Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 05:39 PM EDT

PDB ID	:	4N8G
Title	:	Crystal structure of a TRAP periplasmic solute binding protein from Chromohalobacter salexigens DSM 3043 (Csal_0660), Target EFI-501075, with bound D-alanine-D-alanine
Authors	:	Vetting, M.W.; Al Obaidi, N.F.; Morisco, L.L.; Wasserman, S.R.; Sojitra, S.; Stead, M.; Attonito, J.D.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hillerich, B.; Love, J.; Seidel, R.D.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on	:	2013-10-17
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 (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:

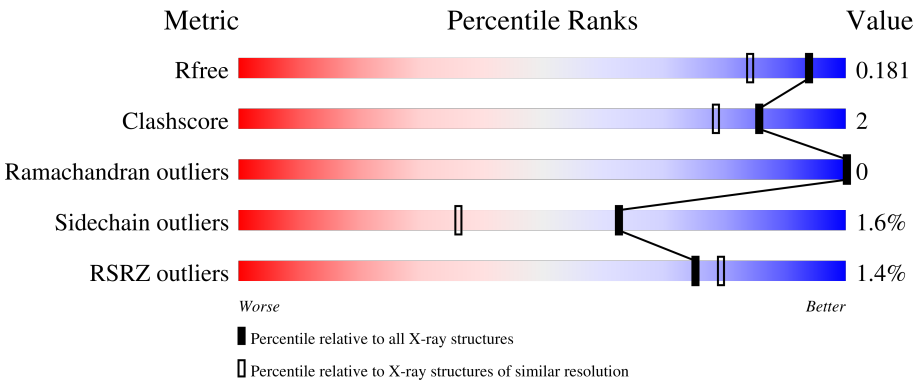
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance (i)

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

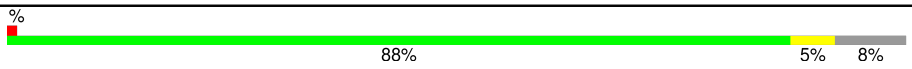
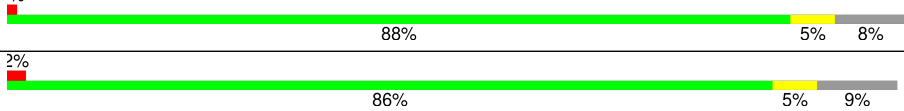
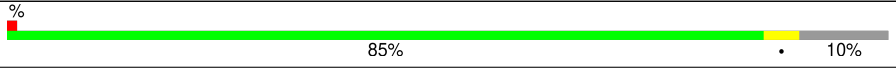
The reported resolution of this entry is 1.50 Å.

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}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (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 <=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	352	
1	B	352	
1	C	352	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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Mol	Chain	Length	Quality of chain
1	D	352	% 83% 5% • 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21284 atoms, of which 9632 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 TRAP dicarboxylate transporter, DctP subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	Se			
1	A	325	5080	1651	2462	417	541	9	0	5	0
1	B	321	4966	1611	2410	410	526	9	0	2	0
1	C	316	4925	1598	2392	405	521	9	0	3	0
1	D	312	4877	1582	2368	402	516	9	0	6	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	ALA	-	EXPRESSION TAG	UNP Q1QZT7
A	347	GLU	-	EXPRESSION TAG	UNP Q1QZT7
A	348	ASN	-	EXPRESSION TAG	UNP Q1QZT7
A	349	LEU	-	EXPRESSION TAG	UNP Q1QZT7
A	350	TYR	-	EXPRESSION TAG	UNP Q1QZT7
A	351	PHE	-	EXPRESSION TAG	UNP Q1QZT7
A	352	GLN	-	EXPRESSION TAG	UNP Q1QZT7
B	346	ALA	-	EXPRESSION TAG	UNP Q1QZT7
B	347	GLU	-	EXPRESSION TAG	UNP Q1QZT7
B	348	ASN	-	EXPRESSION TAG	UNP Q1QZT7
B	349	LEU	-	EXPRESSION TAG	UNP Q1QZT7
B	350	TYR	-	EXPRESSION TAG	UNP Q1QZT7
B	351	PHE	-	EXPRESSION TAG	UNP Q1QZT7
B	352	GLN	-	EXPRESSION TAG	UNP Q1QZT7
C	346	ALA	-	EXPRESSION TAG	UNP Q1QZT7
C	347	GLU	-	EXPRESSION TAG	UNP Q1QZT7
C	348	ASN	-	EXPRESSION TAG	UNP Q1QZT7
C	349	LEU	-	EXPRESSION TAG	UNP Q1QZT7
C	350	TYR	-	EXPRESSION TAG	UNP Q1QZT7
C	351	PHE	-	EXPRESSION TAG	UNP Q1QZT7
C	352	GLN	-	EXPRESSION TAG	UNP Q1QZT7

