Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 04:45 PM EDT

PDB ID	:	8SFG
Title	:	Crystal Structure of the Open Unbound Catalytically Inactive Makes Caterpillars Floppy-like (MCF) Effector from Vibrio vulnificus CMCP6
Authors	:	Minasov, G.; Shuvalova, L.; Rosas-Lemus, M.; Herrera, A.; Satchell, K.J.F.; Center for Structural Biology of Infectious Diseases (CSBID)
Deposited on	:	2023-04-11
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

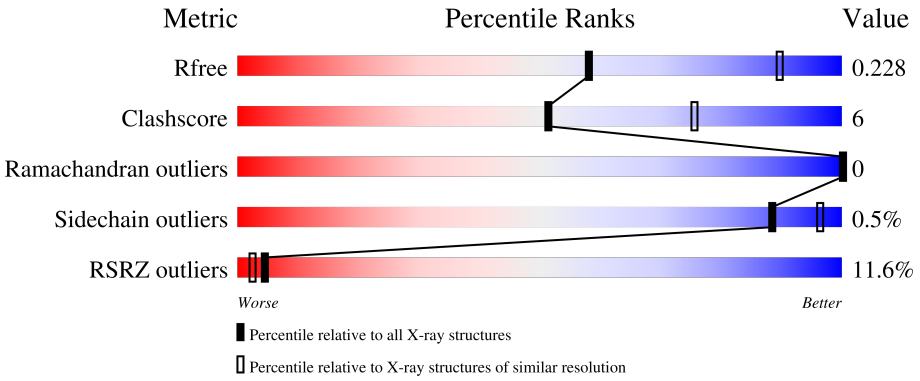
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	365	12% 79% 12% 8%
1	B	365	9% 76% 13% 10%
1	C	365	9% 78% 12% • 10%
1	D	365	11% 76% 12% 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10360 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.

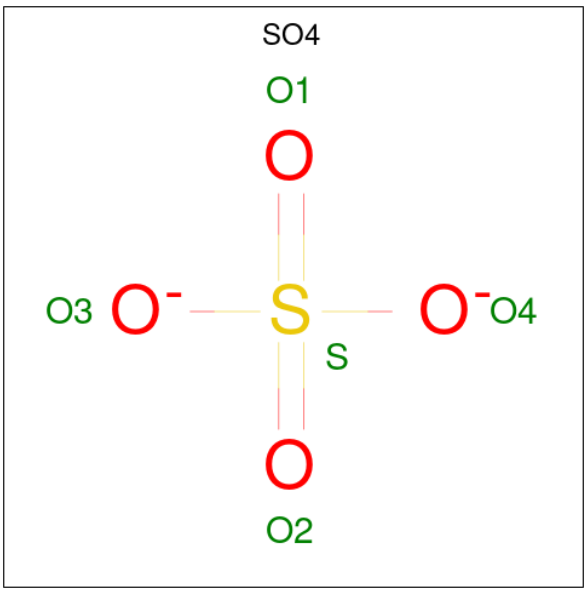
- Molecule 1 is a protein called Autotransporter adhesin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	Se	0	0	0
			2577	1629	440	498	10			
1	B	328	Total	C	N	O	Se	0	0	0
			2530	1601	432	488	9			
1	C	329	Total	C	N	O	Se	0	0	0
			2543	1607	435	492	9			
1	D	322	Total	C	N	O	Se	0	2	0
			2499	1576	428	486	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3215	SER	-	expression tag	UNP A0A3Q0KY79
A	3216	ASN	-	expression tag	UNP A0A3Q0KY79
A	3217	ALA	-	expression tag	UNP A0A3Q0KY79
A	3218	MSE	-	expression tag	UNP A0A3Q0KY79
A	3351	ALA	CYS	engineered mutation	UNP A0A3Q0KY79
B	3215	SER	-	expression tag	UNP A0A3Q0KY79
B	3216	ASN	-	expression tag	UNP A0A3Q0KY79
B	3217	ALA	-	expression tag	UNP A0A3Q0KY79
B	3218	MSE	-	expression tag	UNP A0A3Q0KY79
B	3351	ALA	CYS	engineered mutation	UNP A0A3Q0KY79
C	3215	SER	-	expression tag	UNP A0A3Q0KY79
C	3216	ASN	-	expression tag	UNP A0A3Q0KY79
C	3217	ALA	-	expression tag	UNP A0A3Q0KY79
C	3218	MSE	-	expression tag	UNP A0A3Q0KY79
C	3351	ALA	CYS	engineered mutation	UNP A0A3Q0KY79
D	3215	SER	-	expression tag	UNP A0A3Q0KY79
D	3216	ASN	-	expression tag	UNP A0A3Q0KY79
D	3217	ALA	-	expression tag	UNP A0A3Q0KY79
D	3218	MSE	-	expression tag	UNP A0A3Q0KY79
D	3351	ALA	CYS	engineered mutation	UNP A0A3Q0KY79

