



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 12:51 PM UTC

PDB ID : 1GPF / pdb_00001gpf
Title : CHITINASE B FROM SERRATIA MARCESCENS IN COMPLEX WITH
INHIBITOR PSAMMAPLIN
Authors : Komander, D.; Van Aalten, D.M.
Deposited on : 2001-11-03
Resolution : 1.85 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

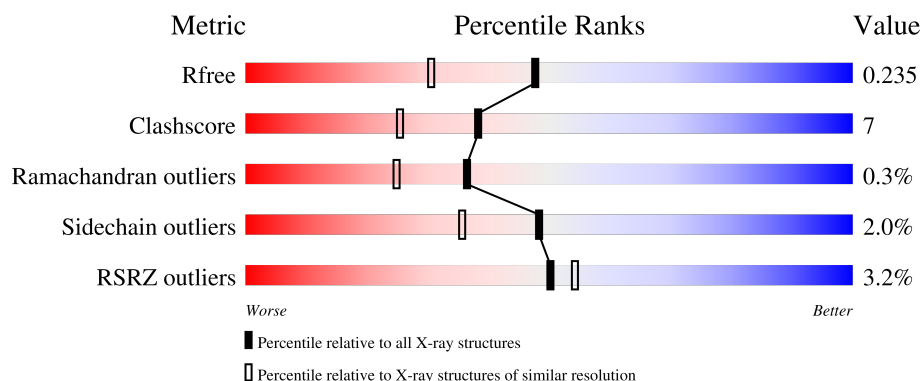
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	499	% 83% 16% .
1	B	499	5% 82% 15% .

2 Entry composition [i](#)

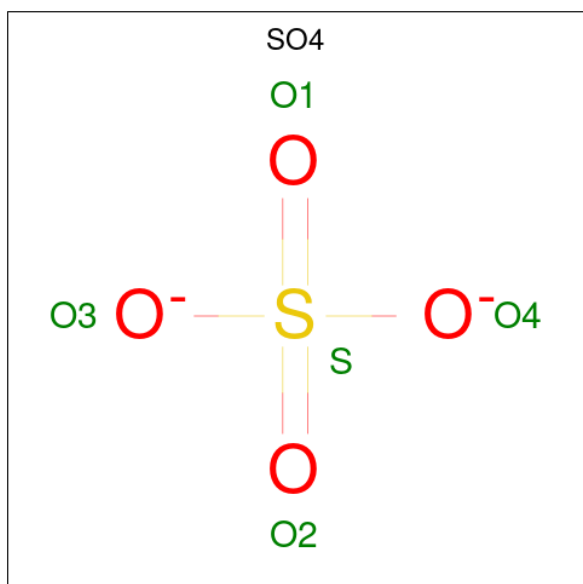
There are 3 unique types of molecules in this entry. The entry contains 8460 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CHITINASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	9	5	1
			3917	2504	657	742	14			
1	B	497	Total	C	N	O	S	10	3	0
			3914	2502	659	739	14			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	328	Total 328	O 328	0	0
3	B	286	Total 286	O 286	0	0