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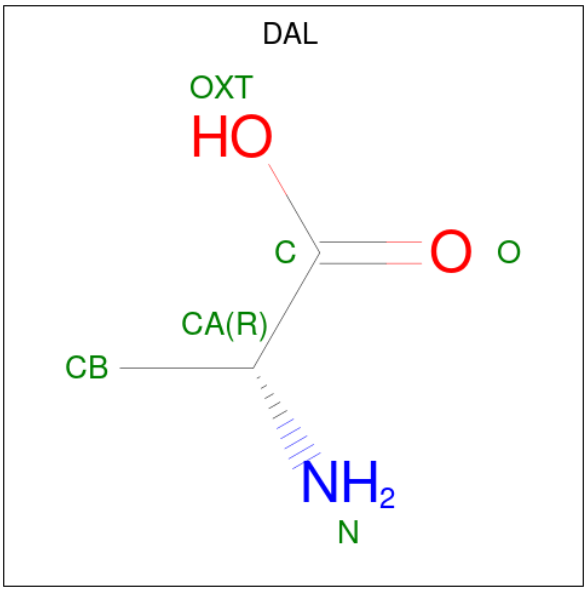
Chain	Residue	Modelled	Actual	Comment	Reference
D	346	ALA	-	EXPRESSION TAG	UNP Q1QZT7
D	347	GLU	-	EXPRESSION TAG	UNP Q1QZT7
D	348	ASN	-	EXPRESSION TAG	UNP Q1QZT7
D	349	LEU	-	EXPRESSION TAG	UNP Q1QZT7
D	350	TYR	-	EXPRESSION TAG	UNP Q1QZT7
D	351	PHE	-	EXPRESSION TAG	UNP Q1QZT7
D	352	GLN	-	EXPRESSION TAG	UNP Q1QZT7

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is D-ALANINE (three-letter code: DAL) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	5	3	1	1	0	0

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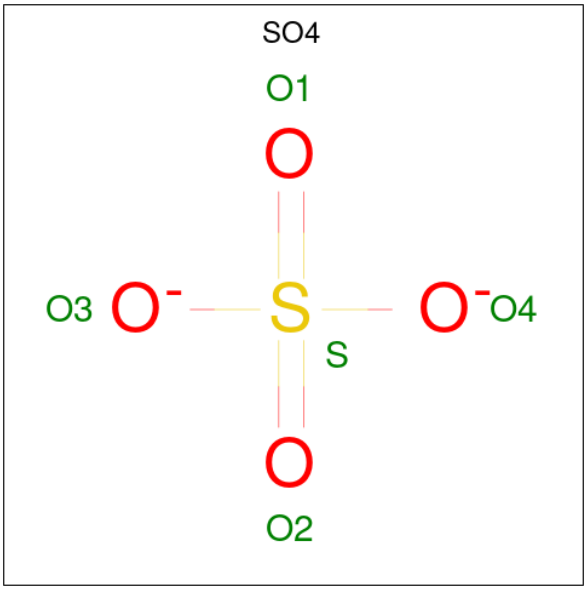
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	6	3	1	2	0	0
3	B	1	5	3	1	1	0	0
3	B	1	6	3	1	2	0	0
3	C	1	5	3	1	1	0	0
3	C	1	6	3	1	2	0	0
3	D	1	5	3	1	1	0	0
3	D	1	6	3	1	2	0	0

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	376	377	377	0	1

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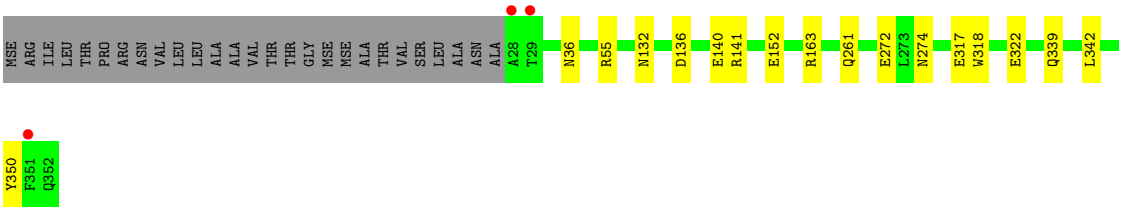
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	335	335	335	0	0
			Total	O		
5	C	315	315	315	0	0
			Total	O		
5	D	356	356	356	0	0

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.