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 10 8 2	0	1
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 10 8 2	0	1
2	C	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 10 8 2	0	1
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total Cl 9 9	0	1
3	B	2	Total Cl 2 2	0	0
3	C	5	Total Cl 5 5	0	0
3	D	7	Total Cl 7 7	0	0

- Molecule 4 is water.

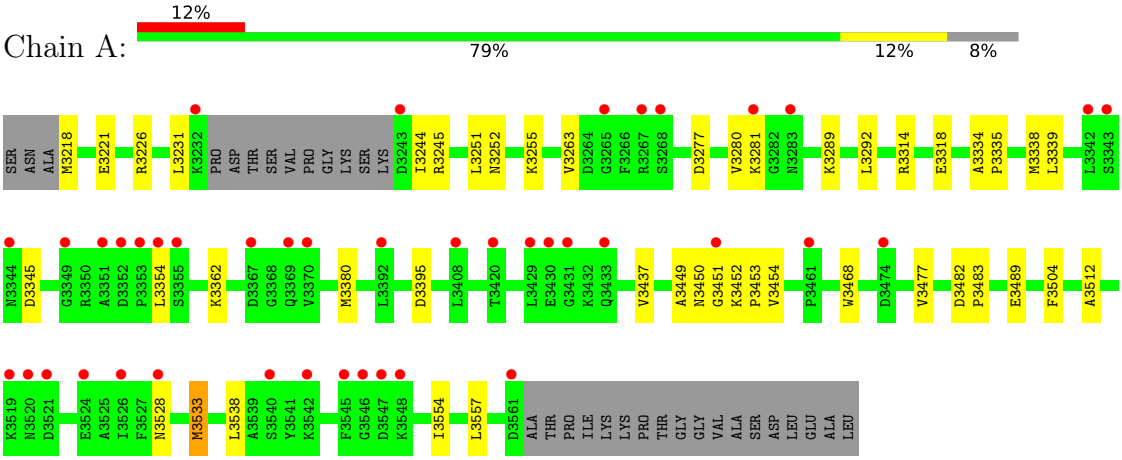
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	15	Total O 16 16	0	1
4	B	17	Total O 17 17	0	0
4	C	24	Total O 24 24	0	0
4	D	26	Total O 26 26	0	0

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.

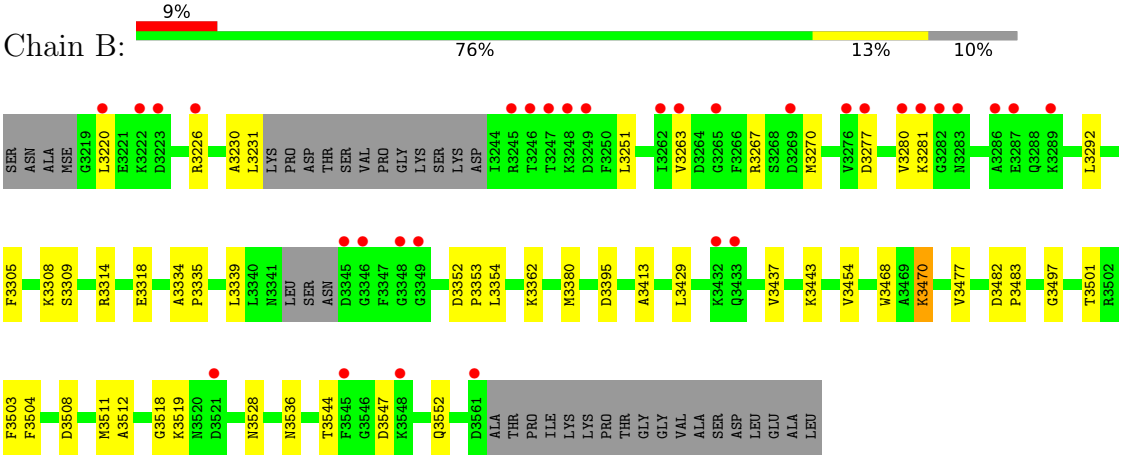
• Molecule 1: Autotransporter adhesin

Chain A:



