



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:45 AM UTC

PDB ID : 3D59 / pdb_00003d59
Title : Crystal structure of human plasma platelet activating factor acetylhydrolase
Authors : Samanta, U.; Bahnson, B.J.
Deposited on : 2008-05-16
Resolution : 1.50 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

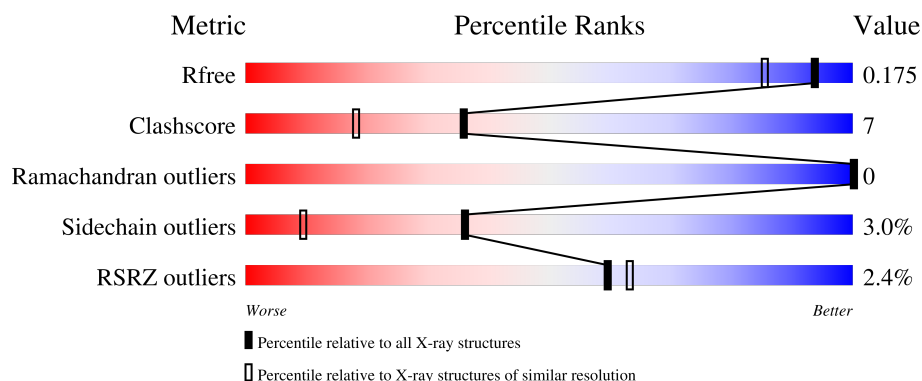
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

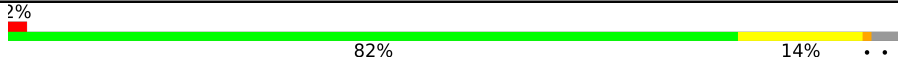
The reported resolution of this entry is 1.50 Å.

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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	383	
1	B	383	

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	ACT	A	11	-	-	X	-
2	ACT	A	16	-	-	X	-
2	ACT	A	24	-	-	X	-
2	ACT	A	33	-	-	X	-
2	ACT	A	36	-	-	X	-
2	ACT	B	23	-	-	X	-

2 Entry composition [i](#)

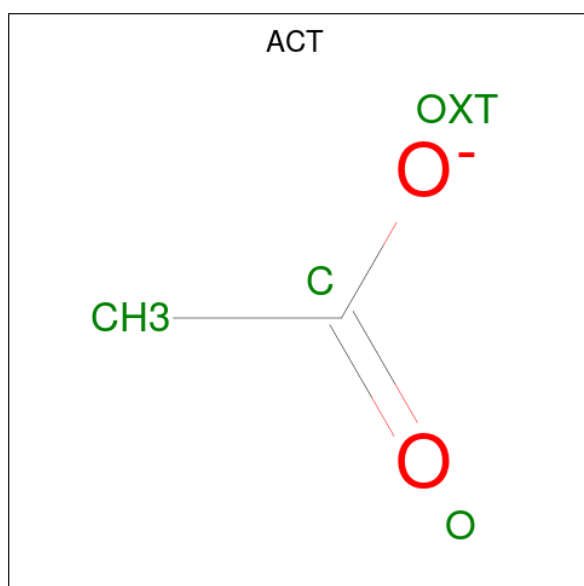
There are 4 unique types of molecules in this entry. The entry contains 6692 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Platelet-activating factor acetylhydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	27	0
			3065	1967	516	568	14			
1	B	374	Total	C	N	O	S	0	11	0
			2990	1913	514	550	13			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