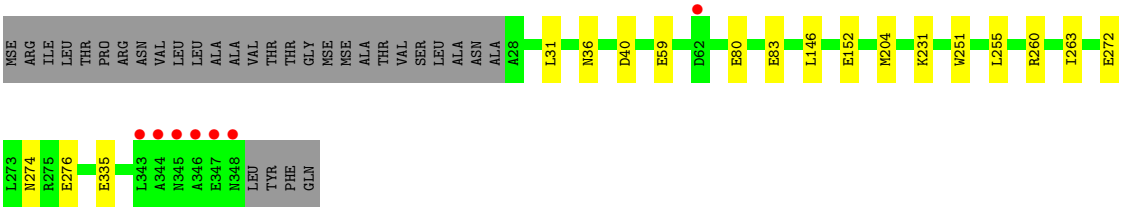
• Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain A:



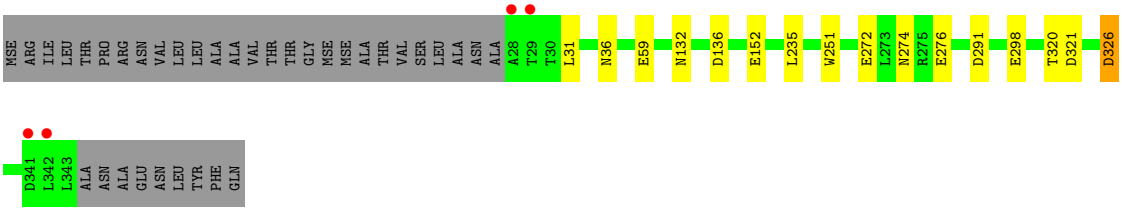
• Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain B:



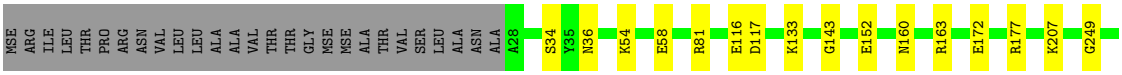
• Molecule 1: TRAP dicarboxylate transporter, DctP subunit

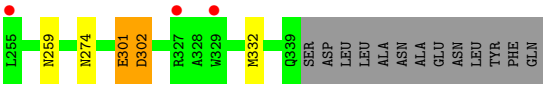
Chain C:



• Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain D:


MSE
ARG
ILE
LEU
THR
PRO
ARG
ASN
VAL
LEU
LEU
ALA
ALA
VAL
THR
THR
GLY
MSE
MSE
ALA
THR
VAL
SER
LEU
ALA
ASN
ALA
A28
S34
Y35
N36
K54
E58
R81
E116
D117
K133
G143
E152
N160
R163
E172
R177
K207
G249


L255
N259
N274
E301
D302
R327
A328
W329
M332
Q339
SER
ASP
LEU
LEU
ALA
ASN
ALA
GLU
ASN
LEU
TYR
PHE
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.54Å 67.96Å 276.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.87 – 1.50 30.87 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.87-1.50) 99.4 (30.87-1.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.42 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.159 , 0.181 0.159 , 0.181	Depositor DCC
R_{free} test set	9860 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	14.8	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	21284	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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 (i)

5.1 Standard geometry (i)

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

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	0.46	0/2678	0.62	1/3622 (0.0%)
1	B	0.47	0/2611	0.61	0/3531
1	C	0.47	0/2587	0.62	0/3499
1	D	0.49	0/2578	0.63	1/3488 (0.0%)
All	All	0.47	0/10454	0.62	2/14140 (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	D	302	ASP	CB-CG-OD1	7.15	124.74	118.30
1	A	163	ARG	NE-CZ-NH2	5.52	123.06	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2618	2462	2447	15	0
1	B	2556	2410	2394	12	0
1	C	2533	2392	2375	10	1
1	D	2509	2368	2342	10	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	11	0	10	0	0
3	B	11	0	10	0	0
3	C	11	0	10	0	0
3	D	11	0	10	0	0
4	A	5	0	0	0	0
5	A	377	0	0	5	0
5	B	335	0	0	7	2
5	C	315	0	0	1	1
5	D	356	0	0	2	0
All	All	11652	9632	9598	43	2