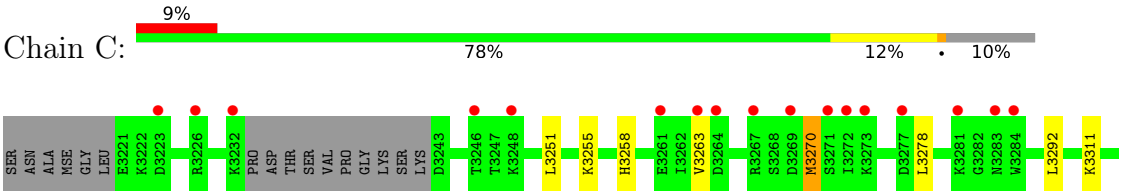
• Molecule 1: Autotransporter adhesin

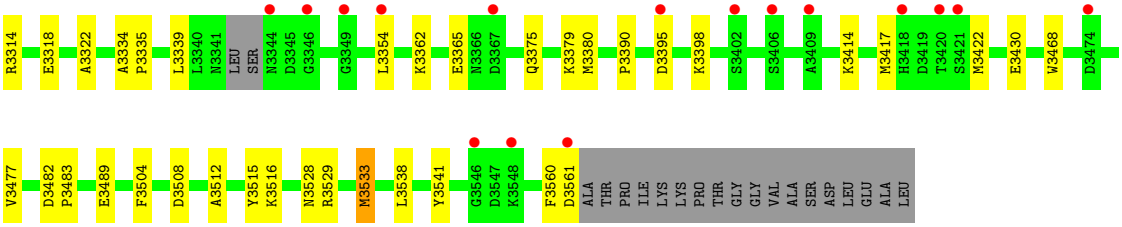
Chain B:



• Molecule 1: Autotransporter adhesin

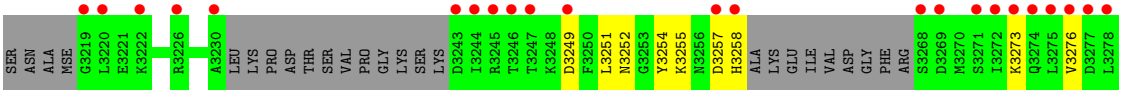
Chain C:

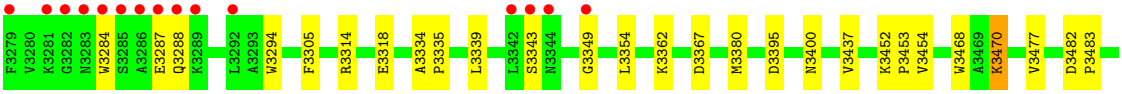


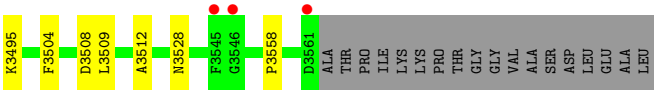


• Molecule 1: Autotransporter adhesin

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.38Å 160.66Å 71.79Å 90.00° 101.28° 90.00°	Depositor
Resolution (Å)	29.87 – 2.80 29.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.87-2.80) 97.6 (29.87-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.189 , 0.230 0.196 , 0.228	Depositor DCC
R_{free} test set	1691 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 63.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10360	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: CL, 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	0.65	0/2612	0.73	2/3502 (0.1%)
1	B	0.65	0/2564	0.74	0/3437
1	C	0.65	0/2577	0.74	3/3454 (0.1%)
1	D	0.65	0/2532	0.74	0/3395
All	All	0.65	0/10285	0.74	5/13788 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3218	MSE	CG-SE-CE	5.81	111.69	98.90
1	C	3422	MSE	CG-SE-CE	5.37	110.71	98.90
1	C	3270	MSE	CG-SE-CE	5.27	110.49	98.90
1	C	3533	MSE	CG-SE-CE	5.18	110.30	98.90
1	A	3533	MSE	CG-SE-CE	5.18	110.29	98.90

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	2577	0	2566	34	0
1	B	2530	0	2517	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2543	0	2526	29	0
1	D	2499	0	2474	34	0
2	A	25	0	0	0	0
2	B	30	0	0	0	0
2	C	25	0	0	1	0
2	D	25	0	0	0	0
3	A	9	0	0	0	0
3	B	2	0	0	0	0
3	C	5	0	0	0	0
3	D	7	0	0	0	0
4	A	16	0	0	0	0
4	B	17	0	0	0	0
4	C	24	0	0	0	0
4	D	26	0	0	0	0
All	All	10360	0	10083	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 6.