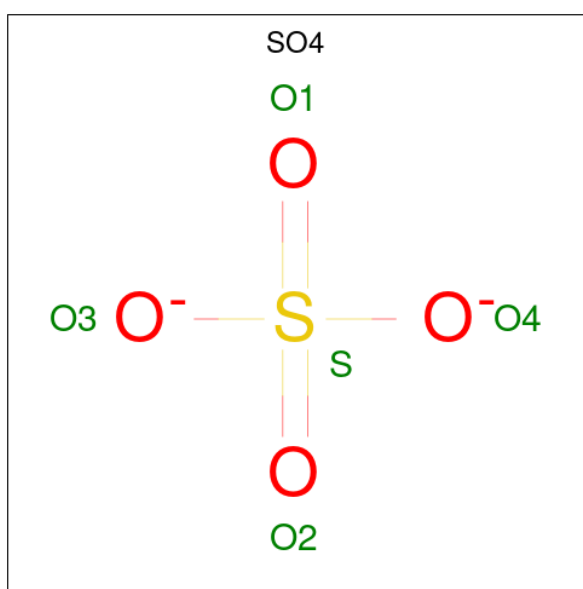
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

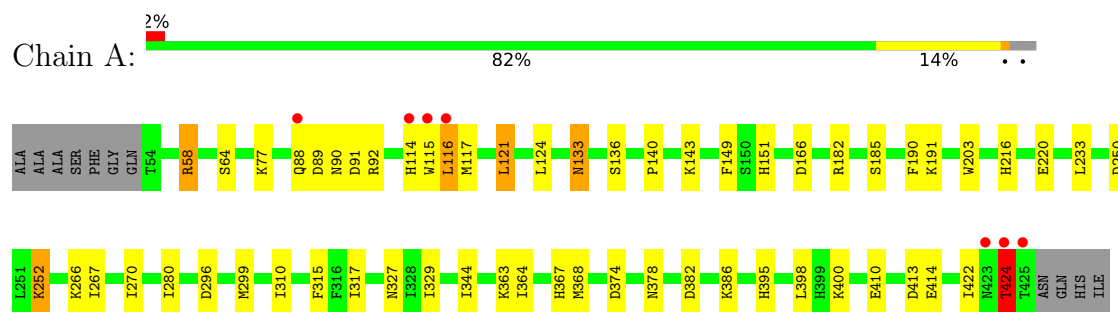
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	293	Total	O	0	0
			293	293		
4	B	218	Total	O	0	0
			218	218		

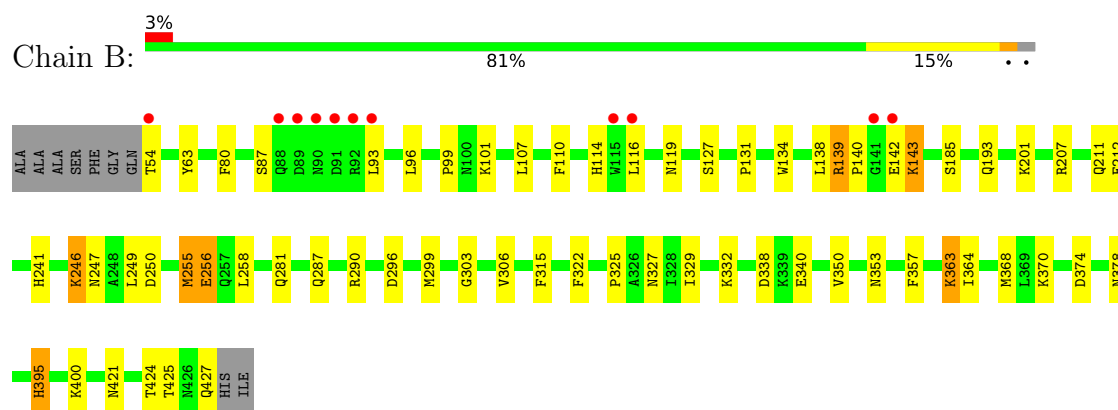
3 Residue-property plots

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: Platelet-activating factor acetylhydrolase



- Molecule 1: Platelet-activating factor acetylhydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.18Å 83.06Å 96.70Å 90.00° 115.09° 90.00°	Depositor
Resolution (Å)	10.00 – 1.50 10.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	91.5 (10.00-1.50) 92.6 (10.00-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 1.40Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.131 , 0.191 0.133 , 0.175	Depositor DCC
R_{free} test set	6764 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 78.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	6692	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ACT

