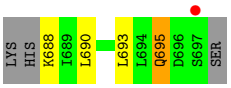
• Molecule 1: Estrogen receptor

Chain B:



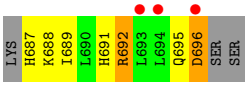
• Molecule 2: GRIP peptide

Chain C:



• Molecule 2: GRIP peptide

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.55Å 79.80Å 58.33Å 90.00° 109.88° 90.00°	Depositor
Resolution (Å)	12.00 – 2.70 11.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.0 (12.00-2.70) 94.0 (11.99-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.227 , 0.297 0.220 , 0.292	Depositor DCC
R_{free} test set	633 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 69.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4042	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.13% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A48

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	0.47	0/1974	0.66	1/2665 (0.0%)
1	B	0.47	0/1921	0.60	0/2593
2	C	0.62	0/85	0.58	0/112
2	D	0.89	1/90 (1.1%)	0.86	0/119
All	All	0.49	1/4070 (0.0%)	0.64	1/5489 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	696	ASP	C-O	5.70	1.34	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	346	LEU	CA-CB-CG	5.37	127.66	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	1932	0	1992	97	0
1	B	1871	0	1917	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	85	0	93	3	0
2	D	89	0	95	9	0
3	A	32	0	29	39	0
3	B	32	0	28	58	0
4	B	1	0	0	0	0
All	All	4042	0	4154	253	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 31.

