Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 08:02 AM EDT

PDB ID	:	3D3X
Title	:	Crystal structure of botulinum neurotoxin serotype E catalytic domain in complex with SNAP-25 substrate peptide
Authors	:	Agarwal, R.; Swaminathan, S.
Deposited on	:	2008-05-13
Resolution	:	2.25 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:

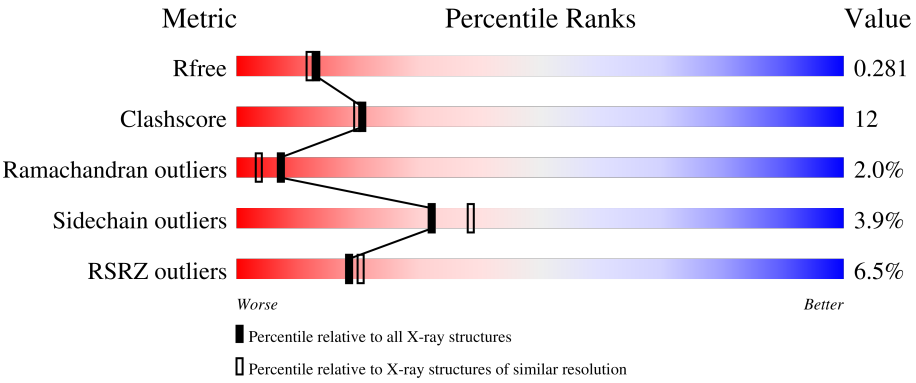
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	427	5% 70% 23% • 5%
1	B	427	7% 69% 22% • 5%
2	C	5	20% 20% 40% 40%
2	D	5	40% 60%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6883 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 Type E botulinum toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3263	2086	545	624	8			
1	B	407	Total	C	N	O	S	0	0	0
			3265	2085	548	625	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	HIS	-	expression tag	UNP Q9K395
A	423	HIS	-	expression tag	UNP Q9K395
A	424	HIS	-	expression tag	UNP Q9K395
A	425	HIS	-	expression tag	UNP Q9K395
A	426	HIS	-	expression tag	UNP Q9K395
A	427	HIS	-	expression tag	UNP Q9K395
B	422	HIS	-	expression tag	UNP Q9K395
B	423	HIS	-	expression tag	UNP Q9K395
B	424	HIS	-	expression tag	UNP Q9K395
B	425	HIS	-	expression tag	UNP Q9K395
B	426	HIS	-	expression tag	UNP Q9K395
B	427	HIS	-	expression tag	UNP Q9K395

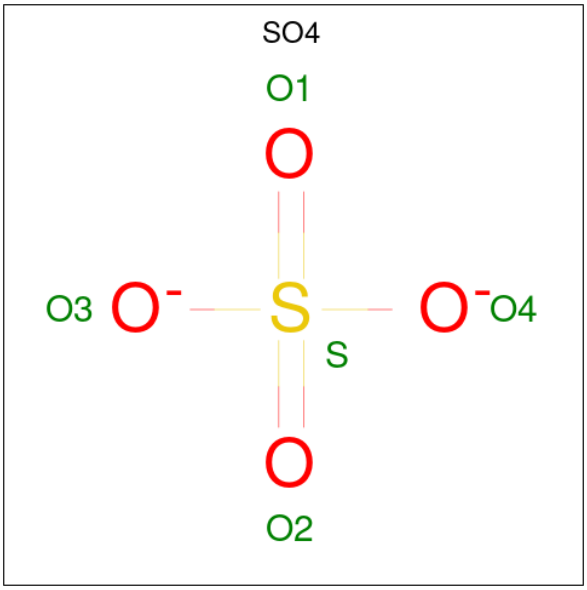
- Molecule 2 is a protein called SNAP-25 substrate peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	S	0	0	0
			21	14	3	3	1			
2	D	5	Total	C	N	O	S	0	1	1
			41	24	8	8	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