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 2.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASN:ND2	1:C:132[B]:ASN:OD1	1.88	1.06
1:A:322[A]:GLU:OE1	5:A:706:HOH:O	1.88	0.91
1:A:272:GLU:OE1	5:A:753:HOH:O	2.02	0.78
1:C:31:LEU:HD11	1:C:251:TRP:CZ2	2.21	0.75
1:A:140:GLU:OE1	5:A:708:HOH:O	2.07	0.72
1:B:83:GLU:OE2	5:B:566:HOH:O	2.14	0.66
1:B:204:MSE:HG3	5:B:803:HOH:O	1.95	0.66
1:B:40:ASP:OD2	5:B:780:HOH:O	2.13	0.65
1:A:322[B]:GLU:CD	1:B:80[B]:GLU:OE2	2.37	0.63
1:C:31:LEU:CD1	1:C:251:TRP:CZ2	2.83	0.61
1:C:235:LEU:HD12	1:C:298:GLU:HG2	1.85	0.58
1:A:322[B]:GLU:OE2	1:B:80[B]:GLU:OE2	2.22	0.58
1:D:301:GLU:CD	1:D:301:GLU:H	2.08	0.57
1:C:320:THR:OG1	1:C:321:ASP:OD2	2.24	0.56
1:D:163:ARG:NH1	1:D:172:GLU:O	2.38	0.55
1:B:231:LYS:HD2	5:B:732:HOH:O	2.06	0.55
1:C:31:LEU:HD11	1:C:251:TRP:CE2	2.42	0.55
1:A:318:TRP:HA	1:A:322[A]:GLU:OE1	2.08	0.52
1:C:272:GLU:OE2	1:C:276:GLU:OE2	2.30	0.50
1:B:260:ARG:HD2	5:B:642:HOH:O	2.11	0.50
1:A:261:GLN:OE1	5:A:819:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:LYS:NZ	5:D:716:HOH:O	2.45	0.48
1:B:59:GLU:OE2	5:B:729:HOH:O	2.21	0.47
1:A:136:ASP:OD2	1:C:136:ASP:OD2	2.34	0.45
1:B:335:GLU:HG3	5:B:679:HOH:O	2.15	0.45
1:A:339:GLN:HB3	1:A:342:LEU:HG	1.99	0.44
1:C:291:ASP:OD2	5:C:608:HOH:O	2.20	0.44
1:C:326:ASP:OD1	1:C:326:ASP:C	2.56	0.44
1:D:116:GLU:HG3	1:D:117:ASP:CG	2.38	0.44
1:D:259:ASN:ND2	5:D:651:HOH:O	2.50	0.44
1:A:318:TRP:CD1	1:A:322[A]:GLU:OE1	2.71	0.43
1:D:143:GLY:O	1:D:249:GLY:HA3	2.18	0.43
1:A:317:GLU:HG3	1:A:350:TYR:CE2	2.54	0.43
1:D:133:LYS:HE3	1:D:332:MSE:SE	2.68	0.43
1:A:55:ARG:NH2	5:A:797:HOH:O	2.53	0.42
1:D:34:SER:HB3	1:D:81:ARG:HD2	2.01	0.42
1:B:255:LEU:HD13	1:B:263:ILE:HD12	2.01	0.42
1:A:140:GLU:OE1	1:A:141:ARG:HG3	2.20	0.42
1:B:272:GLU:OE2	1:B:276:GLU:OE2	2.39	0.41
1:D:54:LYS:O	1:D:58[A]:GLU:HG3	2.20	0.41
1:D:177:ARG:HD3	1:D:177:ARG:C	2.41	0.41
1:B:31:LEU:HD21	1:B:251:TRP:CE2	2.56	0.40
1:A:318:TRP:HD1	1:A:322[A]:GLU:OE1	2.05	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:GLU:OE2	5:B:813:HOH:O[1_545]	2.00	0.20
5:B:722:HOH:O	5:C:726:HOH:O[1_565]	2.07	0.13

