Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:59 PM UTC

PDB ID	:	3DEI / pdb_00003dei
Title	:	Crystal Structures of Caspase-3 with Bound Isoquinoline-1,3,4-trione Derivative Inhibitors
Authors	:	Wu, J.; Du, J.; Li, J.; Ding, J.
Deposited on	:	2008-06-10
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

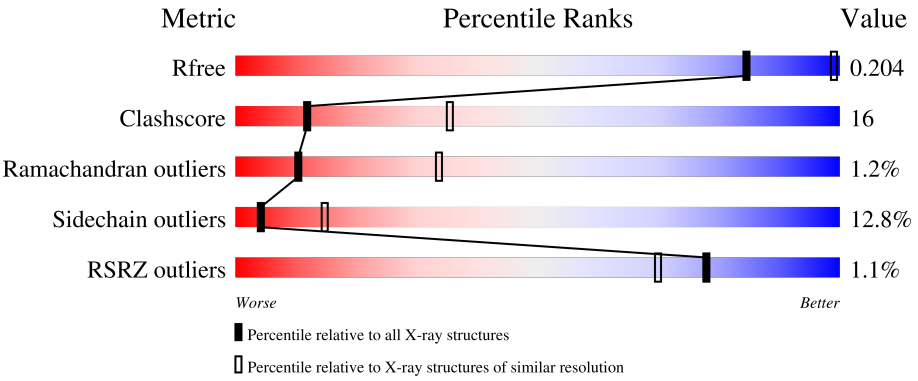
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	249	58% 29% 7% 7%
1	B	249	% 63% 27% • 6%
1	C	249	2% 56% 33% 5% 6%
1	D	249	2% 51% 36% 6% • 6%

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
2	RXB	C	300	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7672 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.

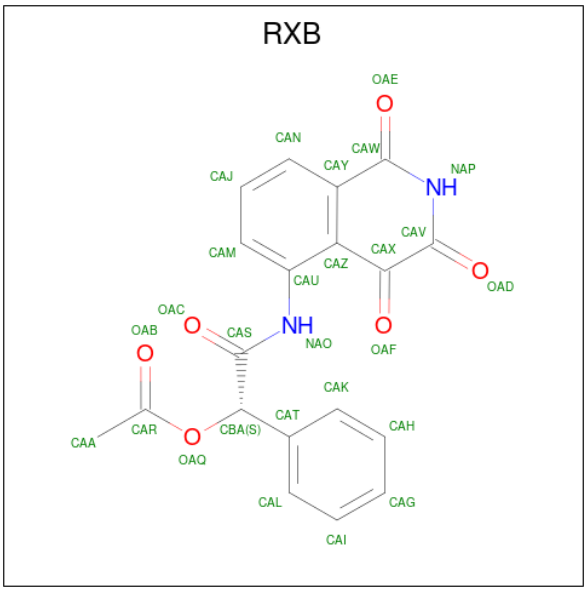
- Molecule 1 is a protein called Caspase-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1883	1192	323	354	14			
1	B	233	Total	C	N	O	S	0	0	0
			1891	1198	324	355	14			
1	C	234	Total	C	N	O	S	0	0	0
			1901	1204	327	356	14			
1	D	234	Total	C	N	O	S	0	0	0
			1896	1201	325	356	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	ASP	GLU	SEE REMARK 999	UNP P42574
B	190	ASP	GLU	SEE REMARK 999	UNP P42574
C	190	ASP	GLU	SEE REMARK 999	UNP P42574
D	190	ASP	GLU	SEE REMARK 999	UNP P42574

- Molecule 2 is (1S)-2-oxo-1-phenyl-2-[(1,3,4-trioxo-1,2,3,4-tetrahydroisoquinolin-5-yl)amino]ethyl acetate (CCD ID: RXB) (formula: $C_{19}H_{14}N_2O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O 27 19 2 6	0	0

- Molecule 3 is water.

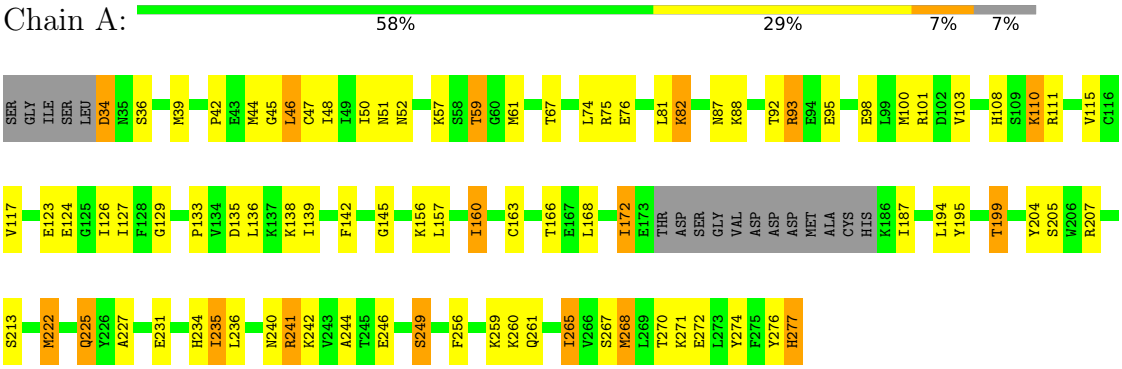
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	29	Total O 29 29	0	0
3	B	24	Total O 24 24	0	0
3	C	18	Total O 18 18	0	0
3	D	3	Total O 3 3	0	0

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.