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	0.73	0/3229	1.34	15/4364 (0.3%)
1	B	0.69	1/3086 (0.0%)	1.36	18/4175 (0.4%)
All	All	0.71	1/6315 (0.0%)	1.35	33/8539 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	250	ASP	C-O	-5.03	1.17	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	ASN	CA-CB-CG	-7.31	105.29	112.60
1	B	249	LEU	CA-C-N	-6.94	112.49	122.77
1	B	249	LEU	C-N-CA	-6.94	112.49	122.77
1	A	115	TRP	CA-C-N	6.88	129.38	120.44
1	A	115	TRP	C-N-CA	6.88	129.38	120.44
1	B	395	HIS	CA-CB-CG	-6.45	107.35	113.80
1	A	395	HIS	CA-CB-CG	-6.34	107.46	113.80
1	B	421	ASN	CA-CB-CG	6.32	118.92	112.60
1	B	315	PHE	CA-CB-CG	6.10	119.90	113.80
1	A	58	ARG	CA-C-N	-6.07	114.58	120.34
1	A	58	ARG	C-N-CA	-6.07	114.58	120.34
1	A	121	LEU	CA-C-O	5.89	126.80	120.55
1	B	281	GLN	OE1-CD-NE2	-5.76	116.84	122.60
1	A	151	HIS	N-CA-C	5.62	117.94	110.53
1	B	378	ASN	CA-CB-CG	-5.56	107.04	112.60
1	A	133	ASN	CA-CB-CG	5.51	118.11	112.60
1	B	241	HIS	CA-CB-CG	-5.45	108.35	113.80
1	A	378	ASN	CA-CB-CG	-5.40	107.20	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	ASP	CA-CB-CG	-5.37	107.23	112.60
1	A	166	ASP	CA-CB-CG	-5.30	107.30	112.60
1	B	54	THR	CA-C-N	-5.18	114.52	122.60
1	B	54	THR	C-N-CA	-5.18	114.52	122.60
1	A	413	ASP	CA-C-O	-5.15	115.23	120.89
1	B	400	LYS	CA-C-N	-5.14	115.00	122.86
1	B	400	LYS	C-N-CA	-5.14	115.00	122.86
1	A	190	PHE	CA-CB-CG	-5.08	108.72	113.80
1	A	140	PRO	CA-C-N	5.06	130.82	120.80
1	A	140	PRO	C-N-CA	5.06	130.82	120.80
1	B	193	GLN	O-C-N	-5.05	116.77	122.12
1	B	80	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	424	THR	CA-C-O	-5.01	115.55	121.16
1	B	87	SER	CA-C-N	-5.01	113.63	120.44
1	B	87	SER	C-N-CA	-5.01	113.63	120.44

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	3065	0	3026	47	0
1	B	2990	0	2912	41	0
2	A	68	0	51	15	0
2	B	48	0	36	6	0
3	B	10	0	0	1	0
4	A	293	0	0	3	0
4	B	218	0	0	3	0
All	All	6692	0	6025	89	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 7.

