



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:43 AM UTC

PDB ID : 2QLJ / pdb_00002qlj
Title : Crystal Structure of Caspase-7 with Inhibitor AC-WEHD-CHO
Authors : Agniswamy, J.; Fang, B.; Weber, I.
Deposited on : 2007-07-12
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

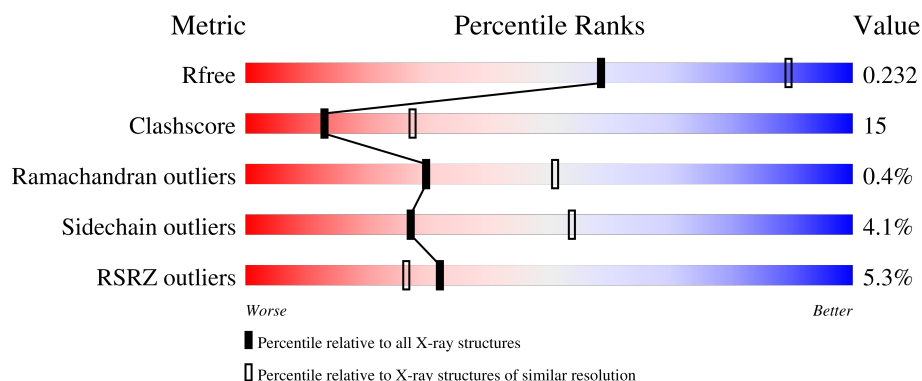
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	173	
1	C	173	
2	B	97	
2	D	97	
3	E	5	

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Mol	Chain	Length	Quality of chain
3	F	5	
4	G	5	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3918 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-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	0	0
			1100	691	188	210	11			
1	C	140	Total	C	N	O	S	0	0	0
			1100	691	188	210	11			

- Molecule 2 is a protein called Caspase-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	92	Total	C	N	O	S	0	0	0
			758	487	128	139	4			
2	D	93	Total	C	N	O	S	0	0	0
			770	496	129	141	4			

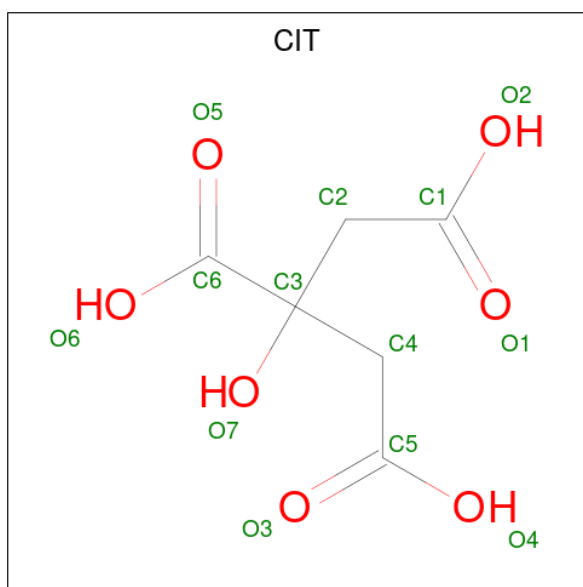
- Molecule 3 is a protein called Inhibitor AC-WEHD-CHO.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			44	28	7	9			
3	F	5	Total	C	N	O	0	0	0
			44	28	7	9			

- Molecule 4 is a protein called Peptide QGHGE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	5	Total	C	N	O	0	0	0
			37	20	8	9			

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		

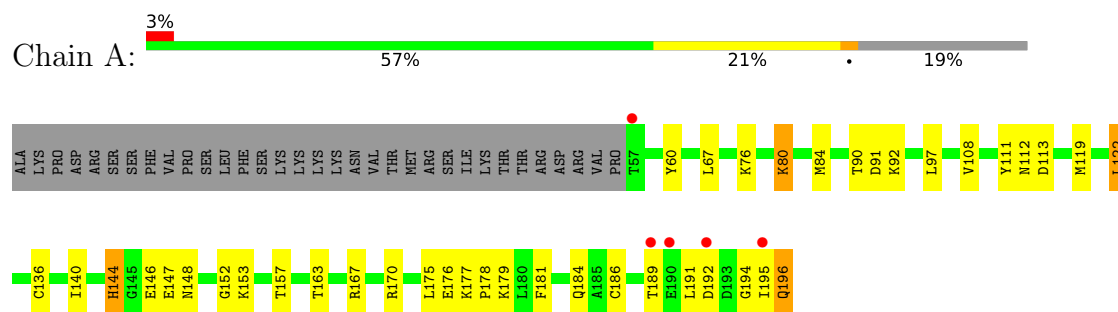
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total	O	0	0
			11	11		
6	B	8	Total	O	0	0
			8	8		
6	C	21	Total	O	0	0
			21	21		
6	D	8	Total	O	0	0
			8	8		
6	F	4	Total	O	0	0
			4	4		