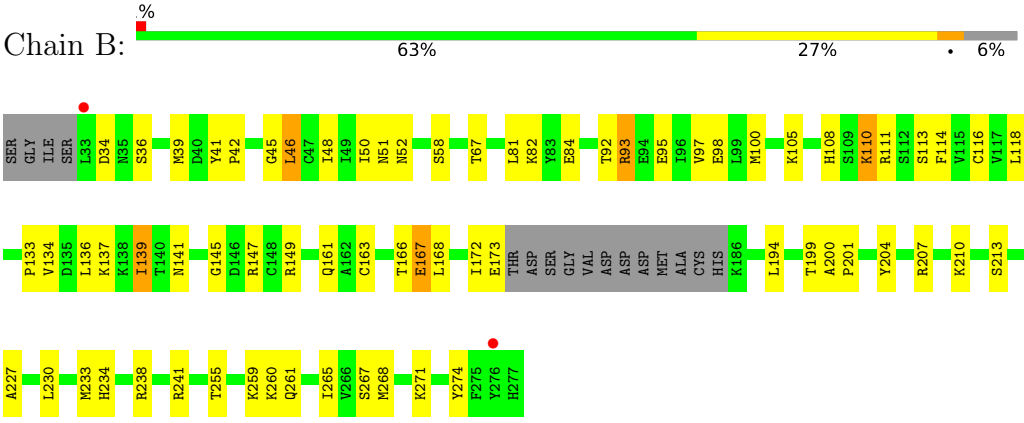
• Molecule 1: Caspase-3

Chain A:



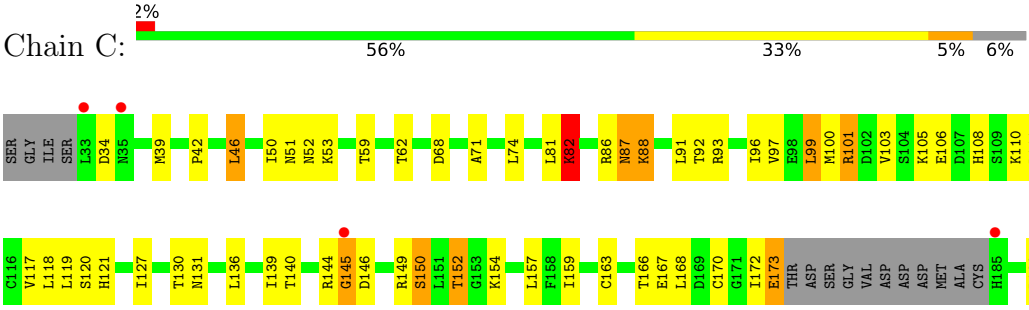
• Molecule 1: Caspase-3

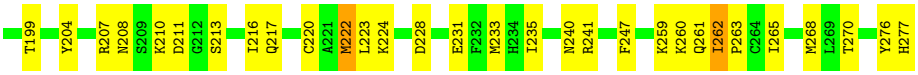
Chain B:



• Molecule 1: Caspase-3

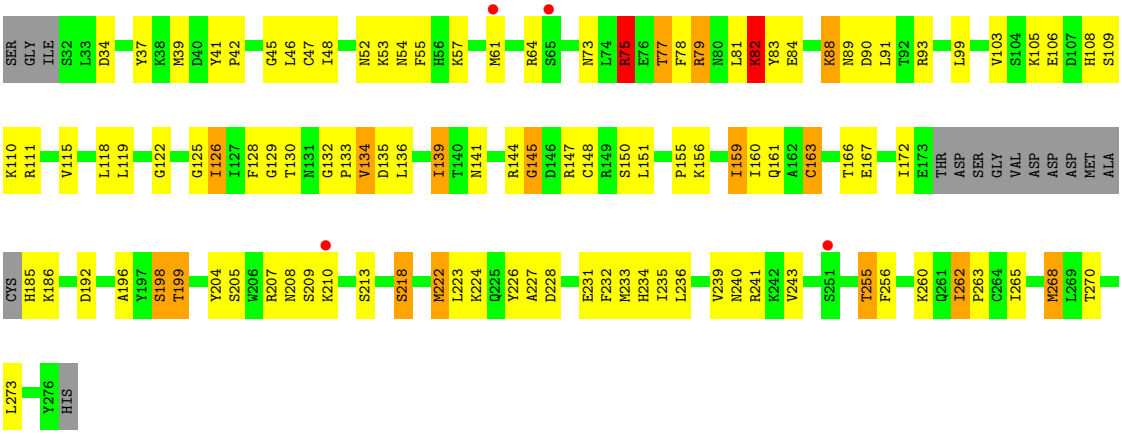
Chain C:





• Molecule 1: Caspase-3

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.52Å 95.98Å 180.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.13 – 2.80 45.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.1 (45.13-2.80) 94.1 (45.13-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.211 , 0.291 0.211 , 0.204	Depositor DCC
R_{free} test set	1384 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	68.4	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7672	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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: RXB, OCS

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	0.74	0/1912	1.05	5/2566 (0.2%)
1	B	0.76	0/1920	1.05	1/2577 (0.0%)
1	C	0.70	0/1931	0.96	1/2592 (0.0%)
1	D	0.59	0/1925	0.92	1/2585 (0.0%)
All	All	0.70	0/7688	1.00	8/10320 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	268	MET	N-CA-C	-6.91	102.02	111.56
1	A	160	ILE	N-CA-C	5.70	115.78	106.72
1	B	230	LEU	N-CA-C	5.60	117.76	110.43
1	A	265	ILE	CB-CA-C	-5.42	104.41	110.96
1	A	267	SER	N-CA-C	5.30	117.60	109.07
1	C	52	ASN	N-CA-C	5.07	116.57	108.41
1	A	129	GLY	N-CA-C	-5.05	104.72	112.85
1	A	52	ASN	N-CA-C	5.02	116.78	108.20

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	1883	0	1852	64	0
1	B	1891	0	1863	48	0
1	C	1901	0	1870	72	0
1	D	1896	0	1868	59	0
2	C	27	0	14	9	0
3	A	29	0	0	1	0
3	B	24	0	0	0	0
3	C	18	0	0	0	0
3	D	3	0	0	1	0
All	All	7672	0	7467	238	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 16.