All (253) 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:343:MET:O	1:A:347:THR:CG2	1.71	1.36
1:A:343:MET:O	1:A:347:THR:HG23	1.15	1.31
3:A:700:A48:HAW2	3:A:700:A48:CAI	1.66	1.24
3:A:700:A48:HAW2	3:A:700:A48:CAJ	1.65	1.24
3:B:800:A48:CAI	3:B:800:A48:HAW2	1.78	1.13
3:B:800:A48:HAW2	3:B:800:A48:CAJ	1.79	1.12
3:B:800:A48:CAJ	3:B:800:A48:CAW	2.28	1.11
1:A:525:LEU:HD13	3:A:700:A48:HAD2	1.24	1.09
1:B:525:LEU:HD13	3:B:800:A48:HAD2	1.09	1.09
3:B:800:A48:CAW	3:B:800:A48:HAJ1	1.83	1.08
1:B:346:LEU:HD12	3:B:800:A48:HAG2	1.15	1.08
1:A:384:LEU:HD13	3:A:700:A48:HBB1	1.34	1.07
3:A:700:A48:CAJ	3:A:700:A48:CAW	2.35	1.04
3:B:800:A48:CAJ	3:B:800:A48:CBD	2.35	1.04
3:B:800:A48:HAQ	3:B:800:A48:CAM	1.91	1.00
1:A:384:LEU:CD1	3:A:700:A48:HBB1	1.90	1.00
1:A:513:HIS:CE1	1:B:458:VAL:HG11	1.97	0.99
1:A:384:LEU:CD1	3:A:700:A48:CBB	2.41	0.98
1:A:334:THR:H	1:A:335:ARG:HH11	1.05	0.98
1:B:525:LEU:HD13	3:B:800:A48:CAD	1.93	0.97
3:B:800:A48:HAJ2	3:B:800:A48:FBE	1.53	0.96
3:B:800:A48:CBD	3:B:800:A48:HAJ2	1.97	0.95
3:B:800:A48:HAJ1	3:B:800:A48:CBD	1.95	0.95
1:A:514:ILE:HA	1:A:517:MET:HG3	1.49	0.93
1:A:519:ASN:HD22	1:B:519:ASN:HD22	1.02	0.93
1:B:347:THR:HA	3:B:800:A48:HAS2	1.46	0.93
1:A:427:MET:HB2	1:A:517:MET:HE1	1.51	0.92
1:B:525:LEU:HD22	3:B:800:A48:HAD3	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:800:A48:CAM	3:B:800:A48:HAD1	1.99	0.92
1:A:513:HIS:NE2	1:B:458:VAL:CG1	2.34	0.91
1:A:384:LEU:HD11	3:A:700:A48:CBB	2.02	0.90
1:B:525:LEU:CD1	3:B:800:A48:HAD2	2.01	0.90
1:A:334:THR:H	1:A:335:ARG:NH1	1.69	0.89
1:A:308:LEU:HD11	1:A:477:ARG:HB3	1.57	0.86
3:A:700:A48:CAW	3:A:700:A48:HAJ1	2.05	0.85
3:A:700:A48:CAI	3:A:700:A48:CAW	2.55	0.83
3:A:700:A48:HAW2	3:A:700:A48:CAH	2.09	0.83
1:A:455:ASN:O	1:A:458:VAL:HG12	1.77	0.82
3:B:800:A48:CAP	3:B:800:A48:HBB3	2.10	0.82
1:A:343:MET:O	1:A:347:THR:HG21	1.78	0.81
1:A:513:HIS:O	1:A:517:MET:HG2	1.81	0.81
1:B:346:LEU:CD1	3:B:800:A48:HAG2	2.06	0.80
1:A:401:LYS:HD3	1:A:409:LEU:HD21	1.63	0.80
3:B:800:A48:CAM	3:B:800:A48:CAQ	2.59	0.80
1:A:334:THR:N	1:A:335:ARG:HH11	1.81	0.79
3:B:800:A48:HAW2	3:B:800:A48:CAH	2.12	0.78
1:A:513:HIS:CE1	1:B:458:VAL:CG1	2.65	0.78
3:B:800:A48:HAJ1	3:B:800:A48:FBF	1.74	0.78
3:A:700:A48:CAW	3:A:700:A48:CAH	2.61	0.78
1:A:384:LEU:HD11	3:A:700:A48:HBB2	1.65	0.77
3:A:700:A48:HAW2	3:A:700:A48:HAJ2	1.62	0.77
1:A:384:LEU:HD13	3:A:700:A48:CBB	2.09	0.76
1:B:525:LEU:HD22	3:B:800:A48:CAD	2.16	0.76
1:B:347:THR:HG22	3:B:800:A48:HAK	1.68	0.75
3:B:800:A48:CAQ	3:B:800:A48:CAV	2.65	0.75
1:A:525:LEU:CD1	3:A:700:A48:HAD2	2.11	0.75
3:B:800:A48:CAI	3:B:800:A48:CAW	2.62	0.74
1:A:519:ASN:ND2	1:B:519:ASN:HD22	1.84	0.74
1:B:315:MET:CE	1:B:365:PRO:HG2	2.17	0.73
1:B:315:MET:HE3	1:B:365:PRO:HG2	1.69	0.73
1:B:343:MET:SD	3:B:800:A48:HAG1	2.29	0.73
1:B:343:MET:O	1:B:347:THR:HG23	1.89	0.73
1:B:542:GLU:OE2	2:D:689:ILE:HG12	1.89	0.72
1:A:519:ASN:HD22	1:B:519:ASN:ND2	1.84	0.71
1:B:447:CYS:O	1:B:451:ILE:HG13	1.91	0.71
1:A:522:MET:HE3	1:A:544:LEU:HD23	1.71	0.71
1:A:427:MET:CB	1:A:517:MET:HE1	2.20	0.71
1:A:534:VAL:HG22	1:A:535:PRO:HD2	1.72	0.70
3:A:700:A48:HAD1	3:A:700:A48:CAV	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:VAL:O	1:B:482:ILE:HG12	1.92	0.70
3:B:800:A48:CAJ	3:B:800:A48:FBF	2.29	0.70
1:B:366:GLY:HA2	1:B:369:ASP:OD2	1.92	0.69
1:B:501[A]:HIS:CE1	1:B:502:GLN:HG3	2.28	0.69
1:B:331:TYR:CE1	1:B:337:PHE:HZ	2.11	0.69
1:B:331:TYR:HE1	1:B:337:PHE:CZ	2.12	0.68
1:B:396:MET:HE1	1:B:435:PHE:HB3	1.74	0.67
3:A:700:A48:HAJ1	3:A:700:A48:N	2.10	0.67
1:A:472:LYS:O	1:A:476:HIS:ND1	2.28	0.67
3:A:700:A48:HAJ2	3:A:700:A48:CBD	2.26	0.66
1:B:384:LEU:HD13	3:B:800:A48:HBB1	1.78	0.66
3:B:800:A48:HAD1	3:B:800:A48:CAV	2.25	0.66
1:B:343:MET:SD	3:B:800:A48:CAG	2.85	0.65
1:B:522:MET:HE2	1:B:522:MET:HA	1.78	0.65
1:A:466:LEU:HA	1:A:469:LEU:HB2	1.79	0.64
1:B:526:TYR:O	1:B:529:LYS:HG3	1.98	0.64
3:B:800:A48:HAQ	3:B:800:A48:CAV	2.25	0.64