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	328/352 (93%)	322 (98%)	6 (2%)	0	100	100
1	B	321/352 (91%)	314 (98%)	7 (2%)	0	100	100
1	C	317/352 (90%)	312 (98%)	5 (2%)	0	100	100
1	D	316/352 (90%)	311 (98%)	5 (2%)	0	100	100
All	All	1282/1408 (91%)	1259 (98%)	23 (2%)	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	280/285 (98%)	277 (99%)	3 (1%)	73	53
1	B	273/285 (96%)	269 (98%)	4 (2%)	65	39
1	C	272/285 (95%)	268 (98%)	4 (2%)	65	39
1	D	271/285 (95%)	265 (98%)	6 (2%)	52	22
All	All	1096/1140 (96%)	1079 (98%)	17 (2%)	62	36

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

Mol	Chain	Res	Type
1	A	36	ASN
1	A	152	GLU
1	A	274	ASN
1	B	36	ASN
1	B	146	LEU
1	B	152	GLU
1	B	274	ASN
1	C	36	ASN
1	C	152	GLU
1	C	274	ASN
1	C	326	ASP
1	D	36	ASN
1	D	152	GLU

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Mol	Chain	Res	Type
1	D	160	ASN
1	D	274	ASN
1	D	301	GLU
1	D	302	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
3	DAL	B	403	3	5,5,5	1.16	0	6,6,6	1.23	1 (16%)
3	DAL	C	402	3	3,4,5	0.60	0	2,4,6	0.74	0
3	DAL	D	402	3	3,4,5	0.65	0	2,4,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	A	404	-	4,4,4	0.29	0	6,6,6	0.21	0
3	DAL	C	403	3	5,5,5	1.06	0	6,6,6	1.26	0
3	DAL	A	402	3	3,4,5	0.71	0	2,4,6	0.80	0
3	DAL	A	403	3	5,5,5	1.20	0	6,6,6	0.80	0
3	DAL	B	402	3	3,4,5	0.69	0	2,4,6	0.96	0
3	DAL	D	403	3	5,5,5	1.07	0	6,6,6	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DAL	B	403	3	-	0/4/4/4	-
3	DAL	C	402	3	-	0/1/2/4	-
3	DAL	D	402	3	-	0/1/2/4	-
3	DAL	C	403	3	-	1/4/4/4	-
3	DAL	A	402	3	-	0/1/2/4	-
3	DAL	A	403	3	-	0/4/4/4	-
3	DAL	B	402	3	-	0/1/2/4	-
3	DAL	D	403	3	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	403	DAL	OXT-C-CA	2.01	120.70	113.79

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	403	DAL	OXT-C-CA-CB

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 (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	316/352 (89%)	-0.40	3 (0%)	84	87	9, 15, 27, 33	0
1	B	312/352 (88%)	-0.23	7 (2%)	62	67	9, 16, 30, 62	0
1	C	307/352 (87%)	-0.31	4 (1%)	77	81	10, 16, 30, 43	0
1	D	303/352 (86%)	-0.39	3 (0%)	82	85	10, 15, 28, 41	0
All	All	1238/1408 (87%)	-0.33	17 (1%)	75	79	9, 16, 29, 62	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	ASN	9.0
1	B	346	ALA	5.8
1	B	344	ALA	4.6
1	C	28	ALA	4.4
1	B	343	LEU	3.8
1	C	341	ASP	3.7
1	B	345	ASN	3.5
1	C	29	THR	3.4
1	B	347	GLU	3.1
1	C	342	LEU	3.1
1	A	28	ALA	3.0
1	A	351	PHE	2.9
1	D	327	ARG	2.7
1	B	62	ASP	2.6
1	D	329	TRP	2.2
1	D	255	LEU	2.1
1	A	29	THR	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 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, 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
4	SO4	A	404	5/5	0.92	0.28	38,39,40,40	0
3	DAL	B	403	6/6	0.96	0.11	9,11,12,12	0
3	DAL	B	402	5/6	0.97	0.12	9,9,11,11	0
3	DAL	D	403	6/6	0.98	0.08	10,10,11,12	0
3	DAL	A	403	6/6	0.98	0.10	8,11,12,12	0
2	CL	C	401	1/1	0.99	0.05	13,13,13,13	0
2	CL	D	401	1/1	0.99	0.07	13,13,13,13	0
3	DAL	C	402	5/6	0.99	0.10	9,10,11,12	0
3	DAL	C	403	6/6	0.99	0.11	9,10,11,12	0
3	DAL	D	402	5/6	0.99	0.11	9,9,10,11	0
3	DAL	A	402	5/6	0.99	0.14	10,10,11,13	0
2	CL	B	401	1/1	0.99	0.06	12,12,12,12	0
2	CL	A	401	1/1	1.00	0.05	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.