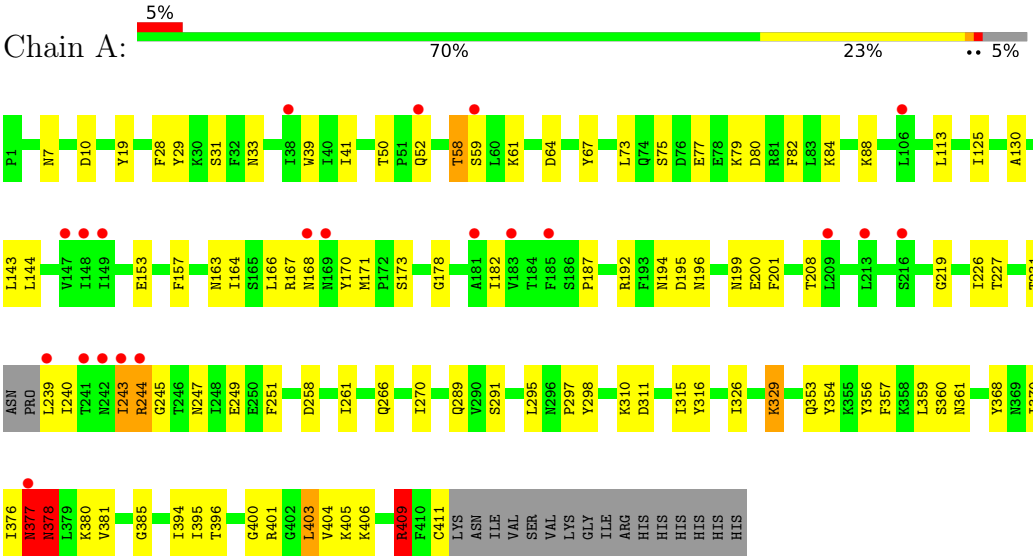
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	148	Total O 148 148	0	0
5	B	102	Total O 102 102	0	0
5	D	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

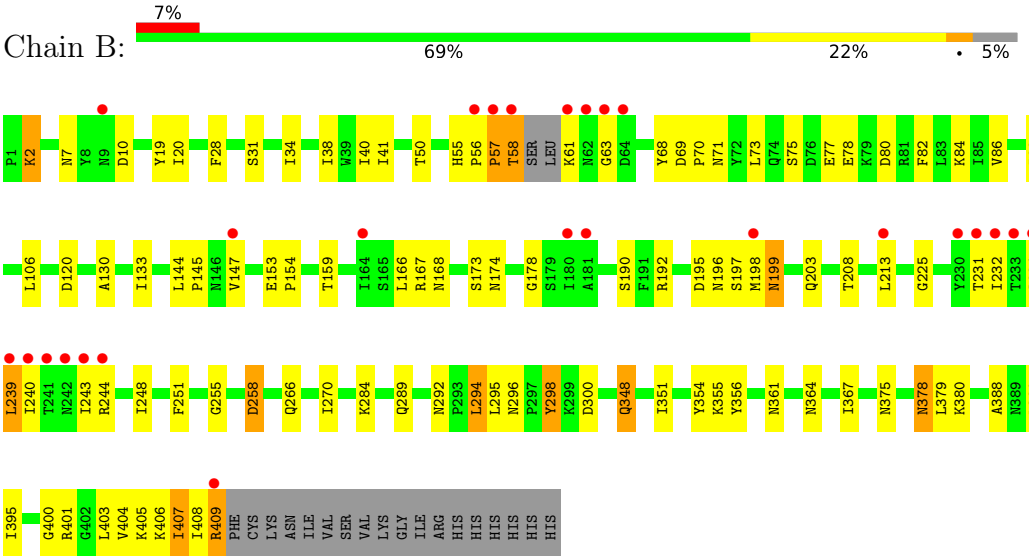
• Molecule 1: Type E botulinum toxin

Chain A:



• Molecule 1: Type E botulinum toxin

Chain B:



• Molecule 2: SNAP-25 substrate peptide

Chain C:

• Molecule 2: SNAP-25 substrate peptide

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	89.41Å 144.74Å 83.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.48 – 2.25 33.47 – 2.25	Depositor EDS
% Data completeness (in resolution range)	91.6 (33.48-2.25) 91.7 (33.47-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.66 (at 2.24Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.288 0.231 , 0.281	Depositor DCC
R_{free} test set	1426 reflections (2.90%)	wwPDB-VP
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.741	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.1	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	0.93	EDS
Total number of atoms	6883	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: SO4, NH2, ZN