All (238) 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:46:LEU:HD12	1:A:46:LEU:H	1.04	1.09
2:C:300:RXB:HAK	2:C:300:RXB:OAF	1.65	0.96
1:D:262:ILE:HD13	1:D:263:PRO:HD2	1.47	0.96
1:A:93:ARG:HH21	1:A:133:PRO:HD2	1.31	0.95
1:A:46:LEU:H	1:A:46:LEU:CD1	1.81	0.93
1:A:51:ASN:HD21	1:A:67:THR:HG23	1.35	0.89
1:D:208:ASN:HD22	1:D:209:SER:H	1.20	0.86
1:A:46:LEU:HD12	1:A:46:LEU:N	1.89	0.86
1:B:48:ILE:HG21	1:B:100:MET:HE1	1.58	0.85
1:D:208:ASN:HD22	1:D:209:SER:N	1.75	0.85
1:C:99:LEU:O	1:C:103:VAL:HG23	1.78	0.84
1:C:222:MET:HE3	1:C:222:MET:HA	1.60	0.83
1:B:222:MET:HE2	1:B:226:TYR:HE2	1.46	0.81
1:A:225:GLN:HG3	1:A:225:GLN:O	1.82	0.79
1:C:222:MET:HA	1:C:222:MET:CE	2.13	0.78
1:D:122:GLY:O	1:D:163:OCS:HB3	1.83	0.78
1:D:45:GLY:HA2	1:D:111:ARG:HD3	1.63	0.78
1:C:42:PRO:HG2	1:C:110:LYS:HB3	1.66	0.77
1:C:46:LEU:HD11	1:C:108:HIS:HE1	1.50	0.77
1:A:51:ASN:HD21	1:A:67:THR:CG2	1.98	0.76
1:A:101:ARG:HG3	1:A:142:PHE:CE1	2.23	0.73
1:D:55:PHE:HE1	1:D:64:ARG:HG3	1.51	0.73
1:A:199:THR:HG21	1:A:204:TYR:O	1.88	0.73
1:B:52:ASN:HB2	1:B:120:SER:HB2	1.71	0.73
1:C:208:ASN:HD22	1:C:211:ASP:H	1.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ASN:ND2	1:B:67:THR:OG1	2.22	0.72
1:C:199:THR:HG21	1:C:204:TYR:O	1.90	0.72
1:C:51:ASN:HD22	1:C:71:ALA:HB2	1.54	0.71
1:A:222:MET:HA	1:A:222:MET:CE	2.21	0.70
1:D:78:PHE:O	1:D:83:TYR:HB2	1.91	0.70
1:D:119:LEU:HD23	1:D:161:GLN:HB3	1.73	0.70
1:B:92:THR:HG23	1:B:95:GLU:OE1	1.92	0.69
1:B:222:MET:HE2	1:B:226:TYR:CE2	2.27	0.69
1:A:207:ARG:HG2	1:A:213:SER:HB3	1.75	0.68
1:C:208:ASN:ND2	1:C:211:ASP:H	1.92	0.68
1:B:222:MET:HE3	1:B:222:MET:HA	1.75	0.67
1:A:50:ILE:HD11	1:A:100:MET:HE3	1.77	0.67
1:C:88:LYS:HG2	1:C:91:LEU:HD11	1.77	0.66
1:C:92:THR:HB	1:C:131:ASN:ND2	2.10	0.65
1:C:51:ASN:ND2	1:C:71:ALA:HB2	2.12	0.65
1:C:101:ARG:HH11	1:C:101:ARG:HB3	1.61	0.64
1:C:222:MET:HE3	1:C:222:MET:CA	2.27	0.64
1:B:233:MET:HE1	1:B:265:ILE:HG21	1.78	0.64
1:C:170:CYS:O	1:D:186:LYS:NZ	2.31	0.64
1:C:51:ASN:HD22	1:C:119:LEU:HD12	1.64	0.62
1:B:168:LEU:HB3	1:B:259:LYS:HD2	1.81	0.62
1:B:108:HIS:HA	1:B:111:ARG:HD2	1.81	0.62
1:A:74:LEU:HD13	1:A:117:VAL:HG11	1.82	0.61
1:A:34:ASP:HA	3:A:288:HOH:O	2.01	0.61
1:A:92:THR:OG1	1:A:95:GLU:HG3	2.01	0.61
1:B:46:LEU:HD12	1:B:46:LEU:H	1.66	0.60
1:C:51:ASN:ND2	1:C:119:LEU:HD12	2.17	0.60
1:A:241:ARG:HH11	1:A:241:ARG:CG	2.15	0.59
1:C:168:LEU:HD13	2:C:300:RXB:HNAO	1.67	0.59
1:B:92:THR:OG1	1:B:95:GLU:HG3	2.01	0.59
1:D:126:ILE:HG22	1:D:135:ASP:HA	1.85	0.58
1:D:148:CYS:SG	1:D:151:LEU:HB2	2.44	0.58
1:C:241:ARG:HH11	1:C:241:ARG:HG3	1.69	0.58
1:C:74:LEU:CD1	1:C:117:VAL:HG11	2.34	0.57
1:D:262:ILE:HD13	1:D:263:PRO:CD	2.28	0.57
1:C:99:LEU:HG	1:C:100:MET:HE2	1.85	0.57
1:C:199:THR:HG22	1:C:261:GLN:HG3	1.87	0.57
1:A:101:ARG:HG3	1:A:142:PHE:HE1	1.69	0.57
1:A:241:ARG:HH11	1:A:241:ARG:HG3	1.70	0.56
1:A:231:GLU:HG3	1:A:272:GLU:HB3	1.88	0.56
1:B:207:ARG:HA	1:B:213:SER:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LYS:HE3	1:C:68:ASP:OD2	2.05	0.56
2:C:300:RXB:OAF	2:C:300:RXB:CAK	2.48	0.56
1:B:194:LEU:HD12	1:B:267:SER:HB2	1.87	0.55
1:B:233:MET:HE1	1:B:265:ILE:CG2	2.36	0.55
1:C:81:LEU:O	1:C:82:LYS:HB2	2.05	0.55
1:A:45:GLY:HA2	1:A:111:ARG:HG2	1.89	0.55
1:C:247:PHE:O	1:C:260:LYS:NZ	2.32	0.55
2:C:300:RXB:CAL	2:C:300:RXB:HAAA	2.36	0.55
1:C:118:LEU:HD13	1:C:127:ILE:HD13	1.88	0.55
1:D:55:PHE:CE1	1:D:64:ARG:HG3	2.39	0.55
1:D:141:ASN:HB3	1:D:147:ARG:HH12	1.72	0.54
1:A:222:MET:HA	1:A:222:MET:HE2	1.89	0.54
1:D:75:ARG:O	1:D:79:ARG:HB2	2.07	0.54
1:C:50:ILE:HG21	1:C:96:ILE:HD11	1.90	0.54
1:D:37:TYR:CD1	1:D:155:PRO:HD3	2.42	0.53