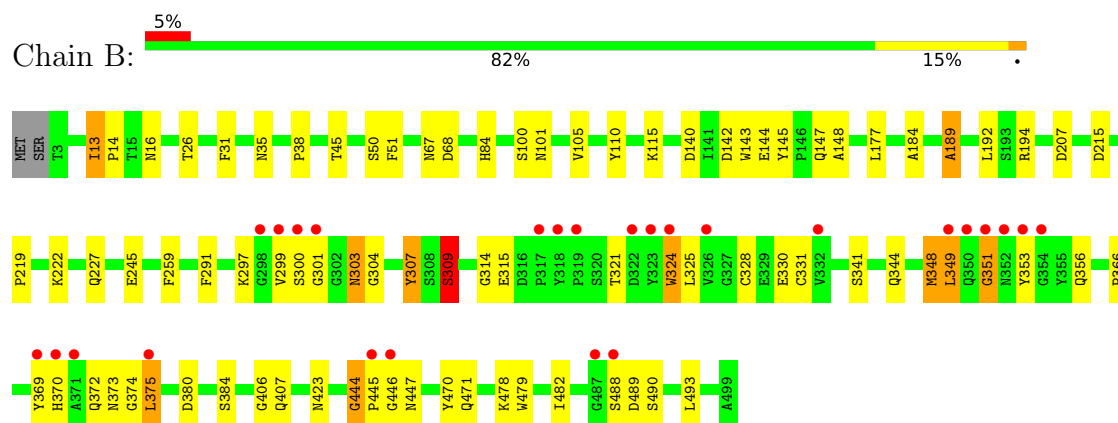
3 Residue-property plots

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: CHITINASE B



• Molecule 1: CHITINASE B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.75Å 103.59Å 186.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.71 – 1.85 29.71 – 1.85	Depositor EDS
% Data completeness (in resolution range)	89.3 (29.71-1.85) 89.4 (29.71-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 1.85Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.200 , 0.245 0.194 , 0.235	Depositor DCC
R_{free} test set	841 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.3	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	0.95	EDS
Total number of atoms	8460	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 3.92% 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: SO4

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	0.68	1/4048 (0.0%)	1.04	18/5520 (0.3%)
1	B	0.66	1/4037 (0.0%)	1.07	24/5501 (0.4%)
All	All	0.67	2/8085 (0.0%)	1.05	42/11021 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	348	MET	SD-CE	-6.72	1.62	1.79
1	A	498	VAL	C-N	-5.67	1.25	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	LYS	N-CA-C	9.66	121.41	111.07
1	A	189	ALA	N-CA-C	7.94	119.93	111.28
1	B	45	THR	N-CA-C	-7.85	104.23	113.88
1	A	100	SER	N-CA-C	7.43	122.52	113.38
1	B	321	THR	N-CA-C	-7.41	103.37	114.64
1	A	45	THR	N-CA-C	-7.39	104.78	113.88
1	B	100	SER	N-CA-C	7.12	122.98	113.72
1	A	309	SER	N-CA-C	-6.96	101.34	110.53
1	B	423	ASN	N-CA-C	6.93	123.25	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	SER	N-CA-C	-6.92	101.39	110.53
1	A	184	ALA	N-CA-C	-6.92	97.46	108.73
1	A	115	LYS	N-CA-C	6.87	118.77	111.28
1	A	485	ALA	N-CA-C	6.85	120.67	110.39
1	A	423	ASN	N-CA-C	6.83	123.12	114.31
1	A	21	TYR	N-CA-C	6.70	120.09	110.24
1	B	444	GLY	CA-C-N	-6.56	111.64	119.84
1	B	444	GLY	C-N-CA	-6.56	111.64	119.84
1	B	207	ASP	N-CA-C	-6.51	103.68	111.69
1	A	105	VAL	N-CA-C	6.15	118.74	111.05
1	A	207	ASP	N-CA-C	-6.07	104.22	111.69
1	A	441	THR	N-CA-C	5.97	119.88	112.59
1	A	324	TRP	N-CA-C	5.95	120.53	113.16
1	B	13	ILE	CA-C-N	5.91	125.87	119.78
1	B	13	ILE	C-N-CA	5.91	125.87	119.78
1	B	291	PHE	N-CA-C	-5.87	106.03	112.72
1	B	189	ALA	N-CA-C	5.86	118.45	111.71
1	B	300	SER	N-CA-C	5.77	123.08	110.80
1	A	405	LEU	N-CA-C	5.75	118.29	111.33
1	B	490	SER	N-CA-C	5.69	119.03	111.75
1	A	259	PHE	N-CA-C	5.67	118.92	108.94
1	A	96	GLY	N-CA-C	-5.56	106.06	112.29
1	B	259	PHE	N-CA-C	5.54	119.05	108.97
1	B	68	ASP	N-CA-C	5.52	117.29	111.28
1	B	184	ALA	N-CA-C	-5.46	100.39	109.46
1	A	107	HIS	N-CA-C	5.46	117.66	111.11
1	B	324	TRP	N-CA-C	5.40	119.74	113.20
1	B	177	LEU	CA-C-N	5.29	125.30	119.90
1	B	177	LEU	C-N-CA	5.29	125.30	119.90
1	A	480	GLY	N-CA-C	5.26	120.90	112.58
1	B	447	ASN	N-CA-C	-5.18	104.77	111.71
1	B	67	ASN	N-CA-C	-5.03	101.91	109.15
1	B	105	VAL	N-CA-C	5.01	117.32	111.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	110	TYR	Sidechain