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	0.44	0/3335	0.70	2/4516 (0.0%)
1	B	0.45	0/3337	0.66	0/4519
2	C	0.60	0/20	0.73	0/25
2	D	0.54	0/43	0.61	0/53
All	All	0.45	0/6735	0.68	2/9113 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	409	ARG	N-CA-C	5.93	127.01	111.00
1	A	378	ASN	N-CA-C	-5.50	96.15	111.00

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	3263	0	3216	83	0
1	B	3265	0	3220	81	0
2	C	21	0	21	3	0
2	D	41	0	40	2	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	30	0	0	1	0
4	B	10	0	0	0	0
5	A	148	0	0	5	0
5	B	102	0	0	4	0
5	D	1	0	0	0	0
All	All	6883	0	6497	162	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 12.

All (162) 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:237:ASN:H	1:B:238:PRO:HD2	1.31	0.95
1:A:409:ARG:HH11	1:A:409:ARG:HG2	1.36	0.90
1:B:2:LYS:HD3	1:B:2:LYS:H	1.37	0.90
1:B:56:PRO:HG3	1:B:68:TYR:HB2	1.57	0.85
1:A:58:THR:HG23	1:A:59:SER:H	1.44	0.82
1:B:153:GLU:HB2	1:B:154:PRO:HD2	1.63	0.79
1:A:409:ARG:HG2	1:A:409:ARG:NH1	1.97	0.75
1:B:237:ASN:N	1:B:238:PRO:HD2	2.02	0.73
1:A:404:VAL:HG23	1:A:405:LYS:H	1.51	0.73
1:B:130:ALA:HB2	1:B:144:LEU:HD23	1.70	0.73
1:B:408:ILE:C	1:B:409:ARG:HD2	2.09	0.73
1:A:377:ASN:HB2	1:A:380:LYS:HD3	1.74	0.70
1:A:58:THR:HG23	1:A:59:SER:N	2.07	0.68
1:B:409:ARG:CA	1:B:409:ARG:HH11	2.07	0.68
1:B:409:ARG:HH11	1:B:409:ARG:N	1.92	0.67
1:A:226:ILE:HB	1:A:270:ILE:HD13	1.78	0.66
1:B:243:ILE:O	1:B:244:ARG:HG2	1.96	0.65
1:B:58:THR:OG1	1:B:61:LYS:HB2	1.99	0.63
1:A:258:ASP:HA	1:A:261:ILE:HD12	1.80	0.61
1:A:7:ASN:HB2	1:A:10:ASP:OD1	2.01	0.60
1:A:409:ARG:HH11	1:A:409:ARG:CG	2.10	0.60
1:B:31:SER:OG	1:B:41:ILE:HG12	2.02	0.60
1:B:106:LEU:HD11	1:B:213:LEU:HB3	1.84	0.60
1:A:231:THR:HG22	1:A:247:ASN:HD22	1.65	0.60
1:A:295:LEU:HD22	5:A:981:HOH:O	2.03	0.59
1:B:295:LEU:H	1:B:295:LEU:HD23	1.67	0.59
1:B:248:ILE:HA	1:B:251:PHE:HD1	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ALA:HB2	1:A:144:LEU:HD23	1.85	0.58
1:B:2:LYS:H	1:B:2:LYS:CD	2.14	0.58
1:A:243:ILE:O	1:A:245:GLY:N	2.37	0.58
1:A:406:LYS:HB2	1:A:406:LYS:NZ	2.19	0.57
1:B:231:THR:O	1:B:232:ILE:HD13	2.05	0.56
1:B:237:ASN:C	1:B:237:ASN:HD22	2.08	0.56
1:B:239:LEU:HD13	1:B:239:LEU:N	2.21	0.56
1:B:356:TYR:HE1	2:D:182:MET:HE1	1.71	0.56
1:B:409:ARG:N	1:B:409:ARG:NH1	2.54	0.56
1:B:55:HIS:ND1	1:B:70:PRO:HG2	2.20	0.56
1:A:404:VAL:HG23	1:A:405:LYS:N	2.20	0.56
1:B:197:SER:O	1:B:198:MET:HG2	2.05	0.55
1:A:50:THR:HG22	1:A:52:GLN:H	1.72	0.55
1:A:73:LEU:HD21	1:A:82:PHE:HB2	1.89	0.55
1:A:163:ASN:ND2	1:A:219:GLY:HA3	2.22	0.54
1:B:7:ASN:HB2	1:B:10:ASP:OD1	2.07	0.54
1:B:401:ARG:O	1:B:405:LYS:HG3	2.08	0.54
1:B:400:GLY:O	1:B:404:VAL:HG23	2.09	0.53