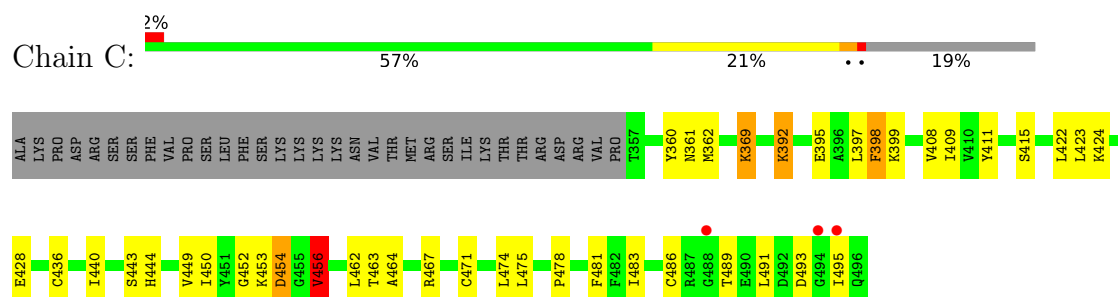
3 Residue-property plots [i](#)

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.

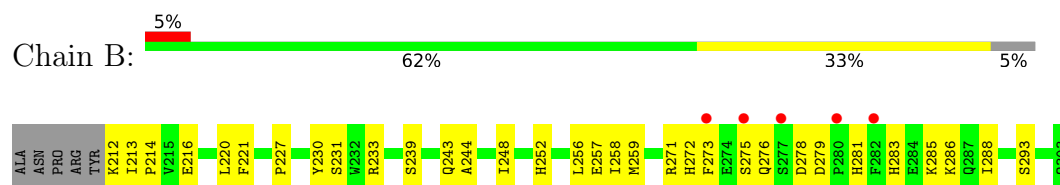
• Molecule 1: Caspase-7



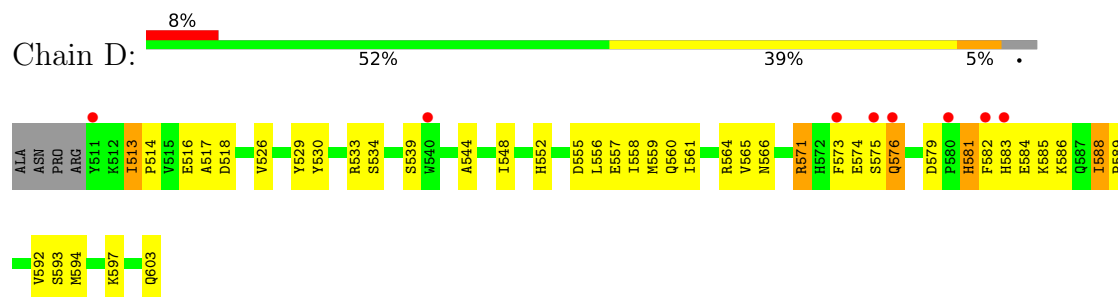
• Molecule 1: Caspase-7



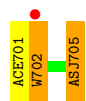
• Molecule 2: Caspase-7



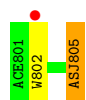
• Molecule 2: Caspase-7



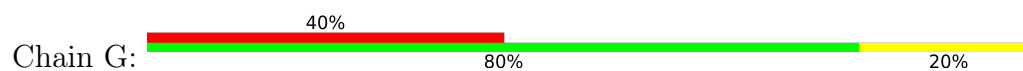
- Molecule 3: Inhibitor AC-WEHD-CHO



- Molecule 3: Inhibitor AC-WEHD-CHO



- Molecule 4: Peptide QGHGE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.50Å 88.50Å 187.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.0 (50.00-2.60) 87.0 (50.00-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.58Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.196 , 0.234 0.195 , 0.232	Depositor DCC
R_{free} test set	1207 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3918	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, ASJ, ACE

