Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 03:15 AM EDT

PDB ID	:	4OA4
Title	:	CRYSTAL STRUCTURE OF A TRAP PERIPLASMIC SOLUTE BINDING PROTEIN FROM SHEWANELLA LOIHICA PV-4 (Shew_1446), TARGET EFI-510273, WITH BOUND SUCCINATE
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	:	2014-01-03
Resolution	:	1.60 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:

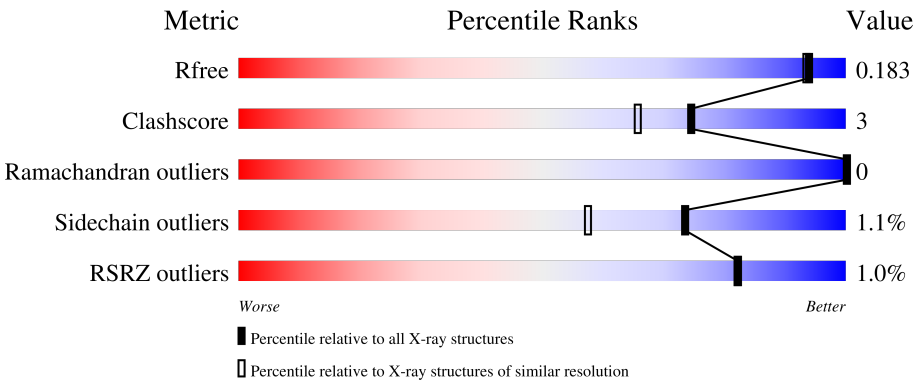
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	328	% 85% 6% • 7%
1	B	328	2% 89% • 7%
1	C	328	% 87% 6% 7%

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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	328	86% 6% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21629 atoms, of which 9782 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	304	4877	1555	2440	415	460	7	0	6	0
1	B	305	4914	1565	2457	417	468	7	0	11	0
1	C	305	4879	1556	2442	411	463	7	0	8	0
1	D	303	4856	1551	2427	410	461	7	0	10	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MSE	-	EXPRESSION TAG	UNP A3QCW5
A	10	HIS	-	EXPRESSION TAG	UNP A3QCW5
A	11	HIS	-	EXPRESSION TAG	UNP A3QCW5
A	12	HIS	-	EXPRESSION TAG	UNP A3QCW5
A	13	HIS	-	EXPRESSION TAG	UNP A3QCW5
A	14	HIS	-	EXPRESSION TAG	UNP A3QCW5
A	15	HIS	-	EXPRESSION TAG	UNP A3QCW5
A	16	SER	-	EXPRESSION TAG	UNP A3QCW5
A	17	SER	-	EXPRESSION TAG	UNP A3QCW5
A	18	GLY	-	EXPRESSION TAG	UNP A3QCW5
A	19	VAL	-	EXPRESSION TAG	UNP A3QCW5
A	20	ASP	-	EXPRESSION TAG	UNP A3QCW5
A	21	LEU	-	EXPRESSION TAG	UNP A3QCW5
A	22	GLY	-	EXPRESSION TAG	UNP A3QCW5
A	23	THR	-	EXPRESSION TAG	UNP A3QCW5
A	24	GLU	-	EXPRESSION TAG	UNP A3QCW5
A	25	ASN	-	EXPRESSION TAG	UNP A3QCW5
A	26	LEU	-	EXPRESSION TAG	UNP A3QCW5
A	27	TYR	-	EXPRESSION TAG	UNP A3QCW5
A	28	PHE	-	EXPRESSION TAG	UNP A3QCW5
A	29	GLN	-	EXPRESSION TAG	UNP A3QCW5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	30	SER	-	EXPRESSION TAG	UNP A3QCW5
A	31	MSE	-	EXPRESSION TAG	UNP A3QCW5
B	9	MSE	-	EXPRESSION TAG	UNP A3QCW5
B	10	HIS	-	EXPRESSION TAG	UNP A3QCW5
B	11	HIS	-	EXPRESSION TAG	UNP A3QCW5
B	12	HIS	-	EXPRESSION TAG	UNP A3QCW5
B	13	HIS	-	EXPRESSION TAG	UNP A3QCW5
B	14	HIS	-	EXPRESSION TAG	UNP A3QCW5
B	15	HIS	-	EXPRESSION TAG	UNP A3QCW5
B	16	SER	-	EXPRESSION TAG	UNP A3QCW5
B	17	SER	-	EXPRESSION TAG	UNP A3QCW5
B	18	GLY	-	EXPRESSION TAG	UNP A3QCW5
B	19	VAL	-	EXPRESSION TAG	UNP A3QCW5
B	20	ASP	-	EXPRESSION TAG	UNP A3QCW5
B	21	LEU	-	EXPRESSION TAG	UNP A3QCW5
B	22	GLY	-	EXPRESSION TAG	UNP A3QCW5
B	23	THR	-	EXPRESSION TAG	UNP A3QCW5
B	24	GLU	-	EXPRESSION TAG	UNP A3QCW5
B	25	ASN	-	EXPRESSION TAG	UNP A3QCW5
B	26	LEU	-	EXPRESSION TAG	UNP A3QCW5
B	27	TYR	-	EXPRESSION TAG	UNP A3QCW5
B	28	PHE	-	EXPRESSION TAG	UNP A3QCW5
B	29	GLN	-	EXPRESSION TAG	UNP A3QCW5
B	30	SER	-	EXPRESSION TAG	UNP A3QCW5
B	31	MSE	-	EXPRESSION TAG	UNP A3QCW5
C	9	MSE	-	EXPRESSION TAG	UNP A3QCW5
C	10	HIS	-	EXPRESSION TAG	UNP A3QCW5
C	11	HIS	-	EXPRESSION TAG	UNP A3QCW5
C	12	HIS	-	EXPRESSION TAG	UNP A3QCW5
C	13	HIS	-	EXPRESSION TAG	UNP A3QCW5
C	14	HIS	-	EXPRESSION TAG	UNP A3QCW5
C	15	HIS	-	EXPRESSION TAG	UNP A3QCW5
C	16	SER	-	EXPRESSION TAG	UNP A3QCW5
C	17	SER	-	EXPRESSION TAG	UNP A3QCW5
C	18	GLY	-	EXPRESSION TAG	UNP A3QCW5
C	19	VAL	-	EXPRESSION TAG	UNP A3QCW5
C	20	ASP	-	EXPRESSION TAG	UNP A3QCW5
C	21	LEU	-	EXPRESSION TAG	UNP A3QCW5
C	22	GLY	-	EXPRESSION TAG	UNP A3QCW5
C	23	THR	-	EXPRESSION TAG	UNP A3QCW5
C	24	GLU	-	EXPRESSION TAG	UNP A3QCW5
C	25	ASN	-	EXPRESSION TAG	UNP A3QCW5