1:A:182:ILE:HD12	1:A:182:ILE:N	2.24	0.52
1:B:409:ARG:NH1	1:B:409:ARG:H	2.07	0.52
1:A:244:ARG:O	1:A:244:ARG:HG2	2.08	0.52
1:A:311:ASP:OD2	1:A:315:ILE:HB	2.09	0.52
1:B:19:TYR:HB3	1:B:28:PHE:HB3	1.91	0.52
1:B:364:ASN:ND2	1:B:367:ILE:HG13	2.25	0.51
1:A:394:ILE:HG13	1:A:395:ILE:HG12	1.92	0.51
1:B:375:ASN:HB3	1:B:380:LYS:HA	1.91	0.51
1:A:231:THR:HG22	1:A:247:ASN:ND2	2.26	0.51
1:A:163:ASN:HD21	1:A:219:GLY:HA3	1.76	0.51
1:B:239:LEU:N	1:B:239:LEU:CD1	2.74	0.51
1:A:153:GLU:HG3	5:A:907:HOH:O	2.12	0.50
1:A:251:PHE:CE2	1:A:261:ILE:HD13	2.46	0.50
1:B:409:ARG:HH11	1:B:409:ARG:HA	1.74	0.50
1:B:61:LYS:N	1:B:61:LYS:HD3	2.27	0.50
1:A:33:ASN:HB2	1:A:39:TRP:CH2	2.46	0.50
1:A:171:MET:HE1	5:A:921:HOH:O	2.12	0.50
1:A:196:ASN:HB2	4:A:897:SO4:O2	2.12	0.50
1:B:2:LYS:HD3	1:B:2:LYS:N	2.16	0.50
1:B:173:SER:HA	1:B:178:GLY:HA2	1.94	0.50
1:B:120:ASP:OD1	1:B:284:LYS:HE2	2.12	0.49
1:B:34:ILE:HD12	1:B:40:ILE:HD11	1.95	0.49
1:B:292:ASN:O	1:B:295:LEU:HD23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:LYS:HB3	1:B:405:LYS:NZ	2.28	0.49
1:A:208:THR:HG23	2:C:181:ILE:HG12	1.94	0.49
1:B:407:ILE:HG22	1:B:407:ILE:O	2.14	0.48
1:B:409:ARG:HD2	1:B:409:ARG:N	2.28	0.48
1:A:58:THR:CG2	1:A:59:SER:H	2.22	0.48
1:A:289:GLN:HG3	1:A:291:SER:H	1.79	0.48
1:A:297:PRO:HG2	1:B:298:TYR:CD2	2.49	0.48
1:B:394:ILE:HG13	1:B:395:ILE:HG13	1.95	0.48
1:A:125:ILE:HD11	1:B:294:LEU:HD13	1.96	0.48
1:A:227:THR:HB	1:A:249:GLU:HB2	1.96	0.48
1:B:167:ARG:O	1:B:168:ASN:HB2	2.14	0.48
1:A:19:TYR:HB3	1:A:28:PHE:HB3	1.96	0.48
1:A:194:ASN:ND2	1:A:200:GLU:HG2	2.29	0.47
1:A:378:ASN:H	1:A:380:LYS:HG2	1.79	0.47
1:A:409:ARG:HA	1:A:409:ARG:HD3	1.41	0.47
1:A:234:GLN:O	1:A:239:LEU:HD23	2.14	0.47
1:A:357:PHE:HB3	1:A:395:ILE:HD12	1.95	0.47
1:A:240:ILE:HG22	1:A:240:ILE:O	2.15	0.47
1:A:251:PHE:HE2	1:A:261:ILE:HD13	1.79	0.47
1:B:238:PRO:O	1:B:239:LEU:HB2	2.15	0.47
1:A:80:ASP:O	1:A:84:LYS:HG2	2.15	0.47
1:A:266:GLN:O	1:A:270:ILE:HG12	2.15	0.47
1:A:360:SER:OG	1:A:396:THR:HG23	2.14	0.47
1:B:82:PHE:O	1:B:86:VAL:HG23	2.15	0.47
1:B:400:GLY:HA2	1:B:403:LEU:HB3	1.97	0.47
1:A:167:ARG:O	1:A:168:ASN:HB2	2.14	0.46
1:A:88:LYS:HG3	1:A:370:ILE:HD11	1.98	0.46
1:A:375:ASN:HD22	1:A:385:GLY:HA3	1.80	0.46
1:A:378:ASN:O	1:A:381:VAL:HG22	2.15	0.46
1:B:255:GLY:O	1:B:258:ASP:HB2	2.16	0.46
1:B:238:PRO:O	1:B:240:ILE:HG13	2.16	0.46
1:A:377:ASN:CB	1:A:380:LYS:HD3	2.45	0.46
1:B:403:LEU:O	1:B:407:ILE:HG13	2.16	0.46
1:A:368:TYR:HA	1:A:373:GLY:O	2.16	0.45
1:B:406:LYS:C	1:B:408:ILE:H	2.19	0.45
1:A:166:LEU:HD12	1:A:170:TYR:HD2	1.82	0.45
1:A:33:ASN:HB2	1:A:39:TRP:CZ2	2.52	0.45
1:B:238:PRO:C	1:B:239:LEU:HD13	2.36	0.45
1:A:173:SER:HA	1:A:178:GLY:HA2	1.99	0.45