1:B:332:ASP:OD2	1:B:334:THR:HB	1.96	0.64
1:A:402:LEU:HD12	1:A:425:PHE:CE2	2.32	0.64
1:B:347:THR:O	1:B:351:ASP:HB2	1.99	0.63
1:B:384:LEU:CD1	3:B:800:A48:CBB	2.76	0.63
1:B:424:ILE:HD11	1:B:524:HIS:NE2	2.13	0.63
3:B:800:A48:CAW	3:B:800:A48:CAH	2.73	0.63
1:B:542:GLU:OE1	2:D:688:LYS:HG2	1.99	0.63
1:B:525:LEU:O	1:B:544:LEU:HD21	1.98	0.62
3:A:700:A48:CAP	3:A:700:A48:HBB3	2.29	0.62
1:A:513:HIS:HE1	1:B:455:ASN:OD1	1.82	0.62
1:B:306:LEU:H	1:B:306:LEU:HD23	1.65	0.62
1:A:496:THR:HG22	1:A:498:GLN:H	1.65	0.62
3:B:800:A48:HBB3	3:B:800:A48:CAQ	2.29	0.62
1:A:464:SER:H	1:A:468:SER:HB2	1.65	0.61
3:A:700:A48:HAD1	3:A:700:A48:CAM	2.29	0.61
1:B:331:TYR:CE1	1:B:337:PHE:CZ	2.89	0.61
1:B:329:SER:HA	1:B:352:ARG:HH22	1.65	0.61
1:A:486:LEU:O	1:A:490:MET:HG3	2.01	0.60
1:A:459:TYR:CE2	1:B:513:HIS:ND1	2.69	0.60
3:B:800:A48:HAW2	3:B:800:A48:HAJ2	1.81	0.60
1:B:331:TYR:HE1	1:B:337:PHE:HZ	1.46	0.60
1:B:385:GLU:HG2	1:B:514:ILE:HG22	1.82	0.60
1:A:474:HIS:O	1:A:478:VAL:HG23	2.03	0.59
1:B:384:LEU:HD11	3:B:800:A48:CBB	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:MET:SD	3:B:800:A48:HAJ3	2.41	0.59
1:A:342:MET:CE	1:A:342:MET:HA	2.34	0.58
1:B:328:TYR:O	1:B:352:ARG:NH1	2.20	0.58
1:B:361:ALA:O	1:B:364:VAL:HB	2.03	0.58
3:A:700:A48:CAJ	3:A:700:A48:CBD	2.82	0.58
1:A:380:GLU:HG3	2:C:690:LEU:HD23	1.85	0.57
1:A:331:TYR:O	1:A:332:ASP:C	2.43	0.57
1:A:401:LYS:HD3	1:A:409:LEU:CD2	2.35	0.57
1:A:481:LYS:O	1:A:485:THR:HG22	2.03	0.57
2:D:687:HIS:C	2:D:687:HIS:CD2	2.77	0.57
3:A:700:A48:CAM	3:A:700:A48:CAQ	2.83	0.57
1:A:482:ILE:HA	1:A:485:THR:HG23	1.87	0.56
1:B:421:MET:CE	3:B:800:A48:HAJ3	2.35	0.56
1:A:388:MET:O	1:A:392:VAL:HG23	2.05	0.56
1:A:466:LEU:O	1:A:470:GLU:HB2	2.05	0.56
1:B:396:MET:O	1:B:436:ARG:NH1	2.34	0.56
1:B:394[A]:ARG:HB2	1:B:403:LEU:HD23	1.87	0.56
1:A:487:ILE:HD13	1:B:501[A]:HIS:HD2	1.70	0.56
3:A:700:A48:CAM	3:A:700:A48:HAQ	2.35	0.56
1:A:481:LYS:O	1:A:485:THR:CG2	2.54	0.56
1:A:524:HIS:CB	3:A:700:A48:HAC2	2.36	0.56
2:D:688:LYS:HB3	2:D:691:HIS:HB2	1.88	0.56
1:A:525:LEU:HD13	3:A:700:A48:CAD	2.16	0.55
1:A:347:THR:HA	3:A:700:A48:HAS2	1.87	0.55
1:A:534:VAL:CG2	1:A:535:PRO:HD2	2.36	0.55
1:B:347:THR:HG21	1:B:536:LEU:HD23	1.86	0.55
1:A:548:ARG:O	1:A:549:LEU:HB2	2.06	0.55
1:A:421:MET:CG	3:A:700:A48:HAF	2.37	0.55
1:B:384:LEU:HD11	3:B:800:A48:HBB2	1.89	0.55
3:B:800:A48:CAM	3:B:800:A48:CAD	2.76	0.55
1:B:372:LEU:HD23	1:B:372:LEU:H	1.72	0.55
1:A:513:HIS:NE2	1:B:458:VAL:HG12	2.22	0.54
1:A:342:MET:HA	1:A:342:MET:HE3	1.90	0.54
1:B:421:MET:HE2	3:B:800:A48:HAJ3	1.89	0.53
1:B:539:LEU:O	1:B:543:MET:HG2	2.09	0.53
1:B:396:MET:CE	1:B:435:PHE:HB3	2.39	0.53
1:B:524:HIS:H	1:B:524:HIS:CD2	2.26	0.53
1:A:514:ILE:HA	1:A:517:MET:CG	2.30	0.53
3:B:800:A48:HAJ1	3:B:800:A48:N	2.22	0.53
1:B:351:ASP:OD1	1:B:540:LEU:HD23	2.09	0.53
1:B:498:GLN:O	1:B:501[A]:HIS:ND1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:ASN:O	1:B:458:VAL:HG12	2.08	0.52
1:A:467:LYS:O	1:A:471:GLU:HB2	2.10	0.52
1:A:421:MET:HG3	3:A:700:A48:HAF	1.91	0.52
1:A:427:MET:CB	1:A:517:MET:CE	2.88	0.52
1:B:384:LEU:CD1	3:B:800:A48:HBB1	2.40	0.51
3:A:700:A48:HAJ2	3:A:700:A48:FBE	2.00	0.51
1:A:483:THR:HG22	1:B:501[A]:HIS:CD2	2.45	0.51
1:A:485:THR:O	1:A:489:LEU:HG	2.11	0.51
1:B:435:PHE:HE1	1:B:510:ILE:HG21	1.76	0.51
2:D:688:LYS:O	2:D:689:ILE:C	2.48	0.51
1:B:413:ASN:C	1:B:413:ASN:HD22	2.14	0.50
3:B:800:A48:CAQ	3:B:800:A48:CBB	2.89	0.50
3:B:800:A48:CAP	3:B:800:A48:CBB	2.85	0.50
1:B:433[B]:SER:OG	1:B:436:ARG:NH2	2.45	0.50
1:B:525:LEU:CD2	3:B:800:A48:HAD3	2.31	0.50
1:A:376:VAL:O	1:A:380:GLU:HB2	2.12	0.49
3:A:700:A48:CAW	3:A:700:A48:HAJ2	2.25	0.49
1:A:335:ARG:HD2	1:A:335:ARG:N	2.28	0.49
1:B:343:MET:HB3	1:B:534:VAL:HG11	1.94	0.48
1:B:474:HIS:O	1:B:478:VAL:HG23	2.13	0.48
1:A:517:MET:HE2	1:A:517:MET:HA	1.95	0.48
1:A:524:HIS:HB2	3:A:700:A48:HAC2	1.95	0.48
1:B:525:LEU:CD1	3:B:800:A48:CAD	2.76	0.48