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	0.41	0/1117	0.91	3/1496 (0.2%)
1	C	0.43	0/1117	0.99	4/1496 (0.3%)
2	B	0.42	0/780	0.92	2/1054 (0.2%)
2	D	0.48	1/793 (0.1%)	1.02	5/1072 (0.5%)
3	E	1.07	0/36	1.99	2/49 (4.1%)
3	F	0.51	0/36	0.91	0/49
4	G	0.44	0/37	0.55	0/46
All	All	0.45	1/3916 (0.0%)	0.97	16/5262 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	588	ILE	CA-CB	5.00	1.58	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	701	ACE	C-N-CA	10.85	154.26	121.70
1	A	152	GLY	N-CA-C	-9.38	99.72	112.57
1	C	452	GLY	N-CA-C	-7.37	99.82	112.64
1	C	456	VAL	N-CA-C	6.92	118.44	108.48
1	A	67	LEU	N-CA-C	-6.72	103.43	111.69
2	D	573	PHE	N-CA-C	6.04	119.46	110.52
2	D	571	ARG	N-CA-C	5.99	122.18	110.56
2	B	293	SER	N-CA-C	5.73	118.25	108.90
2	D	593	SER	N-CA-C	5.44	117.77	108.90
1	C	483	ILE	N-CA-C	5.44	115.82	107.77
2	D	594	MET	N-CA-C	-5.18	105.64	112.94
3	E	701	ACE	O-C-N	5.16	138.48	123.00
1	A	144	HIS	N-CA-C	-5.13	103.62	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	529	TYR	N-CA-C	5.11	117.64	110.14
2	B	273	PHE	N-CA-C	5.10	117.88	109.72
1	C	453	LYS	N-CA-C	-5.02	105.99	111.82

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	1100	0	1085	32	0
1	C	1100	0	1085	38	0
2	B	758	0	731	31	0
2	D	770	0	740	34	0
3	E	44	0	30	4	0
3	F	44	0	31	6	0
4	G	37	0	26	1	0
5	A	13	0	5	2	0
6	A	11	0	0	0	0
6	B	8	0	0	0	0
6	C	21	0	0	1	0
6	D	8	0	0	0	0
6	F	4	0	0	0	0
All	All	3918	0	3733	114	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 15.