1:C:213:SER:HG	1:C:216:ILE:HB	1.73	0.53
1:B:100:MET:HG3	1:B:139:ILE:HB	1.91	0.53
1:A:268:MET:HE1	1:B:201:PRO:HD2	1.91	0.53
1:A:234:HIS:CE1	1:B:234:HIS:CE1	2.96	0.53
1:B:50:ILE:HD11	1:B:100:MET:HE3	1.91	0.53
1:B:81:LEU:O	1:B:82:LYS:HB2	2.09	0.53
2:C:300:RXB:OAF	2:C:300:RXB:OAC	2.26	0.52
1:D:199:THR:HG21	1:D:204:TYR:O	2.08	0.52
1:C:166:THR:O	2:C:300:RXB:HAM	2.09	0.52
1:C:262:ILE:HD13	1:C:263:PRO:HD2	1.91	0.52
1:C:207:ARG:HA	1:C:213:SER:HA	1.92	0.52
1:D:73:ASN:O	1:D:77:THR:OG1	2.28	0.51
1:C:213:SER:OG	1:C:216:ILE:HB	2.09	0.51
1:A:135:ASP:O	1:A:138:LYS:HB3	2.11	0.51
1:A:199:THR:HG23	1:A:261:GLN:HG3	1.91	0.51
1:B:36:SER:HA	1:B:271:LYS:HB3	1.91	0.51
1:A:271:LYS:HE2	1:B:241:ARG:NH1	2.26	0.51
1:C:119:LEU:CD2	1:C:216:ILE:HD11	2.41	0.51
1:A:39:MET:O	1:A:277:HIS:HE1	1.95	0.50
1:A:204:TYR:CG	1:A:205:SER:N	2.80	0.50
1:A:75:ARG:NH1	1:A:87:ASN:OD1	2.40	0.50
2:C:300:RXB:OAF	2:C:300:RXB:CAS	2.59	0.50
1:D:222:MET:HE3	1:D:226:TYR:HE2	1.76	0.50
1:A:46:LEU:HD21	1:A:108:HIS:HE1	1.77	0.50
1:A:136:LEU:HD11	1:A:160:ILE:HD13	1.93	0.50
1:A:39:MET:HE3	1:A:44:MET:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LEU:CD1	1:B:114:PHE:HD1	2.25	0.49
1:D:129:GLY:N	1:D:132:GLY:O	2.36	0.49
1:A:241:ARG:NH2	1:B:34:ASP:HB3	2.27	0.49
1:A:242:LYS:NZ	1:A:246:GLU:OE1	2.44	0.49
1:B:141:ASN:HB3	1:B:147:ARG:NH1	2.28	0.49
1:D:159:ILE:HG13	1:D:196:ALA:HB3	1.93	0.49
1:C:119:LEU:HD21	1:C:216:ILE:HD11	1.95	0.49
1:A:123:GLU:O	1:A:124:GLU:C	2.53	0.49
1:C:127:ILE:HG23	1:C:136:LEU:HG	1.95	0.49
1:D:240:ASN:HA	1:D:263:PRO:HG2	1.95	0.49
1:C:213:SER:O	1:C:217:GLN:HB2	2.12	0.49
1:A:207:ARG:HA	1:A:213:SER:HA	1.94	0.49
1:B:93:ARG:NH2	1:B:133:PRO:HD2	2.28	0.49
1:C:127:ILE:O	1:C:127:ILE:HG13	2.12	0.49
1:C:233:MET:HE1	1:C:265:ILE:HG21	1.94	0.49
1:C:59:THR:HG21	1:C:130:THR:O	2.13	0.48
1:C:228:ASP:HA	1:C:276:TYR:CD2	2.49	0.48
1:A:59:THR:C	1:A:61:MET:H	2.22	0.48
1:C:50:ILE:HG21	1:C:96:ILE:CD1	2.44	0.48
1:C:93:ARG:O	1:C:97:VAL:HG23	2.13	0.48
1:C:115:VAL:HG22	1:C:157:LEU:HD12	1.96	0.47
1:B:39:MET:HG3	1:B:274:TYR:O	2.14	0.47
1:C:144:ARG:O	1:C:146:ASP:N	2.47	0.47
1:D:135:ASP:O	1:D:136:LEU:C	2.58	0.47
1:A:194:LEU:C	1:A:194:LEU:HD23	2.39	0.47
1:C:74:LEU:HD13	1:C:117:VAL:HG11	1.97	0.47
1:D:207:ARG:HA	1:D:213:SER:HA	1.96	0.47
1:D:235:ILE:O	1:D:239:VAL:HG23	2.14	0.47
1:D:55:PHE:HD2	1:D:130:THR:HA	1.79	0.47
1:D:148:CYS:SG	1:D:151:LEU:HD12	2.55	0.47
1:A:222:MET:HA	1:A:222:MET:HE3	1.96	0.47
1:A:207:ARG:HB2	1:A:207:ARG:NH1	2.29	0.47
1:D:128:PHE:CE1	1:D:133:PRO:HB3	2.49	0.46
1:A:46:LEU:HD11	1:A:108:HIS:CE1	2.51	0.46
1:C:233:MET:HE1	1:C:265:ILE:CG2	2.45	0.46
1:A:44:MET:HG3	1:A:81:LEU:O	2.16	0.46
1:B:41:TYR:O	1:B:42:PRO:C	2.58	0.46
1:B:126:ILE:HD13	1:B:133:PRO:CB	2.46	0.46
1:C:168:LEU:HB3	1:C:259:LYS:HD2	1.98	0.46
1:A:39:MET:O	1:A:277:HIS:CE1	2.68	0.46
1:B:199:THR:HG22	1:B:200:ALA:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:TYR:HB3	1:B:110:LYS:O	2.16	0.46
1:C:39:MET:HA	1:C:112:SER:HB3	1.98	0.46
1:A:168:LEU:HG	2:C:300:RXB:HNAP	1.80	0.46
1:B:119:LEU:HD23	1:B:161:GLN:HB3	1.98	0.45
1:D:166:THR:O	1:D:167:GLU:C	2.59	0.45
1:A:48:ILE:HD13	1:A:103:VAL:HG11	1.99	0.45
1:C:150:SER:O	1:C:154:LYS:NZ	2.50	0.45
1:D:42:PRO:HG2	1:D:110:LYS:HD3	1.98	0.45
1:B:199:THR:HG21	1:B:204:TYR:O	2.16	0.45
1:B:46:LEU:HD12	1:B:46:LEU:N	2.28	0.44
1:C:86:ARG:NH2	1:C:106:GLU:OE2	2.42	0.44
1:C:223:LEU:HD23	1:C:235:ILE:HG21	1.98	0.44
1:D:93:ARG:HB2	1:D:134:VAL:HG23	1.99	0.44
1:D:93:ARG:HE	1:D:132:GLY:HA3	1.83	0.44
1:D:231:GLU:OE1	1:D:233:MET:HB2	2.18	0.44
1:A:46:LEU:HD11	1:A:108:HIS:ND1	2.33	0.44