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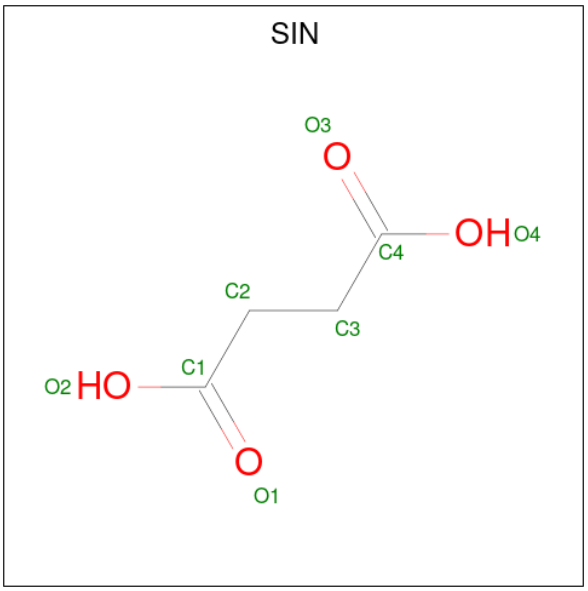
Chain	Residue	Modelled	Actual	Comment	Reference
C	26	LEU	-	EXPRESSION TAG	UNP A3QCW5
C	27	TYR	-	EXPRESSION TAG	UNP A3QCW5
C	28	PHE	-	EXPRESSION TAG	UNP A3QCW5
C	29	GLN	-	EXPRESSION TAG	UNP A3QCW5
C	30	SER	-	EXPRESSION TAG	UNP A3QCW5
C	31	MSE	-	EXPRESSION TAG	UNP A3QCW5
D	9	MSE	-	EXPRESSION TAG	UNP A3QCW5
D	10	HIS	-	EXPRESSION TAG	UNP A3QCW5
D	11	HIS	-	EXPRESSION TAG	UNP A3QCW5
D	12	HIS	-	EXPRESSION TAG	UNP A3QCW5
D	13	HIS	-	EXPRESSION TAG	UNP A3QCW5
D	14	HIS	-	EXPRESSION TAG	UNP A3QCW5
D	15	HIS	-	EXPRESSION TAG	UNP A3QCW5
D	16	SER	-	EXPRESSION TAG	UNP A3QCW5
D	17	SER	-	EXPRESSION TAG	UNP A3QCW5
D	18	GLY	-	EXPRESSION TAG	UNP A3QCW5
D	19	VAL	-	EXPRESSION TAG	UNP A3QCW5
D	20	ASP	-	EXPRESSION TAG	UNP A3QCW5
D	21	LEU	-	EXPRESSION TAG	UNP A3QCW5
D	22	GLY	-	EXPRESSION TAG	UNP A3QCW5
D	23	THR	-	EXPRESSION TAG	UNP A3QCW5
D	24	GLU	-	EXPRESSION TAG	UNP A3QCW5
D	25	ASN	-	EXPRESSION TAG	UNP A3QCW5
D	26	LEU	-	EXPRESSION TAG	UNP A3QCW5
D	27	TYR	-	EXPRESSION TAG	UNP A3QCW5
D	28	PHE	-	EXPRESSION TAG	UNP A3QCW5
D	29	GLN	-	EXPRESSION TAG	UNP A3QCW5
D	30	SER	-	EXPRESSION TAG	UNP A3QCW5
D	31	MSE	-	EXPRESSION TAG	UNP A3QCW5