1:A:487:ILE:HD13	1:B:501[A]:HIS:CD2	2.49	0.48
1:B:335:ARG:HG3	1:B:335:ARG:HH11	1.78	0.48
3:B:800:A48:HAD1	3:B:800:A48:CAL	2.42	0.48
1:B:339:GLU:HG3	1:B:418:VAL:HG22	1.96	0.47
1:B:487:ILE:HD11	1:B:504:LEU:HD22	1.96	0.47
3:B:800:A48:CAM	3:B:800:A48:CAP	2.89	0.47
1:A:459:TYR:HB3	1:B:430:ALA:HB1	1.95	0.47
1:B:384:LEU:HD13	3:B:800:A48:CBB	2.40	0.47
1:B:490:MET:HB3	1:B:495:LEU:HD22	1.97	0.47
1:B:393:TRP:CZ3	1:B:396:MET:HE3	2.49	0.47
1:B:473:ASP:O	1:B:477:ARG:HG2	2.13	0.47
1:B:347:THR:CA	3:B:800:A48:HAS2	2.33	0.47
1:A:435:PHE:O	1:A:439:ASN:N	2.48	0.46
2:D:692:ARG:HA	2:D:695:GLN:HE21	1.80	0.46
1:B:518:SER:O	1:B:522:MET:HG2	2.16	0.46
1:A:331:TYR:CD1	1:A:332:ASP:N	2.84	0.46
1:B:390:GLY:O	1:B:394[A]:ARG:HG2	2.15	0.46
1:B:421:MET:HE3	3:B:800:A48:CAF	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:VAL:CG2	1:A:475:ILE:HD11	2.47	0.45
1:B:412:ARG:NE	1:B:426:ASP:OD1	2.47	0.45
1:A:473:ASP:O	1:A:477:ARG:HG3	2.17	0.45
1:B:526:TYR:O	1:B:529:LYS:CG	2.65	0.45
1:A:424:ILE:HD11	1:A:520:LYS:HB3	1.99	0.45
1:A:547:HIS:C	1:A:548:ARG:HD2	2.37	0.45
1:B:385:GLU:OE2	1:B:456:SER:OG	2.32	0.45
1:A:334:THR:C	1:A:335:ARG:HD2	2.36	0.45
1:A:514:ILE:O	1:A:517:MET:HB2	2.17	0.45
1:A:502:GLN:NE2	1:B:480:ASP:HB3	2.32	0.45
1:B:411:ASP:OD1	1:B:412:ARG:N	2.50	0.44
1:B:330:GLU:O	1:B:345:LEU:HG	2.16	0.44
1:B:547:HIS:C	1:B:548:ARG:HG2	2.38	0.44
1:B:396:MET:HE1	1:B:440:LEU:HB3	2.00	0.44
1:B:525:LEU:CD2	3:B:800:A48:CAD	2.93	0.44
1:B:542:GLU:CD	2:D:689:ILE:HG12	2.38	0.44
1:A:389:ILE:CG2	1:A:390:GLY:N	2.80	0.44
1:A:508:LEU:HD22	1:B:509:LEU:HD21	2.00	0.43
1:B:505:ALA:O	1:B:509:LEU:HG	2.17	0.43
1:A:466:LEU:HD22	1:A:470:GLU:HG2	2.01	0.43
1:A:421:MET:HG2	3:A:700:A48:HAF	2.00	0.43
1:A:513:HIS:NE2	1:B:458:VAL:HG13	2.28	0.43
3:A:700:A48:HBB3	3:A:700:A48:CAX	2.49	0.43
1:B:335:ARG:HG3	1:B:335:ARG:NH1	2.33	0.43
3:A:700:A48:CAM	3:A:700:A48:CAD	2.97	0.43
3:B:800:A48:CAH	3:B:800:A48:HAG3	2.48	0.43
1:B:396:MET:O	1:B:436:ARG:HD3	2.19	0.43
1:B:481:LYS:HB3	1:B:481:LYS:HE3	1.71	0.43
1:A:384:LEU:CD1	3:A:700:A48:HBB2	2.28	0.42
3:A:700:A48:CAP	3:A:700:A48:CAM	2.96	0.42
1:B:310:LEU:HD13	1:B:314:GLN:HB3	2.01	0.42
1:B:413:ASN:HD22	1:B:414:GLN:N	2.16	0.42
1:B:458:VAL:HG22	1:B:458:VAL:O	2.19	0.42
2:D:687:HIS:C	2:D:687:HIS:HD2	2.23	0.42
1:A:364:VAL:O	1:A:365:PRO:C	2.58	0.42
1:A:513:HIS:HE1	1:B:458:VAL:HG11	1.72	0.42
3:B:800:A48:CAD	3:B:800:A48:CAL	2.98	0.42
2:D:695:GLN:O	2:D:696:ASP:C	2.58	0.42
1:B:544:LEU:O	1:B:548:ARG:HG3	2.19	0.42
1:A:534:VAL:HG22	1:A:535:PRO:CD	2.45	0.41
1:B:335:ARG:HA	1:B:335:ARG:HD2	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:MET:CE	1:B:440:LEU:HB3	2.50	0.41
1:A:481:LYS:O	1:A:484:ASP:HB2	2.19	0.41
1:A:434:ARG:HD2	1:A:434:ARG:HA	1.89	0.41
1:A:541:LEU:HD13	1:A:541:LEU:HA	1.97	0.41
3:B:800:A48:HAG3	3:B:800:A48:CAE	2.50	0.41
1:B:343:MET:SD	3:B:800:A48:HAG3	2.60	0.41
1:A:372:LEU:HD21	2:C:695:GLN:HG3	2.02	0.41
1:A:395:SER:HB3	1:A:402:LEU:HA	2.03	0.41
1:A:542:GLU:OE2	2:C:688:LYS:N	2.54	0.41
1:B:487:ILE:HD13	1:B:487:ILE:HA	1.91	0.41
1:A:427:MET:HB3	1:A:517:MET:CE	2.51	0.41
1:B:386:ILE:HA	1:B:389:ILE:HG22	2.03	0.41
1:A:508:LEU:HA	1:A:511:LEU:HG	2.03	0.40
1:A:458:VAL:HG23	1:A:475:ILE:HD11	2.03	0.40
1:A:525:LEU:HD22	3:A:700:A48:CAD	2.51	0.40
3:A:700:A48:CAH	3:A:700:A48:HAG3	2.51	0.40
1:A:402:LEU:HD12	1:A:425:PHE:CD2	2.56	0.40
1:B:384:LEU:CD1	3:B:800:A48:HBB2	2.50	0.40
1:B:521:GLY:O	1:B:525:LEU:HB3	2.22	0.40
1:B:364:VAL:HG21	1:B:453:LEU:HD23	2.03	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	240/258 (93%)	218 (91%)	18 (8%)	4 (2%)	9 23
1	B	233/258 (90%)	219 (94%)	12 (5%)	2 (1%)	17 40
2	C	8/13 (62%)	7 (88%)	1 (12%)	0	100 100
2	D	8/13 (62%)	6 (75%)	2 (25%)	0	100 100
All	All	489/542 (90%)	450 (92%)	33 (7%)	6 (1%)	13 32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	372	LEU
1	B	330	GLU
1	A	331	TYR
1	A	309	SER
1	B	537	SER
1	A	332	ASP