1:D:141:ASN:OD1	1:D:144:ARG:HD3	2.17	0.44
1:A:249:SER:HB3	1:A:259:LYS:H	1.82	0.44
1:C:108:HIS:HA	1:C:111:ARG:HD2	1.98	0.44
1:D:125:GLY:HA2	3:D:279:HOH:O	2.18	0.44
1:D:232:PHE:HA	1:D:235:ILE:HD12	2.00	0.44
1:C:210:LYS:HB3	1:C:210:LYS:HE2	1.78	0.43
2:C:300:RXB:OAC	2:C:300:RXB:CAX	2.66	0.43
1:A:82:LYS:HD3	1:A:82:LYS:N	2.34	0.43
1:A:195:TYR:CD1	1:A:195:TYR:N	2.86	0.43
1:A:270:THR:O	1:B:241:ARG:HB2	2.18	0.43
1:B:222:MET:HA	1:B:222:MET:CE	2.46	0.43
1:D:54:ASN:N	1:D:90:ASP:OD2	2.45	0.43
1:A:172:ILE:HD11	1:B:149:ARG:CZ	2.48	0.43
1:D:198:SER:O	1:D:263:PRO:HA	2.18	0.43
1:A:235:ILE:H	1:A:235:ILE:HG12	1.67	0.43
1:C:231:GLU:O	1:C:235:ILE:HG12	2.19	0.43
1:D:236:LEU:HB3	1:D:265:ILE:CD1	2.49	0.43
1:B:222:MET:HG2	1:B:238:ARG:HB2	2.01	0.43
1:A:241:ARG:CG	1:A:241:ARG:NH1	2.81	0.43
1:C:101:ARG:HH11	1:C:101:ARG:CB	2.30	0.43
1:B:255:THR:O	1:B:259:LYS:HE2	2.19	0.43
1:B:81:LEU:HD21	1:B:227:ALA:HB1	2.00	0.42
1:D:99:LEU:O	1:D:103:VAL:HG23	2.19	0.42
1:B:81:LEU:HD21	1:B:227:ALA:CB	2.49	0.42
1:C:87:ASN:C	1:C:88:LYS:HZ2	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:GLU:HA	1:D:185:HIS:O	2.19	0.42
1:D:47:CYS:HA	1:D:115:VAL:O	2.19	0.42
1:D:192:ASP:OD1	1:D:270:THR:OG1	2.35	0.42
1:C:103:VAL:O	1:C:106:GLU:HB2	2.18	0.42
1:D:108:HIS:HA	1:D:111:ARG:HH11	1.84	0.42
1:A:42:PRO:HG2	1:A:110:LYS:HB3	2.01	0.42
1:C:92:THR:HB	1:C:131:ASN:HD21	1.81	0.42
1:A:81:LEU:O	1:A:82:LYS:HB2	2.20	0.42
1:C:74:LEU:HD23	1:C:220:CYS:SG	2.60	0.42
1:C:117:VAL:HG22	1:C:159:ILE:HG13	2.02	0.42
1:D:144:ARG:O	1:D:145:GLY:C	2.63	0.42
1:A:240:ASN:O	1:A:244:ALA:CB	2.67	0.42
1:D:47:CYS:O	1:D:47:CYS:SG	2.78	0.42
1:A:236:LEU:HB3	1:A:265:ILE:HD12	2.01	0.41
1:D:52:ASN:ND2	1:D:91:LEU:O	2.53	0.41
1:D:218:SER:O	1:D:222:MET:HB2	2.20	0.41
1:B:137:LYS:HG3	1:B:141:ASN:HD21	1.84	0.41
1:D:239:VAL:O	1:D:243:VAL:HG23	2.20	0.41
1:B:45:GLY:HA3	1:B:113:SER:O	2.20	0.41
1:B:166:THR:O	1:B:167:GLU:C	2.62	0.41
1:C:270:THR:O	1:D:241:ARG:HB2	2.19	0.41
1:A:249:SER:OG	1:A:256:PHE:O	2.38	0.41
1:B:116:CYS:SG	1:B:118:LEU:HD21	2.60	0.41
1:C:118:LEU:HD22	1:C:127:ILE:CD1	2.51	0.41
1:C:228:ASP:HA	1:C:276:TYR:HD2	1.86	0.41
1:D:39:MET:HE2	1:D:273:LEU:HD11	2.03	0.41
1:B:126:ILE:HD13	1:B:133:PRO:HB3	2.03	0.41
1:C:92:THR:HB	1:C:131:ASN:CG	2.45	0.41
1:C:120:SER:OG	1:C:121:HIS:N	2.54	0.41
1:A:156:LYS:HE2	1:A:156:LYS:HB2	1.82	0.41
1:C:145:GLY:O	1:C:152:THR:OG1	2.39	0.41
1:C:231:GLU:CG	1:D:234:HIS:HE2	2.34	0.41
1:D:88:LYS:C	1:D:89:ASN:HD22	2.29	0.41
1:D:118:LEU:HD11	1:D:139:ILE:HD11	2.02	0.41
1:D:255:THR:HB	1:D:256:PHE:CD1	2.56	0.41
1:C:199:THR:HG22	1:C:261:GLN:CG	2.49	0.41
1:D:41:TYR:HB3	1:D:42:PRO:HD2	2.03	0.41
1:A:47:CYS:HA	1:A:115:VAL:O	2.21	0.40
1:A:231:GLU:O	1:A:235:ILE:HG12	2.21	0.40
1:A:274:TYR:C	1:A:276:TYR:H	2.29	0.40
1:C:46:LEU:HD12	1:C:114:PHE:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:LEU:HD23	1:D:223:LEU:HA	2.00	0.40
1:A:277:HIS:CD2	1:A:277:HIS:N	2.88	0.40
1:B:93:ARG:O	1:B:97:VAL:HG23	2.21	0.40
1:C:240:ASN:HA	1:C:263:PRO:HD2	2.03	0.40
1:D:226:TYR:O	1:D:228:ASP:N	2.55	0.40
1:A:241:ARG:HH21	1:B:34:ASP:HB3	1.84	0.40
1:D:81:LEU:O	1:D:82:LYS:CB	2.70	0.40
1:C:51:ASN:HD22	1:C:119:LEU:CD1	2.34	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	227/249 (91%)	212 (93%)	13 (6%)	2 (1%)	14	41
1	B	228/249 (92%)	209 (92%)	18 (8%)	1 (0%)	30	60
1	C	229/249 (92%)	219 (96%)	8 (4%)	2 (1%)	14	41
1	D	229/249 (92%)	199 (87%)	24 (10%)	6 (3%)	4	15
All	All	913/996 (92%)	839 (92%)	63 (7%)	11 (1%)	10	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	145	GLY
1	D	34	ASP
1	D	82	LYS
1	D	145	GLY
1	B	145	GLY
1	D	75	ARG
1	D	106	GLU