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:B:3544:THR:HG23	1:B:3547:ASP:HB3	1.60	0.81
1:B:3354:LEU:HD21	1:B:3380:MSE:HE1	1.77	0.65
1:D:3354:LEU:HD21	1:D:3380:MSE:SE	2.47	0.64
1:B:3267:ARG:HG3	1:B:3270:MSE:HG3	1.81	0.63
1:A:3395:ASP:HB3	1:B:3251:LEU:HD13	1.82	0.61
1:C:3354:LEU:HD21	1:C:3380:MSE:SE	2.53	0.58
1:C:3322:ALA:O	1:D:3495:LYS:NZ	2.36	0.58
1:D:3273:LYS:O	1:D:3276:VAL:HG12	2.04	0.58
1:D:3284:TRP:HE3	1:D:3288:GLN:HG2	1.72	0.55
1:D:3314:ARG:O	1:D:3318:GLU:HG3	2.07	0.55
1:B:3552:GLN:HG3	1:D:3367:ASP:O	2.07	0.54
1:D:3257:ASP:O	1:D:3258:HIS:HB3	2.08	0.54
1:B:3339:LEU:N	1:B:3339:LEU:HD12	2.22	0.54
1:B:3280:VAL:HG13	1:B:3281:LYS:N	2.23	0.54
1:B:3314:ARG:O	1:B:3318:GLU:HG3	2.08	0.53
1:A:3339:LEU:HD21	1:B:3305:PHE:CE2	2.45	0.52
1:B:3518:GLY:C	1:B:3519:LYS:HD3	2.30	0.52
1:D:3249:ASP:O	1:D:3287:GLU:HG2	2.10	0.52
1:C:3314:ARG:O	1:C:3318:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3263:VAL:HG11	1:B:3292:LEU:HD21	1.92	0.52
1:A:3314:ARG:O	1:A:3318:GLU:HG3	2.09	0.52
1:D:3339:LEU:HD12	1:D:3339:LEU:N	2.25	0.52
1:B:3230:ALA:C	1:B:3231:LEU:HD12	2.31	0.51
1:B:3536:ASN:HB3	1:D:3453:PRO:HD3	1.91	0.51
1:C:3362:LYS:HE3	1:C:3468:TRP:CZ2	2.46	0.51
1:D:3252:ASN:O	1:D:3255:LYS:HE2	2.11	0.51
1:A:3263:VAL:HG11	1:A:3292:LEU:HD21	1.93	0.50
1:C:3263:VAL:HG11	1:C:3292:LEU:HD21	1.92	0.50
1:C:3339:LEU:CD2	1:D:3305:PHE:CE2	2.95	0.50
1:A:3280:VAL:HG23	1:A:3281:LYS:N	2.26	0.50
1:B:3504:PHE:HB3	1:B:3512:ALA:HB2	1.93	0.50
1:A:3251:LEU:HD13	1:B:3395:ASP:HB3	1.94	0.49
1:A:3226:ARG:NH1	1:A:3277:ASP:OD1	2.44	0.49
1:A:3504:PHE:HB3	1:A:3512:ALA:HB2	1.95	0.49
1:A:3354:LEU:HD21	1:A:3380:MSE:SE	2.63	0.49
1:A:3338:MSE:HE3	1:B:3308:LYS:HA	1.94	0.49
1:A:3452:LYS:HG3	1:A:3453:PRO:HD2	1.94	0.49
1:A:3452:LYS:CG	1:A:3453:PRO:HD2	2.43	0.49
1:C:3398:LYS:HE3	1:D:3254:TYR:O	2.13	0.49
1:A:3338:MSE:CE	1:B:3309:SER:H	2.26	0.48
1:A:3533:MSE:HG2	1:A:3538:LEU:HD22	1.95	0.48
1:D:3354:LEU:CD2	1:D:3380:MSE:SE	3.11	0.48
1:D:3362:LYS:HE3	1:D:3468:TRP:CZ2	2.49	0.48
1:B:3334:ALA:HB3	1:B:3335:PRO:HD3	1.95	0.48
1:C:3339:LEU:HD21	1:D:3305:PHE:CE2	2.48	0.47
1:D:3284:TRP:CE3	1:D:3288:GLN:HG2	2.48	0.47
1:A:3244:ILE:CD1	1:A:3289:LYS:HD2	2.44	0.47
1:B:3470:LYS:HE3	1:B:3477:VAL:HG21	1.95	0.47
1:C:3395:ASP:HB3	1:D:3251:LEU:HD13	1.96	0.47
1:D:3504:PHE:HB3	1:D:3512:ALA:HB2	1.95	0.47
1:A:3477:VAL:CG1	1:A:3489:GLU:HB3	2.44	0.47
1:B:3470:LYS:HE3	1:B:3477:VAL:CG2	2.44	0.47
1:D:3470:LYS:HE3	1:D:3477:VAL:CG2	2.45	0.47