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	220/233 (94%)	193 (88%)	27 (12%)	4 11
1	B	213/233 (91%)	183 (86%)	30 (14%)	3 8
2	C	10/13 (77%)	8 (80%)	2 (20%)	1 3
2	D	10/13 (77%)	9 (90%)	1 (10%)	7 18
All	All	453/492 (92%)	393 (87%)	60 (13%)	4 9

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	ASP
1	A	335	ARG
1	A	337	PHE
1	A	342	MET
1	A	346	LEU
1	A	347	THR
1	A	368	VAL
1	A	372	LEU
1	A	381	CYS
1	A	389	ILE
1	A	395	SER
1	A	437	MET
1	A	450	SER
1	A	465	THR

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Mol	Chain	Res	Type
1	A	467	LYS
1	A	475	ILE
1	A	481	LYS
1	A	482	ILE
1	A	485	THR
1	A	487	ILE
1	A	497	LEU
1	A	517	MET
1	A	518	SER
1	A	536	LEU
1	A	538	ASP
1	A	540	LEU
1	A	541	LEU
1	B	310	LEU
1	B	315	MET
1	B	335	ARG
1	B	345	LEU
1	B	347	THR
1	B	351	ASP
1	B	372	LEU
1	B	394[A]	ARG
1	B	394[B]	ARG
1	B	397	GLU
1	B	411	ASP
1	B	413	ASN
1	B	422	VAL
1	B	423	GLU
1	B	425	PHE
1	B	433[A]	SER
1	B	433[B]	SER
1	B	437	MET
1	B	452	ILE
1	B	470	GLU
1	B	472	LYS
1	B	473	ASP
1	B	492	LYS
1	B	520	LYS
1	B	522	MET
1	B	524	HIS
1	B	528	MET
1	B	529	LYS
1	B	540	LEU

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Mol	Chain	Res	Type
1	B	548	ARG
2	C	693	LEU
2	C	695	GLN
2	D	692	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	513	HIS
1	B	413	ASN
1	B	474	HIS
1	B	519	ASN
1	B	532	ASN
2	C	695	GLN
2	D	687	HIS
2	D	695	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
3	A48	A	700	-	33,34,34	3.79	3 (9%)	46,51,51	2.45	11 (23%)
3	A48	B	800	-	33,34,34	3.58	3 (9%)	46,51,51	3.15	22 (47%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A48	A	700	-	-	3/17/21/21	0/3/3/3
3	A48	B	800	-	-	9/17/21/21	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	A48	CAW-N	17.52	1.55	1.47
3	B	800	A48	CAW-N	16.36	1.54	1.47
3	A	700	A48	B-CAM	-8.79	1.42	1.59
3	A	700	A48	B-CAH	-8.43	1.43	1.59
3	B	800	A48	B-CAM	-8.41	1.43	1.59
3	B	800	A48	B-CAH	-7.88	1.44	1.59