All (89) 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:B:299:MET:H	1:B:327:ASN:HD21	1.19	0.88
1:A:203:TRP:H	2:A:16:ACT:H1	1.40	0.85
1:A:422:ILE:HG22	1:A:424:THR:HG22	1.57	0.84
1:A:299:MET:H	1:A:327:ASN:HD21	1.25	0.82
1:A:90:ASN:HD22	1:A:133:ASN:HD21	1.30	0.80
1:B:138:LEU:HD22	1:B:258:LEU:HD23	1.63	0.79
1:A:364:ILE:O	1:A:368:MET:HG3	1.83	0.78
1:B:350:VAL:H	1:B:353:ASN:HD22	1.29	0.77
1:A:116:LEU:H	1:A:116:LEU:HD13	1.51	0.76
1:A:117:MET:HE3	1:A:121:LEU:HD21	1.69	0.74
1:B:364:ILE:O	1:B:368:MET:HG3	1.88	0.72
1:B:357:PHE:CZ	2:B:23:ACT:H2	2.26	0.70
1:B:114:HIS:CD2	1:B:116:LEU:H	2.11	0.68
1:A:317[B]:ILE:HD13	1:A:344:ILE:HD11	1.73	0.68
1:A:124:LEU:HD22	2:A:24:ACT:H3	1.77	0.67
1:B:107:LEU:HD22	2:B:23:ACT:H1	1.77	0.67
1:B:299:MET:H	1:B:327:ASN:ND2	1.95	0.63
1:B:114:HIS:HD2	1:B:116:LEU:H	1.47	0.63
1:B:350:VAL:H	1:B:353:ASN:ND2	1.96	0.62
1:A:58:ARG:H	2:A:33:ACT:H3	1.64	0.62
1:A:203:TRP:H	2:A:16:ACT:CH3	2.13	0.61
1:A:299:MET:H	1:A:327:ASN:ND2	1.99	0.59
1:A:266:LYS:HD3	1:A:398:LEU:HD23	1.85	0.58
1:A:182:ARG:HH12	2:A:36:ACT:H3	1.69	0.58
1:A:382[B]:ASP:OD1	1:A:386:LYS:HE3	2.04	0.57
1:B:134:TRP:HE1	2:B:13:ACT:C	2.18	0.56
1:B:207:ARG:HD2	3:B:1:SO4:O4	2.05	0.56
1:A:58:ARG:H	2:A:33:ACT:CH3	2.17	0.56
1:A:191:LYS:HZ1	2:A:28:ACT:C	2.21	0.53
1:A:266:LYS:HD3	1:A:398:LEU:CD2	2.40	0.52
1:A:116:LEU:HD22	1:A:117:MET:H	1.75	0.52
1:A:315:PHE:CE2	1:A:317[B]:ILE:HD11	2.45	0.52
1:B:424:THR:HG22	4:B:542:HOH:O	2.10	0.52
1:A:414[A]:GLU:HG2	4:A:583:HOH:O	2.09	0.51
1:B:107:LEU:HD13	2:B:23:ACT:CH3	2.40	0.51
1:B:363[A]:LYS:HG2	1:B:364:ILE:N	2.26	0.51
1:B:142:GLU:HG2	1:B:143:LYS:N	2.24	0.51
1:A:89[B]:ASP:OD1	1:A:136:SER:OG	2.30	0.50
2:A:11:ACT:OXT	2:A:15:ACT:O	2.29	0.50
1:A:367:HIS:HE1	1:A:374:ASP:OD1	1.94	0.50
1:A:203:TRP:HB2	2:A:16:ACT:H1	1.95	0.49
1:A:116:LEU:H	1:A:116:LEU:CD1	2.22	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:GLU:HG2	1:B:395:HIS:CE1	2.48	0.48
1:A:143:LYS:HZ3	2:A:11:ACT:C	2.27	0.48
1:A:252:LYS:HD3	1:A:252:LYS:HA	1.49	0.47
1:B:139:ARG:NH1	1:B:139:ARG:HG2	2.30	0.47