1:A:3345:ASP:C	1:B:3220:LEU:HD23	2.35	0.47
1:D:3470:LYS:HE3	1:D:3477:VAL:HG21	1.97	0.47
1:C:3334:ALA:HB3	1:C:3335:PRO:HD3	1.95	0.47
1:A:3334:ALA:HB3	1:A:3335:PRO:HD3	1.97	0.47
1:B:3226:ARG:NH1	1:B:3277:ASP:OD1	2.48	0.47
1:C:3504:PHE:HB3	1:C:3512:ALA:HB2	1.95	0.47
1:D:3334:ALA:HB3	1:D:3335:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3244:ILE:HD13	1:A:3289:LYS:HD2	1.96	0.46
1:A:3362:LYS:HE3	1:A:3468:TRP:CZ2	2.51	0.46
1:A:3221:GLU:OE2	1:B:3413:ALA:HA	2.15	0.46
1:B:3528:ASN:HD22	1:B:3528:ASN:N	2.13	0.46
1:B:3429:LEU:HD11	1:B:3443:LYS:HE3	1.97	0.46
1:C:3255:LYS:HE3	1:C:3258:HIS:ND1	2.31	0.46
1:C:3533:MSE:HG2	1:C:3538:LEU:HD22	1.98	0.45
1:B:3362:LYS:HE3	1:B:3468:TRP:CZ2	2.52	0.45
1:C:3365:GLU:OE2	2:C:3602[B]:SO4:O4	2.35	0.45
1:A:3449:ALA:O	1:A:3450:ASN:OD1	2.35	0.45
1:C:3311:LYS:HD2	1:D:3509:LEU:HD22	1.99	0.45
1:A:3339:LEU:CD2	1:B:3305:PHE:CE2	3.00	0.44
1:C:3477:VAL:CG1	1:C:3489:GLU:HB3	2.47	0.44
1:A:3528:ASN:N	1:A:3528:ASN:HD22	2.15	0.44
1:C:3528:ASN:HD22	1:C:3528:ASN:N	2.16	0.44
1:C:3354:LEU:CD2	1:C:3380:MSE:SE	3.16	0.44
1:C:3398:LYS:CE	1:D:3254:TYR:O	2.66	0.44
1:C:3270:MSE:HE1	1:C:3278:LEU:HD22	1.99	0.43
1:D:3437:VAL:HG21	1:D:3504:PHE:HB2	1.99	0.43
1:B:3339:LEU:N	1:B:3339:LEU:CD1	2.81	0.43
1:A:3482:ASP:OD1	1:A:3483:PRO:HD2	2.18	0.43
1:C:3560:PHE:O	1:C:3561:ASP:HB2	2.18	0.43
1:B:3280:VAL:HG13	1:B:3281:LYS:H	1.84	0.43
1:A:3252:ASN:O	1:A:3255:LYS:HD3	2.19	0.42
1:C:3251:LEU:HD13	1:D:3395:ASP:HB3	2.01	0.42
1:D:3528:ASN:HD22	1:D:3528:ASN:N	2.16	0.42
1:A:3554:ILE:HA	1:A:3557:LEU:HG	2.00	0.42
1:B:3231:LEU:HD12	1:B:3231:LEU:N	2.34	0.42
1:C:3515:TYR:C	1:C:3516:LYS:HG2	2.40	0.42
1:B:3497:GLY:O	1:B:3501:THR:HG23	2.18	0.42
1:D:3452:LYS:CG	1:D:3453:PRO:HD2	2.49	0.42
1:A:3338:MSE:HE3	1:B:3309:SER:H	1.83	0.42
1:C:3390:PRO:HG3	1:D:3294:TRP:NE1	2.35	0.42
1:B:3454:VAL:O	1:B:3468:TRP:HA	2.20	0.42
1:A:3231:LEU:HD13	1:A:3245:ARG:HD3	2.00	0.42
1:C:3430:GLU:OE2	1:C:3529:ARG:HD2	2.19	0.42
1:C:3375:GLN:O	1:C:3379:LYS:HG3	2.19	0.42
1:B:3482:ASP:OD1	1:B:3483:PRO:HD2	2.20	0.41
1:D:3454:VAL:O	1:D:3468:TRP:HA	2.20	0.41
1:D:3343:SER:O	1:D:3349:GLY:N	2.54	0.41
1:A:3280:VAL:HG23	1:A:3281:LYS:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3449:ALA:C	1:A:3450:ASN:OD1	2.59	0.41
1:A:3450:ASN:CG	1:A:3451:GLY:H	2.24	0.41
1:B:3503:PHE:CE1	1:B:3511:MSE:HG3	2.55	0.41
1:C:3414:LYS:HG2	1:C:3541:TYR:OH	2.21	0.41
1:C:3482:ASP:OD1	1:C:3483:PRO:HD2	2.21	0.41