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	3917	0	3732	53	0
1	B	3914	0	3739	55	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
3	A	328	0	0	2	0
3	B	286	0	0	4	0
All	All	8460	0	7471	105	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 (105) 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:344:GLN:HG3	1:B:348:MET:HE3	1.27	1.06
1:B:344:GLN:HG3	1:B:348:MET:CE	1.98	0.94
1:A:370:HIS:HD2	1:A:373:ASN:H	1.12	0.93
1:A:310:HIS:HD2	1:A:312:THR:H	1.20	0.89
1:A:175:GLN:H	1:A:175:GLN:HE21	1.21	0.86
1:A:444:GLY:H	1:A:447:ASN:HD21	1.22	0.84
1:A:112:ASN:HD22	1:A:115:LYS:HZ3	1.29	0.80
1:A:370:HIS:CD2	1:A:373:ASN:H	1.97	0.79
1:A:444:GLY:H	1:A:447:ASN:ND2	1.81	0.79
1:B:356:GLN:HG3	3:B:2214:HOH:O	1.84	0.78
1:B:328:CYS:HA	1:B:348:MET:HE2	1.66	0.77
1:A:112:ASN:HD22	1:A:115:LYS:NZ	1.82	0.76
1:B:309:SER:HB3	3:B:2199:HOH:O	1.87	0.75
1:B:330:GLU:H	1:B:344:GLN:HE21	1.34	0.73
1:A:112:ASN:ND2	1:A:115:LYS:NZ	2.38	0.72
1:A:310:HIS:CD2	1:A:312:THR:H	2.05	0.70
1:A:112:ASN:ND2	1:A:115:LYS:HZ3	1.90	0.69
1:A:94:ILE:HD12	1:A:141:ILE:CD1	2.23	0.68
1:B:328:CYS:CA	1:B:348:MET:HE2	2.24	0.67
1:A:175:GLN:H	1:A:175:GLN:NE2	1.93	0.65
1:A:372:GLN:HG2	1:A:373:ASN:OD1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:GLU:H	1:B:344:GLN:NE2	1.94	0.63
1:A:22:THR:HG22	1:A:24:THR:H	1.63	0.63
1:A:221:GLU:O	1:A:310:HIS:HE1	1.83	0.61
1:B:344:GLN:CG	1:B:348:MET:HE3	2.17	0.60
1:B:26:THR:HG22	3:B:2025:HOH:O	2.01	0.60
1:B:328:CYS:CB	1:B:348:MET:HE2	2.32	0.59
1:A:484:SER:HB3	1:A:489:ASP:HB2	1.83	0.59
1:B:444:GLY:O	1:B:446:GLY:N	2.35	0.59
1:A:22:THR:HG21	3:A:2017:HOH:O	2.04	0.56
1:B:328:CYS:HB2	1:B:348:MET:CE	2.36	0.56
1:A:498:VAL:HG12	1:A:499:ALA:N	2.21	0.55
1:B:144:GLU:HA	1:B:145:TYR:CG	2.43	0.54
1:A:353:TYR:O	1:A:370:HIS:HE1	1.92	0.53
1:B:307:TYR:N	1:B:307:TYR:CD1	2.77	0.53
1:A:73:ASP:O	1:A:77:ARG:HG3	2.09	0.52
1:B:31:PHE:CG	1:B:406:GLY:HA2	2.45	0.52
1:B:299:VAL:HG22	1:B:374:GLY:O	2.09	0.52
1:B:299:VAL:HG22	1:B:374:GLY:C	2.35	0.52
1:A:278:GLU:HG3	1:A:445:PRO:HB2	1.92	0.52
1:B:147:GLN:HB3	1:B:194:ARG:HD3	1.91	0.52
1:A:498:VAL:CG1	1:A:499:ALA:N	2.73	0.51
1:A:346:GLU:O	1:A:350:GLN:HG2	2.10	0.51
1:A:473:TYR:CD1	1:A:494:LYS:HD3	2.46	0.51
1:B:341:SER:HB2	1:B:407:GLN:HB3	1.94	0.50
1:A:241:ASN:HD22	1:A:241:ASN:C	2.19	0.50
1:B:470:TYR:CD2	1:B:471:GLN:HG3	2.46	0.50
1:B:479:TRP:CD1	1:B:482:ILE:HD11	2.47	0.50
1:A:488:SER:O	1:B:148:ALA:HB2	2.11	0.49
1:B:38:PRO:HG3	1:B:84:HIS:CE1	2.49	0.48
1:B:344:GLN:CG	1:B:348:MET:CE	2.82	0.48
1:B:351:GLY:HA3	1:B:353:TYR:CE2	2.49	0.48
1:B:328:CYS:HB2	1:B:348:MET:HE2	1.95	0.47
1:A:356:GLN:HG3	3:A:2245:HOH:O	2.15	0.47
1:B:370:HIS:CE1	1:B:373:ASN:H	2.31	0.47