All (114) 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:80:LYS:H	1:A:80:LYS:HD2	1.24	0.97
2:D:534:SER:HB2	3:F:802:TRP:CE3	2.11	0.86
2:D:534:SER:HB2	3:F:802:TRP:CZ3	2.11	0.85
2:B:259:MET:HE2	2:D:559:MET:HE2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LYS:HD2	1:A:80:LYS:N	2.02	0.71
2:B:271:ARG:NH1	2:D:513:ILE:HD11	2.06	0.71
1:C:443:SER:HB3	1:C:450:ILE:HD11	1.73	0.70
1:A:147:GLU:HG3	1:A:148:ASN:OD1	1.92	0.69
1:C:423:LEU:HD12	1:C:462:LEU:HD22	1.74	0.67
2:D:533:ARG:HA	2:D:539:SER:HA	1.76	0.67
2:B:286:LYS:HB3	2:D:514:PRO:HG3	1.75	0.67
1:A:84:MET:HE2	1:A:144:HIS:CG	2.30	0.66
1:C:397:LEU:HD13	1:C:440:ILE:HG21	1.77	0.65
1:C:464:ALA:O	1:C:467:ARG:HG3	1.97	0.65
1:C:489:THR:HA	2:D:530:TYR:CE1	2.31	0.65
1:A:80:LYS:H	1:A:80:LYS:CD	1.92	0.64
1:A:195:ILE:O	1:A:196:GLN:HG3	1.98	0.63
2:D:566:ASN:OD1	2:D:589:PRO:HB2	1.98	0.63
1:C:486:CYS:H	3:F:805:ASJ:H	1.64	0.62
1:A:163:THR:HG22	1:A:181:PHE:CE2	2.35	0.61
1:C:392:LYS:NZ	1:C:392:LYS:HB2	2.15	0.61
1:A:186:CYS:H	3:E:705:ASJ:H	1.65	0.61
1:A:163:THR:HG21	2:B:221:PHE:HE1	1.66	0.60
2:D:552:HIS:HB3	2:D:556:LEU:HG	1.83	0.60
2:B:233:ARG:HA	2:B:239:SER:HA	1.84	0.59
1:C:395:GLU:CG	1:C:399:LYS:HE3	2.33	0.59
2:B:276:GLN:HB3	3:E:702:TRP:CZ3	2.39	0.58
1:C:444:HIS:O	1:C:450:ILE:HD12	2.04	0.58
5:A:850:CIT:H22	2:B:227:PRO:HG2	1.87	0.57
1:A:136:CYS:HB3	1:A:178:PRO:HG2	1.87	0.56
1:A:186:CYS:N	3:E:705:ASJ:H	2.20	0.56
1:A:191:LEU:HD23	2:B:285:LYS:HG3	1.88	0.56
2:B:214:PRO:HG3	2:D:586:LYS:HB3	1.88	0.56
1:C:424:LYS:O	1:C:428:GLU:HG3	2.06	0.55
1:A:136:CYS:CB	1:A:178:PRO:HG2	2.36	0.55
1:C:360:TYR:CD1	1:C:478:PRO:HD3	2.42	0.55
2:D:571:ARG:HG2	2:D:571:ARG:HH11	1.72	0.55
1:A:177:LYS:O	1:A:179:LYS:HE2	2.07	0.54
1:C:436:CYS:HB3	1:C:478:PRO:HG2	1.91	0.53
1:A:184:GLN:HE22	2:B:231:SER:HB3	1.73	0.53
4:G:810:GLN:N	4:G:810:GLN:OE1	2.42	0.53
1:C:486:CYS:N	3:F:805:ASJ:H	2.24	0.52
1:C:411:TYR:CG	1:C:422:LEU:HD11	2.45	0.51
1:C:467:ARG:HD3	6:C:50:HOH:O	2.11	0.51
2:B:271:ARG:HH11	2:B:271:ARG:HG3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:LYS:HE2	1:C:409:ILE:CD1	2.41	0.51
1:A:175:LEU:O	1:A:176:GLU:HB2	2.12	0.50
1:C:449:VAL:CG1	1:C:456:VAL:HG13	2.42	0.50
2:D:574:GLU:OE2	2:D:584:GLU:HB3	2.12	0.50
5:A:850:CIT:H41	2:D:592:VAL:HG21	1.94	0.49
2:B:257:GLU:OE2	2:B:258:ILE:HG22	2.12	0.49
2:D:560:GLN:O	2:D:564:ARG:HG3	2.13	0.49
2:B:213:ILE:HD11	2:D:571:ARG:HH12	1.77	0.49
1:C:491:LEU:HD11	2:D:582:PHE:CD2	2.47	0.49
2:D:575:SER:HA	3:F:802:TRP:CD1	2.48	0.49
2:B:257:GLU:OE1	2:B:259:MET:HB2	2.13	0.48
2:D:526:VAL:HG13	2:D:588:ILE:HG23	1.95	0.48
1:C:463:THR:HG22	1:C:481:PHE:CE2	2.49	0.48
2:D:579:ASP:O	2:D:583:HIS:HB2	2.14	0.48
2:B:244:ALA:O	2:B:248:ILE:HG12	2.13	0.48
2:B:281:HIS:O	2:B:285:LYS:HE3	2.14	0.48
1:A:97:LEU:HD13	1:A:140:ILE:HG21	1.95	0.48
1:C:449:VAL:HG11	1:C:456:VAL:HG13	1.95	0.48
2:B:278:ASP:O	2:B:279:ASP:C	2.57	0.48
1:C:449:VAL:CG1	1:C:456:VAL:HG22	2.44	0.48
1:A:111:TYR:CG	1:A:122:LEU:HD21	2.49	0.47