1:D:3482:ASP:OD1	1:D:3483:PRO:HD2	2.21	0.41
1:B:3352:ASP:HB3	1:B:3353:PRO:HD3	2.03	0.41
1:A:3437:VAL:HG21	1:A:3504:PHE:HB2	2.04	0.40
1:A:3454:VAL:O	1:A:3468:TRP:HA	2.21	0.40
1:B:3437:VAL:HG21	1:B:3504:PHE:HB2	2.01	0.40
1:D:3339:LEU:N	1:D:3339:LEU:CD1	2.84	0.40
1:C:3417:MSE:HE2	1:C:3529:ARG:HH21	1.86	0.40
1:D:3400:ASN:HB3	1:D:3558:PRO:O	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	330/365 (90%)	318 (96%)	12 (4%)	0	100	100
1	B	322/365 (88%)	313 (97%)	9 (3%)	0	100	100
1	C	323/365 (88%)	313 (97%)	10 (3%)	0	100	100
1	D	318/365 (87%)	310 (98%)	8 (2%)	0	100	100
All	All	1293/1460 (89%)	1254 (97%)	39 (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	271/285 (95%)	271 (100%)	0	100	100
1	B	265/285 (93%)	263 (99%)	2 (1%)	81	94
1	C	267/285 (94%)	266 (100%)	1 (0%)	91	97
1	D	263/285 (92%)	261 (99%)	2 (1%)	81	94
All	All	1066/1140 (94%)	1061 (100%)	5 (0%)	88	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3470	LYS
1	B	3508	ASP
1	C	3508	ASP
1	D	3470	LYS
1	D	3508	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 44 ligands modelled in this entry, 23 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
2	SO4	C	3603	-	4,4,4	0.39	0	6,6,6	0.06	0
2	SO4	B	3602	-	4,4,4	0.38	0	6,6,6	0.05	0
2	SO4	A	3603	-	4,4,4	0.38	0	6,6,6	0.06	0
2	SO4	B	3604[B]	-	4,4,4	0.39	0	6,6,6	0.06	0
2	SO4	B	3605	-	4,4,4	0.38	0	6,6,6	0.05	0
2	SO4	A	3605	-	4,4,4	0.38	0	6,6,6	0.04	0
2	SO4	C	3602[A]	-	4,4,4	0.40	0	6,6,6	0.06	0
2	SO4	A	3601	-	4,4,4	0.39	0	6,6,6	0.05	0
2	SO4	C	3601	-	4,4,4	0.39	0	6,6,6	0.05	0
2	SO4	A	3602	-	4,4,4	0.40	0	6,6,6	0.07	0
2	SO4	D	3602	-	4,4,4	0.38	0	6,6,6	0.05	0
2	SO4	C	3602[B]	-	4,4,4	0.41	0	6,6,6	0.07	0
2	SO4	D	3603[A]	-	4,4,4	0.39	0	6,6,6	0.05	0
2	SO4	C	3604	-	4,4,4	0.37	0	6,6,6	0.06	0
2	SO4	A	3604	-	4,4,4	0.39	0	6,6,6	0.04	0
2	SO4	B	3601	-	4,4,4	0.38	0	6,6,6	0.06	0
2	SO4	B	3603	-	4,4,4	0.39	0	6,6,6	0.05	0
2	SO4	B	3604[A]	-	4,4,4	0.39	0	6,6,6	0.07	0
2	SO4	D	3604	-	4,4,4	0.39	0	6,6,6	0.04	0
2	SO4	D	3603[B]	-	4,4,4	0.39	0	6,6,6	0.04	0
2	SO4	D	3601	-	4,4,4	0.38	0	6,6,6	0.05	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
2	C	3602[B]	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	324/365 (88%)	0.60	42 (12%)	3 2	42, 71, 123, 172	0
1	B	319/365 (87%)	0.29	32 (10%)	7 4	35, 55, 124, 146	0
1	C	320/365 (87%)	0.37	33 (10%)	6 3	30, 61, 131, 157	0
1	D	313/365 (85%)	0.40	41 (13%)	3 2	29, 48, 151, 173	0