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	800	A48	CBD-CAW-N	12.76	128.94	112.39
3	A	700	A48	CBD-CAW-N	11.47	127.26	112.39
3	A	700	A48	FBE-CBD-CAW	-6.69	101.16	112.13
3	B	800	A48	CAX-CAP-N	6.36	124.85	120.92
3	B	800	A48	CAJ-CAI-CAF	-5.03	110.20	119.49
3	B	800	A48	CAI-CAH-CAE	-4.97	112.96	117.65
3	B	800	A48	CAA-CAE-CAH	4.32	123.66	120.19
3	B	800	A48	CAJ-CAI-CAH	4.28	126.63	121.76
3	B	800	A48	FBE-CBD-CAW	-4.12	105.38	112.13
3	B	800	A48	CAV-CAM-CAL	-3.82	114.04	117.65
3	A	700	A48	CAX-CAP-N	3.81	123.28	120.92
3	B	800	A48	CAF-CAI-CAH	3.72	123.17	120.19
3	B	800	A48	CAU-CAV-CAM	3.72	123.17	120.19
3	B	800	A48	CBB-CAV-CAU	-3.67	112.70	119.49
3	A	700	A48	CAF-CAI-CAH	3.09	122.67	120.19
3	B	800	A48	CAQ-CAP-N	-3.05	119.03	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	800	A48	CAK-CAL-CAM	2.95	122.56	120.19
3	A	700	A48	B-CAH-CAE	2.83	125.05	121.22
3	B	800	A48	CAC-CAB-CAF	-2.74	116.88	120.94
3	B	800	A48	CAC-CAB-CAA	2.69	124.92	120.94
3	B	800	A48	B-CAM-CAL	2.62	124.76	121.22
3	B	800	A48	FBF-CBD-CAW	2.30	115.89	112.13
3	B	800	A48	B-CAH-CAE	2.27	124.29	121.22
3	B	800	A48	CAR-CAQ-CAP	2.27	123.30	120.32
3	A	700	A48	CAQ-CAP-N	-2.22	119.55	120.92
3	A	700	A48	CAU-CAV-CAM	2.19	121.95	120.19
3	A	700	A48	CAV-CAU-CAT	-2.15	119.96	122.17
3	B	800	A48	CAG-CAL-CAM	-2.12	119.35	121.76
3	B	800	A48	CAE-CAA-CAB	-2.10	120.01	122.17
3	A	700	A48	CAC-CAB-CAF	-2.10	117.83	120.94
3	B	800	A48	CBB-CAV-CAM	2.08	124.12	121.76
3	A	700	A48	CAI-CAH-CAE	-2.05	115.72	117.65
3	A	700	A48	CAJ-CAI-CAF	-2.00	115.79	119.49

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	700	A48	N-CAW-CBD-FBF
3	A	700	A48	N-CAW-CBD-FBC
3	B	800	A48	N-B-CAH-CAE
3	B	800	A48	CAM-B-CAH-CAE
3	B	800	A48	CAM-B-CAH-CAI
3	B	800	A48	CAQ-CAP-N-B
3	B	800	A48	CAX-CAP-N-B
3	B	800	A48	N-CAW-CBD-FBF
3	B	800	A48	N-CAW-CBD-FBE
3	B	800	A48	N-CAW-CBD-FBC
3	B	800	A48	N-B-CAH-CAI
3	A	700	A48	N-CAW-CBD-FBE

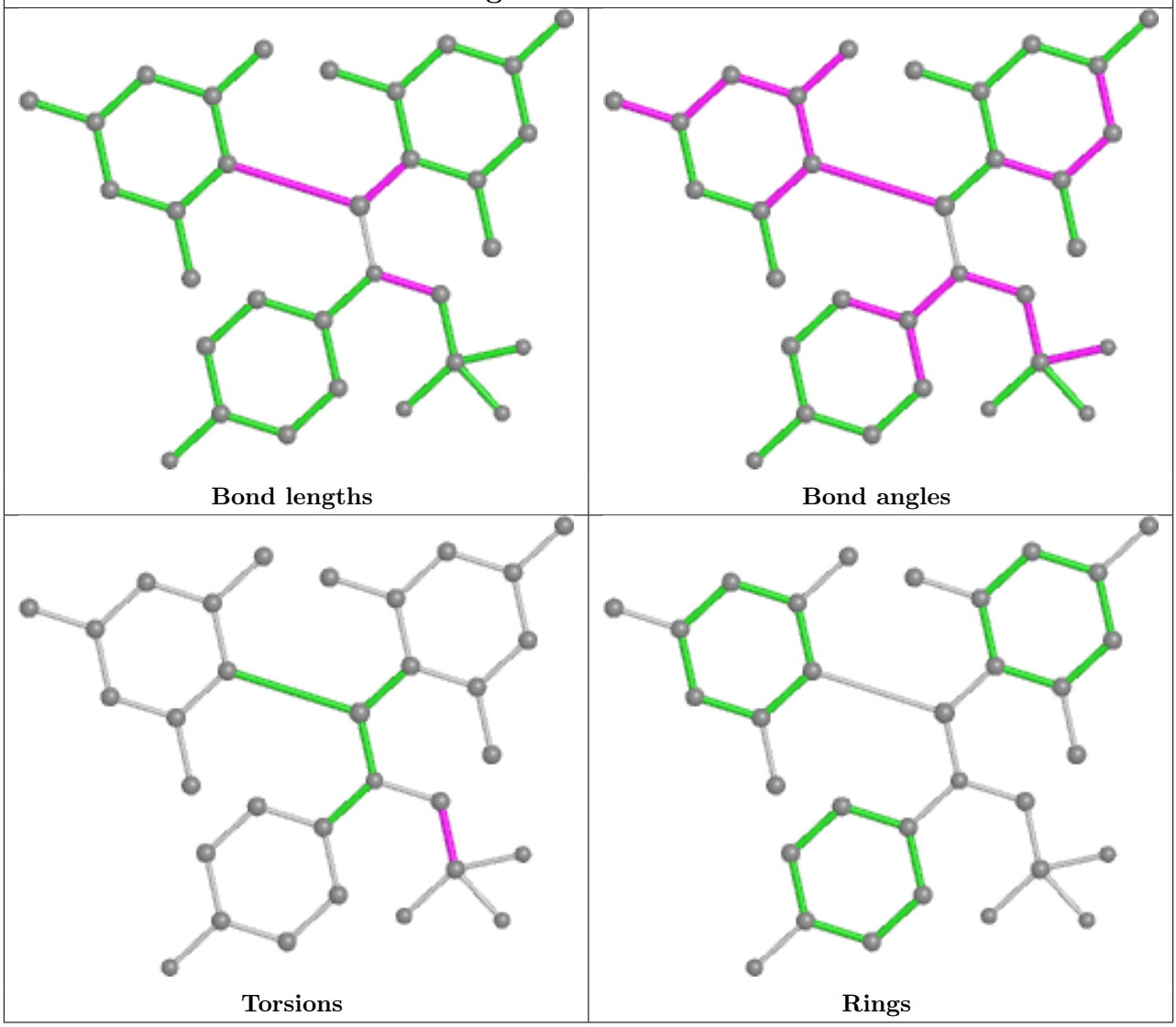
There are no ring outliers.