1:A:144:GLU:HA	1:A:145:TYR:CG	2.49	0.47
1:A:294:ARG:HG2	1:A:339:ILE:CD1	2.45	0.47
1:A:140:ASP:OD2	1:A:142[B]:ASP:OD1	2.32	0.47
1:B:219:PRO:HB2	1:B:314:GLY:HA2	1.96	0.46
1:B:140:ASP:OD2	1:B:142[A]:ASP:OD1	2.33	0.46
1:B:215:ASP:H	1:B:227:GLN:HE21	1.64	0.46
1:B:14:PRO:HB2	1:B:16[B]:ASN:ND2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:LEU:HD23	1:B:349:LEU:HA	1.69	0.46
1:B:315:GLU:H	1:B:315:GLU:CD	2.24	0.46
1:A:456:TYR:CE2	1:A:485:ALA:HB2	2.51	0.46
1:B:50:SER:HA	1:B:51:PHE:HA	1.78	0.45
1:B:328:CYS:CB	1:B:348:MET:CE	2.93	0.45
1:A:28:VAL:HG13	1:A:29:VAL:N	2.31	0.45
1:A:50:SER:HB2	1:A:51:PHE:CG	2.52	0.45
1:A:13:ILE:HA	1:A:14:PRO:HD3	1.86	0.44
1:A:294:ARG:HG2	1:A:339:ILE:HD13	1.97	0.44
1:A:333:ARG:NH1	1:A:334:ASP:OD2	2.51	0.44
1:B:325:LEU:HD23	1:B:331:CYS:SG	2.57	0.44
1:B:101:ASN:HA	1:B:144:GLU:O	2.17	0.44
1:B:215:ASP:H	1:B:227:GLN:NE2	2.14	0.44
1:B:50:SER:HB2	1:B:51:PHE:CG	2.53	0.44
1:B:304:GLY:HA2	1:B:369:TYR:CD2	2.52	0.44
1:A:447:ASN:H	1:A:447:ASN:HD22	1.66	0.43
1:B:366:PRO:HD3	1:B:384:SER:HB3	2.00	0.43
1:A:101:ASN:HA	1:A:144:GLU:O	2.18	0.43
1:A:467:LEU:HD23	1:A:476:GLN:HB2	2.00	0.43
1:A:245:GLU:OE1	1:B:478:LYS:NZ	2.42	0.43
1:A:478:LYS:NZ	1:B:245:GLU:OE1	2.43	0.43
1:A:444:GLY:N	1:A:447:ASN:HD21	2.02	0.42
1:B:13:ILE:HA	1:B:14:PRO:HD3	1.84	0.42
1:B:370:HIS:HB3	1:B:375:LEU:HB2	2.01	0.42
1:A:121:ALA:O	1:A:125[A]:GLN:HG3	2.19	0.42
1:B:189:ALA:HA	1:B:192:LEU:HB3	2.01	0.42
1:B:444:GLY:O	1:B:445:PRO:C	2.61	0.42
1:A:50:SER:HA	1:A:51:PHE:HA	1.81	0.42
1:B:143:TRP:O	1:B:145:TYR:HA	2.20	0.42
1:B:35:ASN:ND2	3:B:2028:HOH:O	2.52	0.41
1:B:303:ASN:HD22	1:B:303:ASN:HA	1.61	0.41
1:A:8:ILE:HG12	1:A:46:HIS:HB2	2.02	0.41
1:A:140:ASP:HA	1:A:182:THR:O	2.20	0.41
1:A:353:TYR:O	1:A:370:HIS:CE1	2.72	0.41
1:A:294:ARG:NH1	1:A:339:ILE:HD11	2.35	0.41
1:A:479:TRP:CD1	1:A:482:ILE:HD11	2.56	0.41
1:A:349:LEU:HD23	1:A:349:LEU:HA	1.93	0.41
1:B:297:LYS:HD3	1:B:324:TRP:CE2	2.55	0.41
1:B:478:LYS:HE2	1:B:493:LEU:HB2	2.03	0.40
1:A:31:PHE:CG	1:A:406:GLY:HA2	2.56	0.40
1:B:13:ILE:HG23	1:B:13:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:SER:O	1:B:489:ASP:C	2.63	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	500/499 (100%)	491 (98%)	9 (2%)	0	100	100
1	B	498/499 (100%)	477 (96%)	18 (4%)	3 (1%)	21	10
All	All	998/998 (100%)	968 (97%)	27 (3%)	3 (0%)	36	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	301	GLY
1	B	372	GLN
1	B	351	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	407/405 (100%)	398 (98%)	9 (2%)	45	32
1	B	405/405 (100%)	398 (98%)	7 (2%)	53	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	812/810 (100%)	796 (98%)	16 (2%)	48 36