1:A:91[A]:ASP:OD1	1:B:101:LYS:NZ	2.46	0.47
1:A:400:LYS:HE2	4:A:626:HOH:O	2.15	0.47
1:A:317[B]:ILE:HD13	1:A:344:ILE:CD1	2.44	0.47
1:B:63:TYR:HE1	1:B:139:ARG:HE	1.61	0.47
1:B:332:LYS:HD3	1:B:332:LYS:HA	1.60	0.47
1:A:90:ASN:ND2	1:A:133:ASN:HD21	2.08	0.46
1:B:424:THR:HA	4:B:542:HOH:O	2.15	0.46
1:A:88:GLN:HG3	1:A:89[A]:ASP:OD2	2.15	0.46
1:B:93:LEU:HB3	1:B:131:PRO:HA	1.96	0.46
1:B:322:PHE:HD1	2:B:14:ACT:H3	1.81	0.46
1:A:410:GLU:O	2:A:39:ACT:OXT	2.32	0.46
1:A:149:PHE:HA	1:A:270:ILE:O	2.16	0.46
2:A:19:ACT:H2	4:A:662:HOH:O	2.16	0.46
1:B:139:ARG:NH1	1:B:140:PRO:O	2.48	0.46
1:B:139:ARG:NH2	1:B:142:GLU:OE1	2.49	0.45
1:A:280:ILE:HG23	1:A:310:ILE:HD11	1.98	0.45
1:B:287:GLN:NE2	1:B:290[B]:ARG:NH1	2.64	0.45
1:A:64:SER:OG	1:A:90:ASN:HB2	2.17	0.45
1:A:203:TRP:N	2:A:16:ACT:H1	2.20	0.45
1:A:233:LEU:HD11	1:A:267[A]:ILE:HD13	1.98	0.45
1:A:124:LEU:HD22	2:A:24:ACT:CH3	2.45	0.44
1:A:182:ARG:HH12	2:A:36:ACT:CH3	2.29	0.43
1:B:325:PRO:O	1:B:329:ILE:HG13	2.19	0.43
1:A:364:ILE:HD12	1:A:364:ILE:N	2.33	0.43
1:B:96:LEU:HD23	1:B:99:PRO:HA	2.01	0.42
1:B:201:LYS:NZ	4:B:640:HOH:O	2.53	0.42
1:B:246:LYS:HD3	1:B:247:ASN:O	2.19	0.42
1:B:303:GLY:O	1:B:306:VAL:HG12	2.19	0.42
1:B:255:MET:HE1	1:B:258:LEU:HD12	2.01	0.42
1:B:287:GLN:NE2	1:B:290[B]:ARG:HH12	2.18	0.42
1:B:255:MET:CE	1:B:258:LEU:HD12	2.50	0.42
1:A:117:MET:O	1:A:121:LEU:HG	2.21	0.41
1:A:116:LEU:CD2	1:A:117:MET:H	2.33	0.41
1:A:114:HIS:C	1:A:116:LEU:HD22	2.46	0.41
1:B:212:GLU:H	1:B:212:GLU:CD	2.28	0.41
1:B:110:PHE:O	2:B:34:ACT:OXT	2.38	0.41
1:B:425:THR:HG23	1:B:427:GLN:H	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:HIS:NE2	1:A:220[B]:GLU:OE2	2.54	0.41
1:A:329:ILE:HA	1:A:329:ILE:HD12	1.91	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	394/383 (103%)	384 (98%)	10 (2%)	0	100	100
1	B	378/383 (99%)	368 (97%)	10 (3%)	0	100	100
All	All	772/766 (101%)	752 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	344/329 (105%)	335 (97%)	9 (3%)	40	13
1	B	321/329 (98%)	309 (96%)	12 (4%)	30	6
All	All	665/658 (101%)	644 (97%)	21 (3%)	36	8