2 monomers are involved in 97 short contacts:

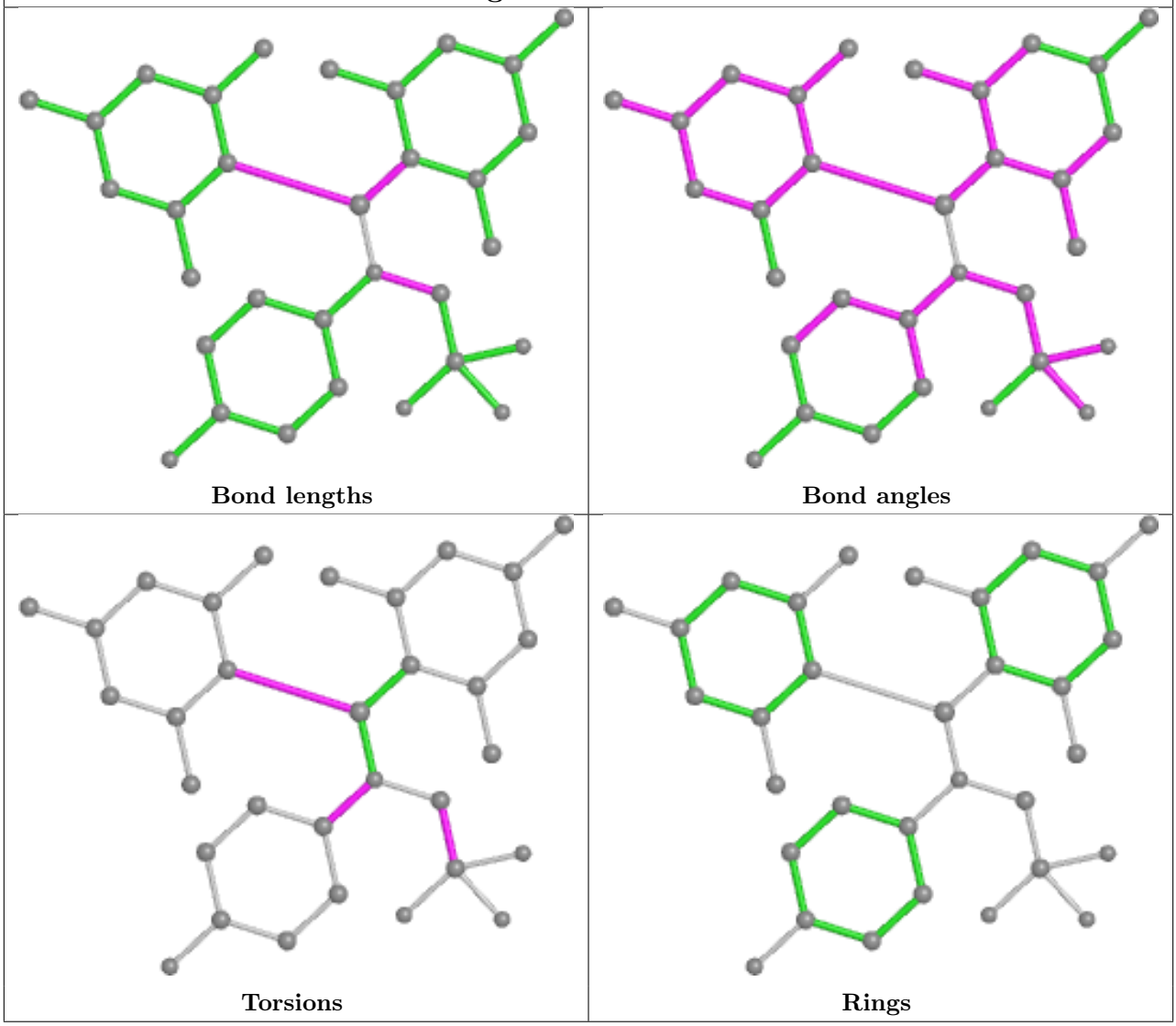
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	700	A48	39	0
3	B	800	A48	58	0

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 A48 A 700



Ligand A48 B 800



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	242/258 (93%)	0.07	9 (3%)	41	41	7, 18, 44, 50	0
1	B	233/258 (90%)	0.31	21 (9%)	9	7	3, 20, 44, 49	0
2	C	10/13 (76%)	0.72	1 (10%)	7	5	18, 20, 24, 27	0
2	D	10/13 (76%)	1.64	3 (30%)	0	0	41, 42, 46, 47	0
All	All	495/542 (91%)	0.23	34 (6%)	16	15	3, 19, 45, 50	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	466	LEU	6.0
2	D	696	ASP	4.9
1	B	535	PRO	4.5
2	C	697	SER	4.2
1	B	472	LYS	4.1
1	B	306	LEU	4.1
1	B	470	GLU	3.9
1	B	420	GLY	3.5
1	B	532	ASN	3.3
2	D	693	LEU	3.1
1	B	321	ASP	3.1
1	A	321	ASP	3.0
1	B	368	VAL	3.0
1	B	417	CYS	2.9
1	B	458	VAL	2.9
1	B	531	LYS	2.8
2	D	694	LEU	2.7
1	B	533	VAL	2.6
1	B	528	MET	2.6
1	B	337	PHE	2.5
1	B	527	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	470	GLU	2.4
1	B	545	ASP	2.4
1	B	419	GLU	2.3
1	B	526	TYR	2.3
1	A	437	MET	2.3
1	B	471	GLU	2.2
1	A	549	LEU	2.1
1	A	460	THR	2.1
1	A	373	HIS	2.1
1	A	332	ASP	2.1
1	B	477	ARG	2.1
1	A	538	ASP	2.0
1	B	457	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