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Mol	Chain	Res	Type
1	A	227	ALA
1	C	82	LYS
1	D	227	ALA
1	A	145	GLY

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	207/221 (94%)	180 (87%)	27 (13%)	4 14
1	B	208/221 (94%)	186 (89%)	22 (11%)	6 22
1	C	209/221 (95%)	183 (88%)	26 (12%)	4 16
1	D	209/221 (95%)	177 (85%)	32 (15%)	3 10
All	All	833/884 (94%)	726 (87%)	107 (13%)	4 15

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	36	SER
1	A	46	LEU
1	A	57	LYS
1	A	59	THR
1	A	76	GLU
1	A	82	LYS
1	A	88	LYS
1	A	93	ARG
1	A	98	GLU
1	A	110	LYS
1	A	126	ILE
1	A	127	ILE
1	A	139	ILE
1	A	157	LEU
1	A	166	THR
1	A	172	ILE

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Mol	Chain	Res	Type
1	A	187	ILE
1	A	199	THR
1	A	222	MET
1	A	225	GLN
1	A	235	ILE
1	A	241	ARG
1	A	249	SER
1	A	260	LYS
1	A	268	MET
1	A	277	HIS
1	B	46	LEU
1	B	58	SER
1	B	84	GLU
1	B	93	ARG
1	B	98	GLU
1	B	105	LYS
1	B	110	LYS
1	B	120	SER
1	B	126	ILE
1	B	127	ILE
1	B	134	VAL
1	B	136	LEU
1	B	139	ILE
1	B	167	GLU
1	B	172	ILE
1	B	173	GLU
1	B	210	LYS
1	B	222	MET
1	B	224	LYS
1	B	260	LYS
1	B	261	GLN
1	B	268	MET
1	C	34	ASP
1	C	46	LEU
1	C	62	THR
1	C	82	LYS
1	C	87	ASN
1	C	88	LYS
1	C	99	LEU
1	C	101	ARG
1	C	105	LYS
1	C	112	SER

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Mol	Chain	Res	Type
1	C	139	ILE
1	C	140	THR
1	C	149	ARG
1	C	150	SER
1	C	152	THR
1	C	167	GLU
1	C	172	ILE
1	C	173	GLU
1	C	190	ASP
1	C	192	ASP
1	C	194	LEU
1	C	222	MET
1	C	224	LYS
1	C	262	ILE
1	C	268	MET
1	C	277	HIS
1	D	46	LEU
1	D	48	ILE
1	D	53	LYS
1	D	57	LYS
1	D	61	MET
1	D	75	ARG
1	D	77	THR
1	D	79	ARG
1	D	82	LYS
1	D	84	GLU
1	D	88	LYS
1	D	105	LYS
1	D	109	SER
1	D	126	ILE
1	D	134	VAL
1	D	139	ILE
1	D	150	SER
1	D	156	LYS
1	D	159	ILE
1	D	160	ILE
1	D	172	ILE
1	D	198	SER
1	D	199	THR
1	D	205	SER
1	D	210	LYS
1	D	218	SER

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Mol	Chain	Res	Type
1	D	222	MET
1	D	224	LYS
1	D	255	THR
1	D	260	LYS
1	D	262	ILE
1	D	268	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	51	ASN
1	A	56	HIS
1	A	217	GLN
1	A	234	HIS
1	A	277	HIS
1	B	51	ASN
1	B	54	ASN
1	B	87	ASN
1	C	35	ASN
1	C	51	ASN
1	C	73	ASN
1	C	80	ASN
1	C	208	ASN
1	D	51	ASN
1	D	56	HIS
1	D	73	ASN
1	D	89	ASN
1	D	208	ASN
1	D	225	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	OCS	D	163	1	6,8,9	0.92	0	7,11,13	2.14	4 (57%)
1	OCS	B	163	1	6,8,9	1.20	1 (16%)	7,11,13	2.45	3 (42%)
1	OCS	A	163	1	6,8,9	1.42	1 (16%)	7,11,13	3.40	4 (57%)
1	OCS	C	163	1	6,8,9	1.55	1 (16%)	7,11,13	3.82	5 (71%)

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
1	OCS	D	163	1	-	0/4/7/9	-
1	OCS	B	163	1	-	3/4/7/9	-
1	OCS	A	163	1	-	2/4/7/9	-
1	OCS	C	163	1	-	1/4/7/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	163	OCS	OD3-SG	2.94	1.53	1.45
1	A	163	OCS	OD3-SG	2.52	1.52	1.45
1	B	163	OCS	OD3-SG	2.37	1.51	1.45