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LYS
1	A	92	ARG
1	A	116	LEU
1	A	185[A]	SER
1	A	185[B]	SER
1	A	252	LYS
1	A	296	ASP
1	A	363	LYS
1	A	424	THR
1	B	127	SER
1	B	139	ARG
1	B	143	LYS
1	B	185[A]	SER
1	B	185[B]	SER
1	B	211	GLN
1	B	246	LYS
1	B	255	MET
1	B	256[A]	GLU
1	B	296	ASP
1	B	363[A]	LYS
1	B	374	ASP

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

Mol	Chain	Res	Type
1	A	60	ASN
1	A	90	ASN
1	A	119	ASN
1	A	135	ASN
1	A	241	HIS
1	A	327	ASN
1	A	367	HIS
1	A	415	ASN
1	B	100	ASN
1	B	114	HIS
1	B	193	GLN
1	B	211	GLN
1	B	327	ASN
1	B	353	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

31 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	$\# Z > 2$
2	ACT	A	29	-	3,3,3	0.92	0	3,3,3	0.84	0
2	ACT	A	33	-	3,3,3	0.79	0	3,3,3	1.13	0
2	ACT	B	18	-	3,3,3	0.81	0	3,3,3	1.47	0
2	ACT	A	15	-	3,3,3	0.80	0	3,3,3	1.29	0
2	ACT	B	34	-	3,3,3	0.70	0	3,3,3	1.54	0
3	SO4	B	1	-	4,4,4	1.15	0	6,6,6	1.48	1 (16%)
2	ACT	A	12	-	3,3,3	0.76	0	3,3,3	1.85	1 (33%)
2	ACT	A	19	-	3,3,3	0.91	0	3,3,3	0.98	0
2	ACT	A	20	-	3,3,3	0.70	0	3,3,3	1.28	0
2	ACT	B	31	-	3,3,3	0.84	0	3,3,3	1.35	0
2	ACT	A	28	-	3,3,3	0.88	0	3,3,3	2.20	1 (33%)
2	ACT	A	30	-	3,3,3	0.85	0	3,3,3	1.34	0
2	ACT	B	21	-	3,3,3	0.84	0	3,3,3	0.97	0
3	SO4	B	2	-	4,4,4	0.93	0	6,6,6	1.22	1 (16%)
2	ACT	B	38	-	3,3,3	0.87	0	3,3,3	1.50	0
2	ACT	A	11	-	3,3,3	0.84	0	3,3,3	1.23	0
2	ACT	B	37	-	3,3,3	0.86	0	3,3,3	1.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	A	16	-	3,3,3	0.82	0	3,3,3	1.07	0
2	ACT	A	25	-	3,3,3	0.68	0	3,3,3	0.76	0
2	ACT	B	23	-	3,3,3	0.87	0	3,3,3	1.48	0
2	ACT	B	27	-	3,3,3	0.86	0	3,3,3	1.20	0
2	ACT	B	14	-	3,3,3	0.67	0	3,3,3	1.64	1 (33%)
2	ACT	A	24	-	3,3,3	0.74	0	3,3,3	1.26	0
2	ACT	A	35	-	3,3,3	0.75	0	3,3,3	1.62	1 (33%)
2	ACT	A	22	-	3,3,3	0.82	0	3,3,3	1.21	0
2	ACT	A	32	-	3,3,3	0.82	0	3,3,3	1.62	1 (33%)
2	ACT	B	17	-	3,3,3	1.04	0	3,3,3	1.68	2 (66%)
2	ACT	B	13	-	3,3,3	0.80	0	3,3,3	1.37	0
2	ACT	B	26	-	3,3,3	0.84	0	3,3,3	1.01	0
2	ACT	A	36	-	3,3,3	0.81	0	3,3,3	1.88	2 (66%)
2	ACT	A	39	-	3,3,3	0.88	0	3,3,3	0.65	0