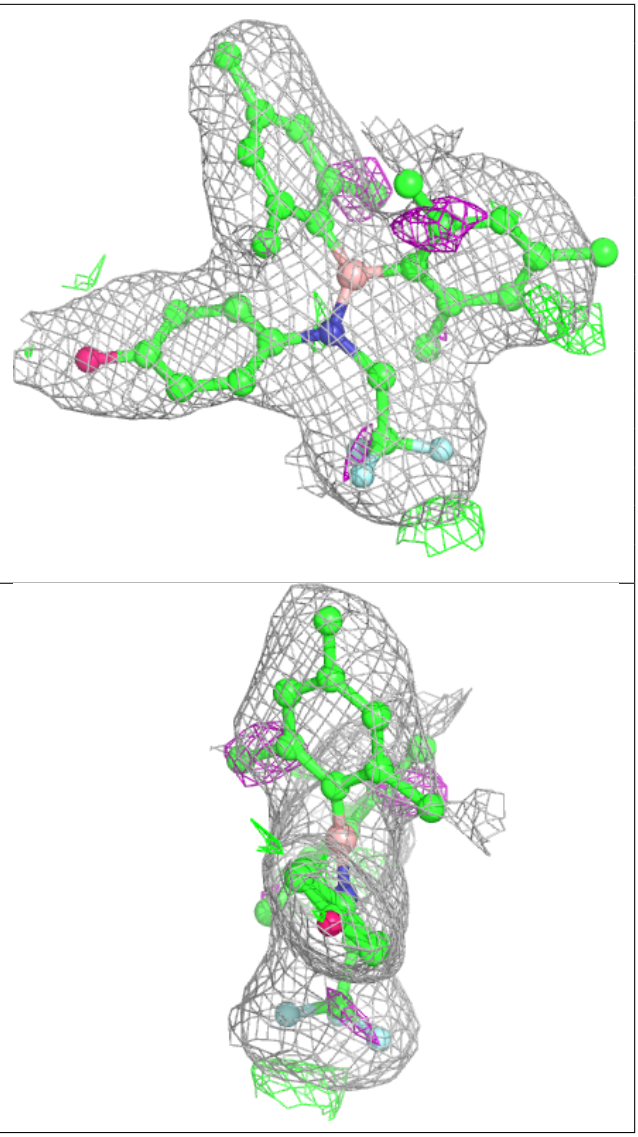
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	A48	A	700	32/32	0.86	0.20	36,41,44,44	0
3	A48	B	800	32/32	0.90	0.17	29,35,38,40	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.

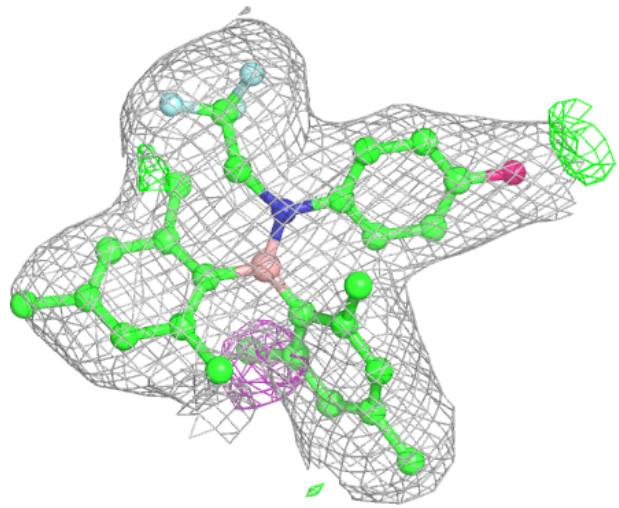
Electron density around A48 A 700:

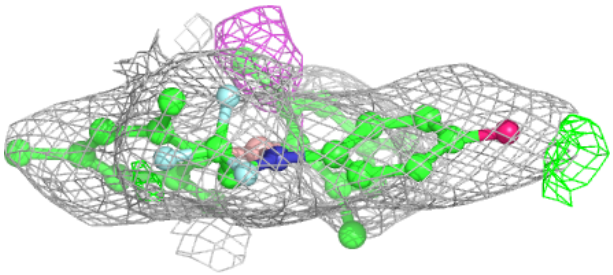
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

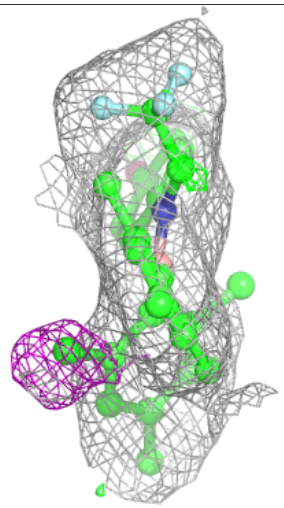


Electron density around A48 B 800:

$2mF_o$-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.