1:A:196:GLN:HG2	1:C:475:LEU:CD2	2.43	0.47
1:C:398:PHE:CD1	1:C:398:PHE:C	2.93	0.47
2:B:216:GLU:HB2	2:D:588:ILE:HG21	1.96	0.47
1:A:163:THR:HG21	2:B:221:PHE:CE1	2.47	0.47
2:D:557:GLU:OE2	2:D:558:ILE:HG22	2.14	0.47
2:B:283:HIS:O	2:B:285:LYS:HE2	2.14	0.47
2:D:561:ILE:O	2:D:565:VAL:HG23	2.15	0.47
1:A:60:TYR:CD1	1:A:178:PRO:HD3	2.49	0.47
1:C:493:ASP:HA	2:D:585:LYS:HD2	1.95	0.46
1:C:436:CYS:CB	1:C:478:PRO:HG2	2.45	0.46
1:A:167:ARG:NH1	1:A:170:ARG:NH2	2.64	0.46
1:C:369:LYS:HE2	1:C:409:ILE:HD11	1.98	0.46
1:A:146:GLU:O	1:A:147:GLU:C	2.58	0.46
2:B:213:ILE:HD11	2:D:571:ARG:NH1	2.32	0.45
1:C:415:SER:HB2	1:C:454:ASP:OD2	2.16	0.45
1:C:449:VAL:HG11	1:C:456:VAL:CG1	2.45	0.45
1:A:196:GLN:HG2	1:C:475:LEU:HD21	1.99	0.45
1:C:395:GLU:HG2	1:C:399:LYS:HE3	1.99	0.45
2:D:557:GLU:OE1	2:D:559:MET:HB2	2.17	0.45
1:A:163:THR:HG22	1:A:181:PHE:CD2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:CYS:SG	1:C:474:LEU:HD12	2.57	0.44
2:B:252:HIS:HB3	2:B:256:LEU:HD12	2.00	0.44
2:B:288:ILE:O	2:B:288:ILE:HG23	2.18	0.44
1:C:411:TYR:CD1	1:C:422:LEU:HD11	2.52	0.44
1:C:392:LYS:HB2	1:C:392:LYS:HZ3	1.81	0.44
2:B:220:LEU:C	2:B:220:LEU:HD23	2.43	0.43
1:A:189:THR:HA	2:B:230:TYR:CE1	2.54	0.42
2:B:275:SER:OG	2:B:285:LYS:HB2	2.20	0.42
2:B:288:ILE:HG21	2:D:516:GLU:HB2	2.01	0.42
1:A:112:ASN:O	1:A:113:ASP:C	2.62	0.42
2:B:239:SER:O	2:B:243:GLN:HG3	2.19	0.42
2:D:576:GLN:H	3:F:802:TRP:CD1	2.37	0.42
2:D:571:ARG:HG2	2:D:571:ARG:NH1	2.35	0.42
1:A:194:GLY:HA2	2:D:513:ILE:O	2.19	0.42
1:A:97:LEU:HD22	1:A:140:ILE:HD13	2.02	0.42
1:C:449:VAL:HG11	1:C:456:VAL:CG2	2.50	0.42
2:B:285:LYS:HA	2:B:285:LYS:HD3	1.88	0.41
2:B:212:LYS:HA	1:C:495:ILE:O	2.21	0.41
2:B:276:GLN:HB3	3:E:702:TRP:CE3	2.56	0.41
2:D:517:ALA:O	2:D:518:ASP:HB2	2.21	0.41
2:D:555:ASP:O	2:D:556:LEU:HD23	2.21	0.41
1:C:360:TYR:CD2	2:D:597:LYS:HB2	2.56	0.40
1:A:76:LYS:HB2	1:A:90:THR:HG21	2.04	0.40
1:A:76:LYS:HD2	1:A:91:ASP:OD2	2.21	0.40
1:A:119:MET:HE3	1:A:157:THR:HG21	2.03	0.40
1:C:491:LEU:HD13	2:D:581:HIS:O	2.22	0.40
1:C:361:ASN:O	1:C:362:MET:HE2	2.22	0.40
2:D:544:ALA:O	2:D:548:ILE:HG12	2.21	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	138/173 (80%)	132 (96%)	6 (4%)	0	100	100
1	C	138/173 (80%)	133 (96%)	5 (4%)	0	100	100
2	B	90/97 (93%)	82 (91%)	7 (8%)	1 (1%)	11	25
2	D	91/97 (94%)	87 (96%)	4 (4%)	0	100	100
3	E	3/5 (60%)	1 (33%)	1 (33%)	1 (33%)	0	0
3	F	3/5 (60%)	3 (100%)	0	0	100	100
4	G	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
All	All	466/555 (84%)	440 (94%)	24 (5%)	2 (0%)	30	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	702	TRP
2	B	272	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	120/152 (79%)	113 (94%)	7 (6%)	18	39
1	C	120/152 (79%)	114 (95%)	6 (5%)	22	46
2	B	84/88 (96%)	84 (100%)	0	100	100
2	D	85/88 (97%)	81 (95%)	4 (5%)	23	48
3	E	3/3 (100%)	3 (100%)	0	100	100
3	F	3/3 (100%)	3 (100%)	0	100	100
4	G	3/3 (100%)	3 (100%)	0	100	100
All	All	418/489 (86%)	401 (96%)	17 (4%)	27	54