All	All	1276/1460 (87%)	0.42	148 (11%)	4 2	29, 59, 136, 173	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3344	ASN	11.0
1	A	3546	GLY	10.6
1	D	3281	LYS	8.1
1	D	3344	ASN	8.1
1	D	3268	SER	7.0
1	B	3349	GLY	6.7
1	C	3283	ASN	6.6
1	A	3561	ASP	6.1
1	A	3343	SER	5.9
1	C	3223	ASP	5.9
1	C	3561	ASP	5.8
1	D	3343	SER	5.6
1	D	3247	THR	5.6
1	D	3243	ASP	5.4
1	D	3287	GLU	5.3
1	D	3269	ASP	4.9
1	D	3258	HIS	4.9
1	A	3265	GLY	4.8
1	D	3288	GLN	4.8
1	B	3561	ASP	4.7
1	C	3546	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	3283	ASN	4.6
1	B	3265	GLY	4.5
1	C	3344	ASN	4.5
1	B	3286	ALA	4.4
1	B	3283	ASN	4.4
1	C	3273	LYS	4.2
1	A	3353	PRO	4.2
1	C	3281	LYS	4.1
1	D	3282	GLY	4.1
1	C	3248	LYS	4.0
1	A	3354	LEU	4.0
1	D	3219	GLY	3.9
1	A	3548	LYS	3.8
1	A	3433	GLN	3.8
1	D	3272	ILE	3.8
1	B	3281	LYS	3.7
1	B	3277	ASP	3.7
1	D	3285	SER	3.7
1	A	3542	LYS	3.6
1	D	3274	GLN	3.6
1	A	3355	SER	3.6
1	A	3420	THR	3.6
1	A	3351	ALA	3.6
1	D	3342	LEU	3.6
1	C	3548	LYS	3.5
1	A	3232	LYS	3.5
1	A	3547	ASP	3.4
1	B	3348	GLY	3.4
1	D	3246	THR	3.4
1	B	3545	PHE	3.4
1	D	3546	GLY	3.3
1	D	3545	PHE	3.3
1	C	3284	TRP	3.3
1	D	3257	ASP	3.3
1	A	3281	LYS	3.2
1	D	3275	LEU	3.2
1	D	3245	ARG	3.2
1	D	3273	LYS	3.1
1	C	3246	THR	3.1
1	D	3226	ARG	3.1
1	B	3222	LYS	3.1
1	B	3521	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	3278	LEU	3.0
1	C	3420	THR	2.9
1	C	3418	HIS	2.9
1	B	3282	GLY	2.9
1	A	3267	ARG	2.9
1	D	3271	SER	2.9
1	B	3346	GLY	2.9
1	A	3545	PHE	2.9
1	B	3263	VAL	2.9
1	A	3283	ASN	2.9
1	D	3277	ASP	2.8
1	B	3249	ASP	2.8
1	A	3342	LEU	2.8
1	C	3421	SER	2.8
1	D	3284	TRP	2.8
1	A	3540	SER	2.8
1	B	3246	THR	2.8
1	C	3346	GLY	2.8
1	A	3520	ASN	2.7
1	B	3223	ASP	2.7
1	A	3526	ILE	2.7
1	D	3279	PHE	2.7
1	A	3268	SER	2.7
1	A	3369	GLN	2.7
1	A	3352	ASP	2.6
1	B	3226	ARG	2.6
1	B	3432	LYS	2.6
1	B	3280	VAL	2.6
1	C	3367	ASP	2.6
1	D	3292	LEU	2.6
1	D	3286	ALA	2.6
1	A	3431	GLY	2.5
1	B	3289	LYS	2.5
1	A	3524	GLU	2.5
1	A	3408	LEU	2.5
1	C	3232	LYS	2.5
1	C	3409	ALA	2.5
1	D	3561	ASP	2.4
1	A	3451	GLY	2.4
1	C	3261	GLU	2.4
1	D	3222	LYS	2.4
1	A	3474	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	3248	LYS	2.4
1	A	3461	PRO	2.4
1	D	3249	ASP	2.4
1	C	3272	ILE	2.4
1	B	3345	ASP	2.4
1	A	3528	ASN	2.4
1	B	3269	ASP	2.3
1	A	3429	LEU	2.3
1	B	3433	GLN	2.3
1	B	3548	LYS	2.3
1	B	3262	ILE	2.3
1	A	3367	ASP	2.3
1	D	3230	ALA	2.3
1	B	3247	THR	2.2
1	C	3349	GLY	2.2
1	B	3276	VAL	2.2
1	D	3289	LYS	2.2
1	D	3276	VAL	2.2
1	C	3395	ASP	2.2
1	D	3244	ILE	2.2
1	A	3521	ASP	2.2
1	C	3271	SER	2.2