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	163	OCS	OD3-SG-CB	7.76	118.34	106.76
1	A	163	OCS	OD3-SG-CB	7.48	117.92	106.76
1	B	163	OCS	OD3-SG-CB	4.81	113.94	106.76
1	C	163	OCS	OD2-SG-CB	-3.61	99.00	105.97
1	C	163	OCS	OD2-SG-OD3	3.52	120.19	111.40
1	D	163	OCS	CA-CB-SG	-3.41	108.54	113.61
1	A	163	OCS	OD2-SG-OD1	-3.10	103.64	111.40
1	C	163	OCS	OD3-SG-OD1	-3.07	103.83	113.82
1	B	163	OCS	OD2-SG-CB	3.07	111.89	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	OCS	OD3-SG-OD1	-2.89	104.44	113.82
1	D	163	OCS	OD3-SG-CB	2.74	110.85	106.76
1	D	163	OCS	OD1-SG-CB	2.40	110.33	106.76
1	A	163	OCS	OD2-SG-OD3	2.17	116.84	111.40
1	C	163	OCS	OD2-SG-OD1	-2.04	106.30	111.40
1	D	163	OCS	OD3-SG-OD1	-2.03	107.22	113.82
1	B	163	OCS	OD2-SG-OD1	-2.02	106.33	111.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	163	OCS	CA-CB-SG-OD1
1	B	163	OCS	CA-CB-SG-OD1
1	B	163	OCS	CA-CB-SG-OD2
1	B	163	OCS	CA-CB-SG-OD3
1	A	163	OCS	CA-CB-SG-OD3
1	C	163	OCS	CA-CB-SG-OD3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	163	OCS	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\|>2$
2	RXB	C	300	-	29,29,29	2.98	5 (17%)	41,41,41	3.27	16 (39%)

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	RXB	C	300	-	-	7/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	300	RXB	CAV-CAX	-12.32	1.38	1.53
2	C	300	RXB	OAQ-CAR	7.11	1.50	1.35
2	C	300	RXB	CAY-CAW	-3.92	1.40	1.47
2	C	300	RXB	OAE-CAW	2.71	1.29	1.23
2	C	300	RXB	OAF-CAX	2.26	1.28	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	300	RXB	OAQ-CBA-CAT	11.04	123.88	107.67
2	C	300	RXB	OAQ-CAR-CAA	8.26	125.82	111.09
2	C	300	RXB	CBA-OAQ-CAR	7.42	126.39	115.66
2	C	300	RXB	CBA-CAS-NAO	6.14	126.10	115.06
2	C	300	RXB	OAC-CAS-CBA	-5.52	113.21	120.11
2	C	300	RXB	CAZ-CAU-NAO	4.21	123.78	118.46
2	C	300	RXB	CAX-CAV-NAP	3.55	120.78	116.39
2	C	300	RXB	OAQ-CAR-OAB	-3.42	116.39	122.99
2	C	300	RXB	OAD-CAV-CAX	-3.42	117.24	121.13
2	C	300	RXB	CAT-CBA-CAS	-3.01	104.54	110.43
2	C	300	RXB	CAU-NAO-CAS	-2.61	119.74	126.98
2	C	300	RXB	CAN-CAY-CAW	-2.59	116.33	120.13
2	C	300	RXB	OAF-CAX-CAZ	2.50	126.58	122.06
2	C	300	RXB	OAQ-CBA-CAS	2.44	113.31	109.65
2	C	300	RXB	CAJ-CAM-CAU	2.13	123.03	118.69
2	C	300	RXB	CAN-CAY-CAZ	2.12	123.15	120.16

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	300	RXB	CAT-CBA-OAQ-CAR
2	C	300	RXB	OAB-CAR-OAQ-CBA
2	C	300	RXB	CAA-CAR-OAQ-CBA
2	C	300	RXB	CAS-CBA-OAQ-CAR
2	C	300	RXB	CAK-CAT-CBA-CAS
2	C	300	RXB	CAL-CAT-CBA-CAS
2	C	300	RXB	CAZ-CAU-NAO-CAS

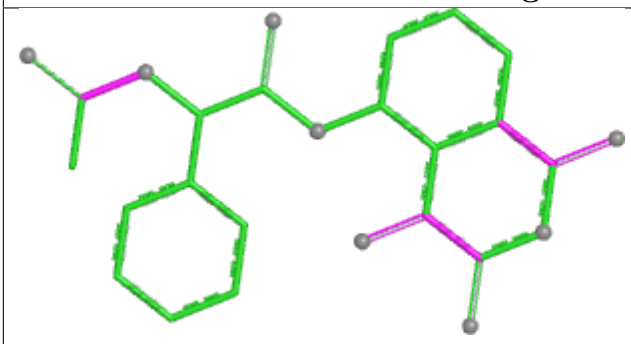
There are no ring outliers.

1 monomer is involved in 9 short contacts:

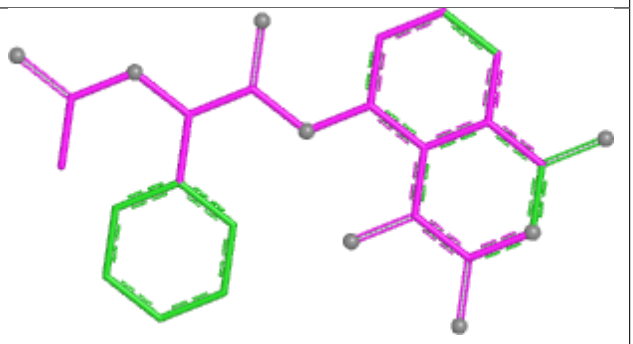
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	300	RXB	9	0

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.