1:A:192:ARG:HA	1:A:201:PHE:O	2.17	0.45
1:B:174:ASN:HB3	1:B:225:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ILE:CD1	1:B:147:VAL:HB	2.47	0.44
1:B:355:LYS:HA	5:B:938:HOH:O	2.17	0.44
1:A:326:ILE:HA	1:A:329:LYS:HE3	1.99	0.44
1:B:89:ILE:O	1:B:93:ILE:HG13	2.17	0.44
1:A:400:GLY:O	1:A:403:LEU:HB2	2.17	0.44
1:A:67:TYR:HB2	1:A:157:PHE:CZ	2.53	0.44
1:A:133:ILE:HG21	1:A:143:LEU:HB2	1.99	0.44
1:A:356:TYR:HE1	2:C:182:MET:SD	2.41	0.44
1:B:190:SER:OG	1:B:203:GLN:HB3	2.18	0.44
1:A:61:LYS:HB3	1:A:64:ASP:OD1	2.17	0.44
1:B:388:ALA:HB1	1:B:395:ILE:HD11	1.99	0.44
1:A:130:ALA:HB2	1:A:144:LEU:CD2	2.47	0.44
1:B:75:SER:OG	1:B:78:GLU:HG3	2.17	0.43
1:B:192:ARG:O	1:B:354:TYR:HB3	2.18	0.43
1:B:73:LEU:HD21	1:B:82:PHE:HB2	1.99	0.43
1:A:19:TYR:HA	1:A:29:TYR:O	2.18	0.43
1:B:153:GLU:HB2	1:B:154:PRO:CD	2.43	0.43
1:B:56:PRO:HA	1:B:57:PRO:HD3	1.76	0.43
1:B:348:GLN:O	1:B:348:GLN:HG3	2.16	0.43
1:B:378:ASN:ND2	5:B:920:HOH:O	2.51	0.43
1:A:381:VAL:O	1:A:381:VAL:HG23	2.19	0.43
1:B:80:ASP:OD1	1:B:84:LYS:HE3	2.19	0.43
1:B:390:LEU:O	1:B:390:LEU:HD23	2.19	0.43
1:A:226:ILE:CB	1:A:270:ILE:HD13	2.47	0.42
1:A:113:LEU:HD22	1:A:125:ILE:HG12	2.00	0.42
1:A:310:LYS:HD3	1:A:316:TYR:CE1	2.54	0.42
1:B:289:GLN:HA	5:B:941:HOH:O	2.19	0.42
1:B:266:GLN:O	1:B:270:ILE:HG12	2.19	0.42
1:B:69:ASP:OD1	1:B:71:ASN:HB2	2.19	0.42
1:B:409:ARG:HH11	1:B:409:ARG:CG	2.32	0.42
1:A:77:GLU:O	1:A:77:GLU:OE1	2.37	0.42
1:A:164:ILE:HD11	1:A:182:ILE:HD11	2.02	0.42
1:B:159:THR:HG21	1:B:208:THR:HG22	2.00	0.42
1:A:375:ASN:HD22	1:A:385:GLY:CA	2.33	0.42
1:B:166:LEU:HB3	5:B:927:HOH:O	2.18	0.42
1:A:133:ILE:HD11	1:A:141:ASP:HB3	2.01	0.41
1:B:234:GLN:C	1:B:236:GLN:H	2.24	0.41
1:B:409:ARG:NH1	1:B:409:ARG:HG3	2.35	0.41
1:A:31:SER:OG	1:A:41:ILE:HG12	2.20	0.41
1:A:195:ASP:OD1	1:A:199:ASN:HB2	2.21	0.41
1:B:20:ILE:HG12	1:B:133:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:THR:HG23	2:D:181:ILE:HG12	2.03	0.41
1:B:393:ARG:HH11	1:B:393:ARG:HG3	1.85	0.41
1:A:75:SER:O	1:A:79:LYS:HG3	2.20	0.41
1:A:187:PRO:O	1:A:359:LEU:HD12	2.21	0.41
1:A:354:TYR:HD2	2:C:182:MET:HG3	1.86	0.41
1:A:61:LYS:HE2	5:A:929:HOH:O	2.21	0.41
1:B:199:ASN:HD22	1:B:199:ASN:HA	1.56	0.41
1:A:227:THR:HG23	5:A:958:HOH:O	2.21	0.41
1:A:405:LYS:HB3	1:A:405:LYS:HE2	1.89	0.40
1:A:226:ILE:HB	1:A:270:ILE:CD1	2.50	0.40
1:A:409:ARG:NH1	1:A:409:ARG:CG	2.71	0.40
1:B:379:LEU:CD1	1:B:391:ASN:HD21	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	403/427 (94%)	374 (93%)	22 (6%)	7 (2%)	9 4
1	B	403/427 (94%)	363 (90%)	31 (8%)	9 (2%)	6 3
2	C	1/5 (20%)	1 (100%)	0	0	100 100
2	D	4/5 (80%)	4 (100%)	0	0	100 100
All	All	811/864 (94%)	742 (92%)	53 (6%)	16 (2%)	7 4