1	C	3406	SER	2.2
1	B	3287	GLU	2.2
1	C	3263	VAL	2.2
1	A	3349	GLY	2.2
1	A	3430	GLU	2.1
1	C	3264	ASP	2.1
1	C	3474	ASP	2.1
1	A	3519	LYS	2.1
1	A	3370	VAL	2.1
1	C	3226	ARG	2.1
1	C	3277	ASP	2.1
1	A	3392	LEU	2.1
1	B	3220	LEU	2.1
1	B	3245	ARG	2.1
1	C	3402	SER	2.0
1	D	3220	LEU	2.0
1	C	3354	LEU	2.0
1	C	3269	ASP	2.0
1	D	3349	GLY	2.0
1	C	3267	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	3243	ASP	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
2	SO4	D	3602	5/5	0.67	0.28	116,120,129,132	0
3	CL	A	3606	1/1	0.69	0.11	88,88,88,88	0
3	CL	D	3609	1/1	0.72	0.18	85,85,85,85	0
3	CL	D	3611	1/1	0.73	0.32	73,73,73,73	0
3	CL	D	3610	1/1	0.77	0.38	86,86,86,86	0
2	SO4	A	3605	5/5	0.79	0.35	114,117,129,137	0
2	SO4	C	3604	5/5	0.80	0.41	95,98,109,114	0
3	CL	C	3608	1/1	0.81	0.16	83,83,83,83	0
3	CL	C	3606	1/1	0.82	0.17	90,90,90,90	0
2	SO4	B	3604[A]	5/5	0.83	0.31	53,57,61,61	5
2	SO4	B	3604[B]	5/5	0.83	0.31	67,67,75,76	5
3	CL	C	3605	1/1	0.84	0.15	81,81,81,81	0
3	CL	C	3607	1/1	0.84	0.20	74,74,74,74	0
2	SO4	A	3602	5/5	0.85	0.31	88,96,98,101	0
2	SO4	B	3605	5/5	0.85	0.20	103,110,124,128	0
3	CL	C	3609	1/1	0.86	0.13	86,86,86,86	0
3	CL	A	3609	1/1	0.86	0.15	72,72,72,72	0
3	CL	A	3608	1/1	0.87	0.34	98,98,98,98	0
2	SO4	B	3602	5/5	0.88	0.27	108,109,116,119	0
3	CL	D	3607	1/1	0.88	0.11	69,69,69,69	0
2	SO4	D	3603[A]	5/5	0.88	0.24	59,61,65,69	5
2	SO4	D	3603[B]	5/5	0.88	0.24	50,52,56,56	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	B	3607	1/1	0.88	0.12	79,79,79,79	0
3	CL	D	3605	1/1	0.89	0.14	77,77,77,77	0
3	CL	A	3610	1/1	0.91	0.20	81,81,81,81	0
2	SO4	C	3601	5/5	0.91	0.41	110,113,118,121	0
3	CL	A	3613[B]	1/1	0.92	0.12	61,61,61,61	1
2	SO4	A	3604	5/5	0.92	0.14	95,103,110,114	0
2	SO4	B	3603	5/5	0.92	0.32	100,102,107,108	0
2	SO4	C	3602[A]	5/5	0.92	0.21	44,46,52,52	5
2	SO4	C	3602[B]	5/5	0.92	0.21	27,30,31,37	5
3	CL	A	3613[A]	1/1	0.92	0.12	53,53,53,53	1
3	CL	D	3608	1/1	0.93	0.13	86,86,86,86	0
3	CL	A	3612	1/1	0.93	0.07	84,84,84,84	0
3	CL	A	3611	1/1	0.94	0.12	79,79,79,79	0
2	SO4	A	3603	5/5	0.94	0.12	76,86,100,101	0
3	CL	D	3606	1/1	0.94	0.06	72,72,72,72	0
2	SO4	D	3604	5/5	0.94	0.26	92,92,95,100	0
2	SO4	D	3601	5/5	0.95	0.14	67,70,76,79	0
3	CL	B	3606	1/1	0.95	0.07	67,67,67,67	0
2	SO4	A	3601	5/5	0.95	0.12	77,80,84,84	0
2	SO4	C	3603	5/5	0.97	0.19	80,86,88,94	0
2	SO4	B	3601	5/5	0.98	0.10	50,58,63,65	0
3	CL	A	3607	1/1	0.99	0.05	70,70,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.