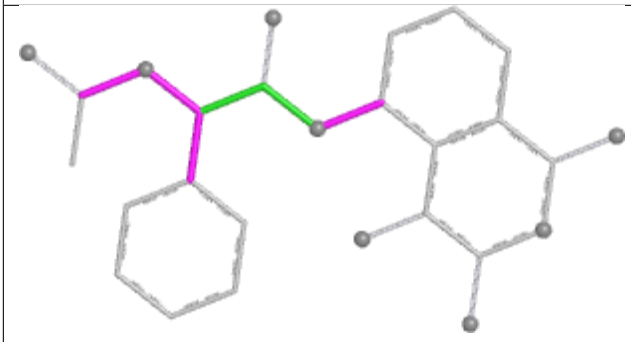
Ligand RXB C 300



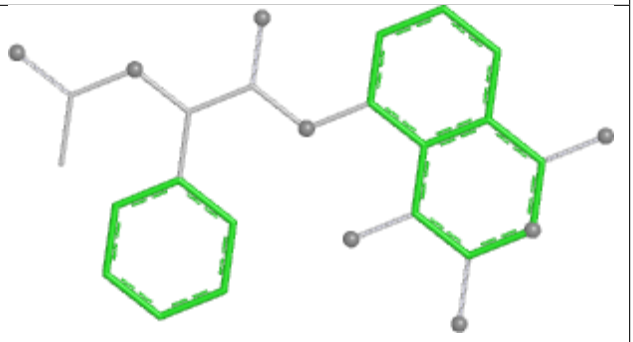
Bond lengths



Bond angles



Torsions



Rings

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	231/249 (92%)	-0.37	0 100 100	36, 59, 89, 125	0
1	B	232/249 (93%)	-0.33	2 (0%) 81 74	33, 58, 89, 119	0
1	C	233/249 (93%)	-0.05	4 (1%) 69 60	39, 72, 106, 161	0
1	D	233/249 (93%)	0.39	4 (1%) 69 60	54, 90, 125, 171	0
All	All	929/996 (93%)	-0.09	10 (1%) 78 70	33, 68, 113, 171	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	LEU	2.8
1	B	276	TYR	2.8
1	C	185	HIS	2.6
1	D	251	SER	2.3
1	D	65	SER	2.3
1	C	35	ASN	2.2
1	D	61	MET	2.2
1	C	145	GLY	2.2
1	D	210	LYS	2.1
1	C	33	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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
1	OCS	C	163	9/10	0.87	0.12	49,51,58,61	0
1	OCS	D	163	9/10	0.88	0.12	95,97,98,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	OCS	B	163	9/10	0.93	0.11	55,57,68,68	0
1	OCS	A	163	9/10	0.94	0.10	44,46,57,61	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

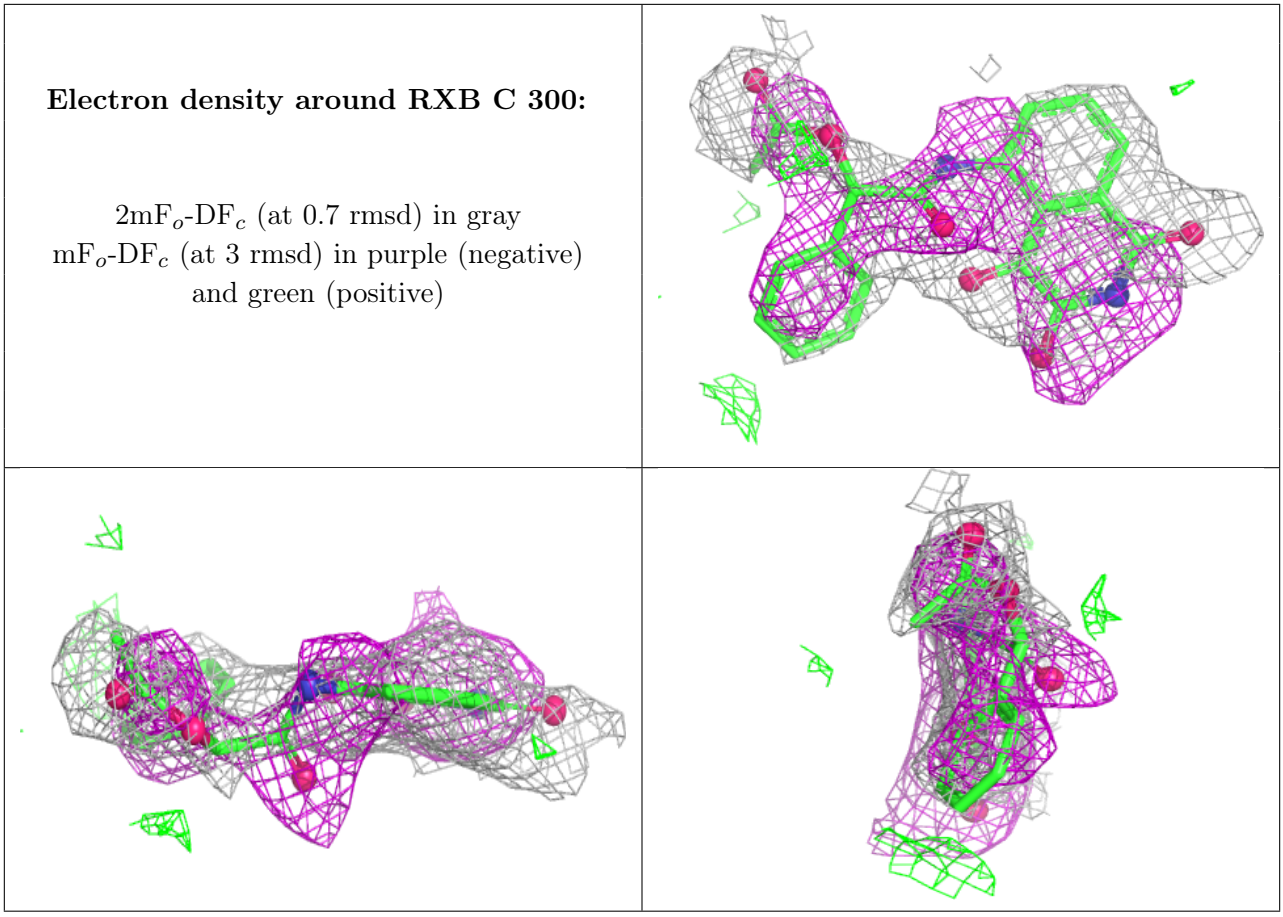
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	RXB	C	300	27/27	0.68	0.19	55,61,66,67	0

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

Electron density around RXB C 300:

$2mF_o$-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.