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	243	ILE
1	A	244	ARG

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Mol	Chain	Res	Type
1	A	378	ASN
1	B	57	PRO
1	A	361	ASN
1	A	376	ILE
1	B	237	ASN
1	A	377	ASN
1	B	63	GLY
1	B	195	ASP
1	B	235	LYS
1	B	361	ASN
1	B	407	ILE
1	B	196	ASN
1	B	238	PRO

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	367/387 (95%)	357 (97%)	10 (3%)	44 54
1	B	367/387 (95%)	349 (95%)	18 (5%)	25 27
2	C	2/4 (50%)	2 (100%)	0	100 100
2	D	5/4 (125%)	3 (60%)	2 (40%)	0 0
All	All	741/782 (95%)	711 (96%)	30 (4%)	32 37

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	ASP
1	A	298	TYR
1	A	329	LYS
1	A	353	GLN
1	A	377	ASN
1	A	378	ASN
1	A	401	ARG
1	A	403	LEU

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Mol	Chain	Res	Type
1	A	409	ARG
1	A	411	CYS
1	B	2	LYS
1	B	50	THR
1	B	58	THR
1	B	77	GLU
1	B	145	PRO
1	B	199	ASN
1	B	237	ASN
1	B	239	LEU
1	B	258	ASP
1	B	294	LEU
1	B	296	ASN
1	B	298	TYR
1	B	300	ASP
1	B	348	GLN
1	B	351	ILE
1	B	378	ASN
1	B	393	ARG
1	B	409	ARG
2	D	183[A]	GLU
2	D	183[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	163	ASN
1	A	174	ASN
1	A	194	ASN
1	A	196	ASN
1	A	247	ASN
1	A	266	GLN
1	A	296	ASN
1	A	353	GLN
1	A	375	ASN
1	B	9	ASN
1	B	33	ASN
1	B	95	ASN
1	B	124	HIS
1	B	163	ASN
1	B	168	ASN