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LYS
1	A	92	LYS
1	A	108	VAL
1	A	122	LEU
1	A	153	LYS
1	A	192	ASP
1	A	196	GLN
1	C	369	LYS
1	C	392	LYS
1	C	398	PHE
1	C	408	VAL
1	C	454	ASP
1	C	456	VAL
2	D	513	ILE
2	D	576	GLN
2	D	581	HIS
2	D	603	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	184	GLN
2	B	283	HIS
1	C	359	GLN
1	C	388	ASN
1	C	448	ASN
4	G	810	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
3	ASJ	F	805	3,1	7,7,7	1.09	0	5,8,8	2.18	1 (20%)
3	ASJ	E	705	3,1	7,7,7	0.78	0	5,8,8	1.43	1 (20%)

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	ASJ	F	805	3,1	-	4/6/6/6	-
3	ASJ	E	705	3,1	-	2/6/6/6	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	F	805	ASJ	CB-CA-C	-4.16	104.68	112.21
3	E	705	ASJ	CB-CA-C	-2.52	107.65	112.21

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	705	ASJ	O-C-CA-N
3	E	705	ASJ	O-C-CA-CB
3	F	805	ASJ	O-C-CA-N
3	F	805	ASJ	O-C-CA-CB
3	F	805	ASJ	C-CA-CB-CG
3	F	805	ASJ	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	805	ASJ	2	0
3	E	705	ASJ	2	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	$\# Z > 2$
5	CIT	A	850	-	12,12,12	1.48	1 (8%)	17,17,17	1.40	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CIT	A	850	-	-	10/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	850	CIT	C2-C3	3.91	1.58	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	850	CIT	O6-C6-C3	3.63	120.11	113.14

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	850	CIT	C2-C3-C6-O5

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Mol	Chain	Res	Type	Atoms
5	A	850	CIT	O7-C3-C6-O5
5	A	850	CIT	O7-C3-C4-C5
5	A	850	CIT	C1-C2-C3-C4
5	A	850	CIT	C2-C3-C6-O6
5	A	850	CIT	C6-C3-C4-C5
5	A	850	CIT	C4-C3-C6-O6
5	A	850	CIT	C1-C2-C3-C6
5	A	850	CIT	C4-C3-C6-O5
5	A	850	CIT	O7-C3-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	850	CIT	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	140/173 (80%)	0.09	5 (3%)	46 40	51, 72, 96, 113	0
1	C	140/173 (80%)	-0.15	3 (2%)	63 58	47, 59, 92, 125	0
2	B	92/97 (94%)	0.19	5 (5%)	31 26	49, 68, 138, 144	0
2	D	93/97 (95%)	0.21	8 (8%)	16 12	48, 62, 137, 145	0
3	E	3/5 (60%)	1.76	1 (33%)	1 1	97, 97, 106, 120	0
3	F	3/5 (60%)	0.96	1 (33%)	1 1	77, 77, 79, 92	0
4	G	5/5 (100%)	2.09	2 (40%)	1 0	111, 115, 121, 121	0
All	All	476/555 (85%)	0.10	25 (5%)	32 26	47, 65, 121, 145	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	702	TRP	4.5
2	D	575	SER	3.6
2	D	511	TYR	3.5
2	D	573	PHE	3.5
1	C	495	ILE	3.3
2	B	280	PRO	3.3
2	B	282	PHE	3.3
2	D	580	PRO	3.0
1	A	57	THR	3.0
3	F	802	TRP	2.8
1	C	494	GLY	2.8
4	G	813	GLY	2.7
4	G	814	GLU	2.7
2	D	576	GLN	2.7
2	D	583	HIS	2.6
2	B	275	SER	2.5
1	A	192	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	582	PHE	2.5
1	A	189	THR	2.5
1	A	190	GLU	2.4
2	D	540	TRP	2.3
2	B	277	SER	2.3
2	B	273	PHE	2.2
1	C	488	GLY	2.2
1	A	195	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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	ASJ	E	705	8/8	0.93	0.10	80,82,84,87	0
3	ASJ	F	805	8/8	0.95	0.10	69,71,73,74	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CIT	A	850	13/13	0.82	0.19	109,111,113,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.