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	SO4	O4-S-O3	3.27	126.56	108.54
2	A	28	ACT	OXT-C-CH3	3.03	127.77	115.05
3	B	2	SO4	O4-S-O3	2.60	122.85	108.54
2	A	12	ACT	OXT-C-CH3	2.46	125.35	115.05
2	A	32	ACT	OXT-C-O	-2.33	113.39	122.03
2	A	36	ACT	OXT-C-CH3	2.31	124.74	115.05
2	A	36	ACT	OXT-C-O	-2.29	113.52	122.03
2	A	35	ACT	OXT-C-CH3	2.26	124.51	115.05
2	B	14	ACT	OXT-C-O	-2.12	114.17	122.03
2	B	17	ACT	OXT-C-O	-2.06	114.39	122.03
2	B	17	ACT	OXT-C-CH3	2.05	123.66	115.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	33	ACT	2	0
2	A	15	ACT	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	34	ACT	1	0
3	B	1	SO4	1	0
2	A	19	ACT	1	0
2	A	28	ACT	1	0
2	A	11	ACT	2	0
2	A	16	ACT	4	0
2	B	23	ACT	3	0
2	B	14	ACT	1	0
2	A	24	ACT	2	0
2	B	13	ACT	1	0
2	A	36	ACT	2	0
2	A	39	ACT	1	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 [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	372/383 (97%)	-0.54	7 (1%) 66 70	9, 20, 44, 84	27 (7%)
1	B	374/383 (97%)	-0.33	11 (2%) 53 58	12, 25, 52, 80	11 (2%)
All	All	746/766 (97%)	-0.43	18 (2%) 59 63	9, 22, 50, 84	38 (5%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	91	ASP	5.8
1	B	115	TRP	4.9
1	B	88	GLN	4.6
1	B	54	THR	4.5
1	B	90	ASN	4.2
1	A	423	ASN	4.2
1	A	116	LEU	4.0
1	B	92	ARG	3.7
1	B	89	ASP	3.6
1	A	115	TRP	3.2
1	A	114	HIS	2.9
1	B	116	LEU	2.8
1	A	425	THR	2.5
1	B	93	LEU	2.4
1	B	142	GLU	2.2
1	B	141	GLY	2.2
1	A	424	THR	2.1
1	A	88	GLN	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
2	ACT	B	13	4/4	0.58	0.16	62,72,74,78	0
2	ACT	A	35	4/4	0.61	0.16	49,66,76,78	0
2	ACT	B	23	4/4	0.63	0.15	105,113,117,121	0
2	ACT	B	34	4/4	0.63	0.13	48,67,74,76	0
2	ACT	B	38	4/4	0.66	0.10	93,101,102,106	0
2	ACT	A	22	4/4	0.67	0.15	77,91,93,95	0
2	ACT	B	37	4/4	0.69	0.11	67,68,77,81	0
2	ACT	B	31	4/4	0.71	0.11	76,77,80,85	0
2	ACT	B	27	4/4	0.71	0.13	51,59,62,69	0
2	ACT	A	30	4/4	0.72	0.10	78,80,81,86	0
2	ACT	A	39	4/4	0.73	0.19	44,51,58,61	0
2	ACT	A	32	4/4	0.73	0.11	63,64,65,66	0
2	ACT	B	17	4/4	0.75	0.13	57,61,63,63	0
2	ACT	A	33	4/4	0.78	0.14	41,53,58,89	0
2	ACT	A	36	4/4	0.80	0.11	59,66,67,70	0
2	ACT	A	19	4/4	0.81	0.15	66,72,86,86	0
2	ACT	B	26	4/4	0.82	0.11	49,53,59,61	0
2	ACT	A	24	4/4	0.84	0.15	79,104,105,113	0
2	ACT	A	29	4/4	0.86	0.14	40,41,47,49	0
2	ACT	B	21	4/4	0.86	0.11	35,42,42,55	0
2	ACT	A	20	4/4	0.86	0.13	50,52,59,65	0
2	ACT	A	16	4/4	0.87	0.14	46,60,71,72	0
2	ACT	B	18	4/4	0.87	0.13	39,39,43,44	0
2	ACT	A	12	4/4	0.88	0.08	48,53,59,62	0
2	ACT	A	28	4/4	0.88	0.14	51,70,85,102	0
2	ACT	A	25	4/4	0.90	0.09	32,40,43,45	0
2	ACT	A	11	4/4	0.90	0.11	43,54,55,56	0
3	SO4	B	1	5/5	0.90	0.08	58,66,79,86	0
2	ACT	A	15	4/4	0.91	0.12	57,57,63,77	0
2	ACT	B	14	4/4	0.92	0.10	29,36,36,47	0
3	SO4	B	2	5/5	0.92	0.09	46,47,51,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.