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	213	THR
1	A	303	ASN
1	A	325	LEU
1	A	358	LEU
1	A	378	THR
1	A	380	ASP
1	A	447	ASN
1	A	498	VAL
1	B	222	LYS
1	B	303	ASN
1	B	307	TYR
1	B	309	SER
1	B	349	LEU
1	B	375	LEU
1	B	380	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	109	ASN
1	A	112	ASN
1	A	167	GLN
1	A	175	GLN
1	A	201	GLN
1	A	241	ASN
1	A	310	HIS
1	A	347	GLN
1	A	370	HIS
1	A	447	ASN
1	A	464	GLN
1	A	471	GLN
1	B	17	GLN
1	B	35	ASN
1	B	57	ASN

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Mol	Chain	Res	Type
1	B	84	HIS
1	B	112	ASN
1	B	147	GLN
1	B	167	GLN
1	B	180	GLN
1	B	227	GLN
1	B	273	GLN
1	B	303	ASN
1	B	344	GLN
1	B	347	GLN
1	B	356	GLN
1	B	394	GLN
1	B	431	GLN
1	B	464	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	SO4	A	1499	-	4,4,4	0.37	0	6,6,6	0.15	0
2	SO4	B	1501	-	4,4,4	0.38	0	6,6,6	0.09	0
2	SO4	B	1500	-	4,4,4	0.40	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	497/499 (99%)	-0.09	6 (1%) 76 80	11, 25, 40, 55	7 (1%)
1	B	497/499 (99%)	0.09	26 (5%) 33 35	12, 26, 50, 61	6 (1%)
All	All	994/998 (99%)	-0.00	32 (3%) 50 54	11, 26, 45, 61	13 (1%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	498	VAL	4.8
1	A	499	ALA	4.6
1	B	351	GLY	3.9
1	B	352	ASN	3.5
1	B	445	PRO	3.3
1	B	354	GLY	3.2
1	B	446	GLY	3.1
1	B	350	GLN	3.0
1	B	332	VAL	3.0
1	B	324	TRP	3.0
1	B	371	ALA	3.0
1	B	369	TYR	2.9
1	B	317	PRO	2.8
1	B	322	ASP	2.7
1	B	319	PRO	2.7
1	B	300	SER	2.7
1	A	28	VAL	2.6
1	B	326	VAL	2.6
1	B	487	GLY	2.5
1	B	488	SER	2.5
1	B	353	TYR	2.4
1	A	26	THR	2.4
1	B	299	VAL	2.3
1	B	349	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	375	LEU	2.3
1	B	323	TYR	2.3
1	B	298	GLY	2.3
1	B	318	TYR	2.2
1	B	301	GLY	2.2
1	B	370	HIS	2.1
1	A	22	THR	2.1
1	A	319	PRO	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
2	SO4	B	1500	5/5	0.86	0.09	73,74,74,75	0
2	SO4	B	1501	5/5	0.88	0.10	71,71,72,72	0
2	SO4	A	1499	5/5	0.93	0.08	54,54,55,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.