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Mol	Chain	Res	Type
1	B	174	ASN
1	B	199	ASN
1	B	237	ASN
1	B	266	GLN
1	B	268	ASN
1	B	296	ASN
1	B	321	ASN
1	B	353	GLN
1	B	375	ASN
1	B	377	ASN
1	B	389	ASN
1	B	391	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	$\#\|Z\| > 2$
4	SO4	A	891	-	4,4,4	0.35	0	6,6,6	0.16	0
4	SO4	A	894	-	4,4,4	0.36	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	A	896	-	4,4,4	0.42	0	6,6,6	0.12	0
4	SO4	A	892	-	4,4,4	0.48	0	6,6,6	0.13	0
4	SO4	B	895	-	4,4,4	0.40	0	6,6,6	0.15	0
4	SO4	A	897	-	4,4,4	0.35	0	6,6,6	0.08	0
4	SO4	B	890	-	4,4,4	0.37	0	6,6,6	0.18	0
4	SO4	A	893	-	4,4,4	0.35	0	6,6,6	0.12	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	897	SO4	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

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	407/427 (95%)	0.15	21 (5%) 27 30	21, 35, 46, 58	0
1	B	407/427 (95%)	0.38	31 (7%) 13 15	26, 39, 51, 56	0
2	C	3/5 (60%)	1.45	1 (33%) 0 0	46, 46, 49, 54	0
2	D	4/5 (80%)	0.62	0 100 100	43, 43, 46, 49	0
All	All	821/864 (95%)	0.27	53 (6%) 18 20	21, 37, 49, 58	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	THR	5.6
1	B	237	ASN	5.6
1	B	61	LYS	5.1
1	B	239	LEU	5.0
1	B	233	THR	4.9
1	B	57	PRO	4.6
1	B	235	LYS	4.4
1	B	238	PRO	4.3
1	A	244	ARG	3.8
1	B	244	ARG	3.6
1	B	64	ASP	3.4
1	B	242	ASN	3.3
1	B	241	THR	3.3
1	A	213	LEU	3.1
1	B	63	GLY	3.1
1	A	169	ASN	3.1
2	C	181	ILE	3.1
1	A	149	ILE	3.0
1	B	56	PRO	3.0
1	B	230	TYR	2.9
1	A	377	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	147	VAL	2.8
1	B	147	VAL	2.7
1	B	97	LEU	2.7
1	B	243	ILE	2.7
1	A	59	SER	2.7
1	B	181	ALA	2.7
1	A	242	ASN	2.6
1	A	168	ASN	2.6
1	B	62	ASN	2.6
1	A	243	ILE	2.5
1	B	234	GLN	2.5
1	A	183	VAL	2.5
1	B	232	ILE	2.5
1	B	231	THR	2.4
1	A	38	ILE	2.4
1	B	236	GLN	2.3
1	A	209	LEU	2.3
1	A	216	SER	2.3
1	A	185	PHE	2.3
1	B	9	ASN	2.3
1	A	52	GLN	2.3
1	B	213	LEU	2.2
1	A	148	ILE	2.2
1	B	240	ILE	2.2
1	B	164	ILE	2.2
1	A	241	THR	2.2
1	B	180	ILE	2.1
1	A	181	ALA	2.1
1	A	239	LEU	2.0
1	A	106	LEU	2.0
1	B	409	ARG	2.0
1	B	198	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	SO4	B	895	5/5	0.85	0.27	60,61,61,62	5
4	SO4	A	892	5/5	0.87	0.16	51,51,52,53	5
4	SO4	A	894	5/5	0.93	0.17	50,52,52,53	5
4	SO4	A	896	5/5	0.94	0.15	54,54,55,55	5
4	SO4	B	890	5/5	0.94	0.11	46,46,48,49	4
4	SO4	A	891	5/5	0.94	0.13	40,44,44,45	5
4	SO4	A	897	5/5	0.95	0.17	50,50,51,51	5
4	SO4	A	893	5/5	0.96	0.17	52,53,53,54	5
3	ZN	A	428	1/1	0.98	0.09	50,50,50,50	0
3	ZN	B	822	1/1	0.99	0.04	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.