- Molecule 2 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	12	4	4	4	0	0
2	B	1	12	4	4	4	0	0
2	C	1	12	4	4	4	0	0
2	D	1	12	4	4	4	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	3	3	3	0	0
3	B	2	2	2	0	0
3	C	2	2	2	0	0
3	D	2	2	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	508	508	508	0	0

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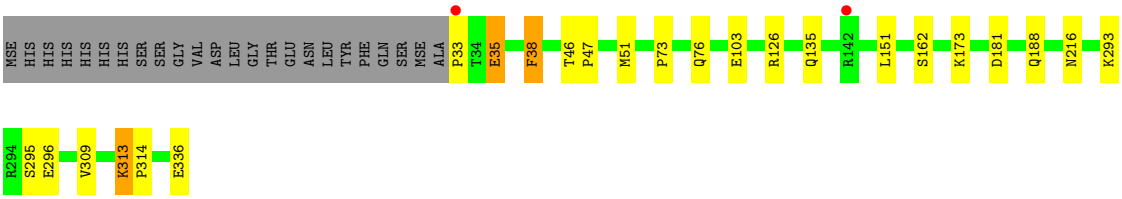
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	502	502	502	0	0
			Total	O		
4	C	496	496	496	0	0
			Total	O		
4	D	540	540	540	0	0

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.

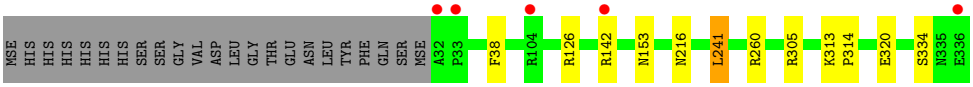
• Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain A:



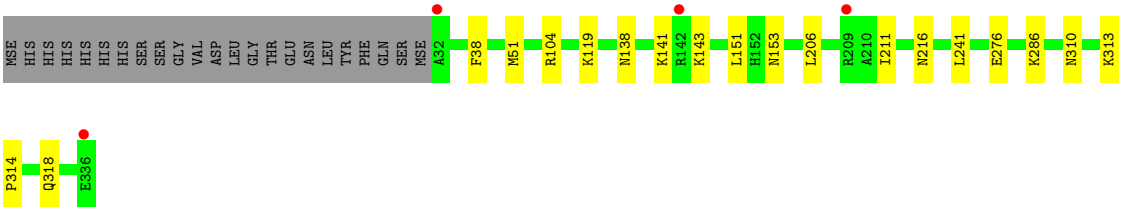
• Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain B:



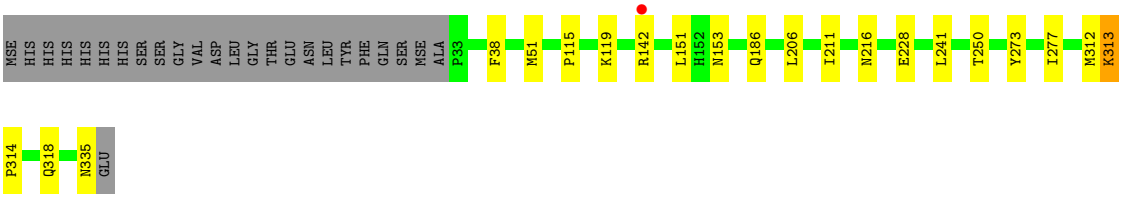
• Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain C:



• Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.22Å 117.95Å 89.43Å 90.00° 93.00° 90.00°	Depositor
Resolution (Å)	25.22 – 1.60 25.22 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (25.22-1.60) 99.5 (25.22-1.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.154 , 0.182 0.156 , 0.183	Depositor DCC
R_{free} test set	10901 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	15.3	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 55.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	21629	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: CL, SIN

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	0.52	0/2502	0.59	0/3369
1	B	0.46	0/2532	0.60	1/3410 (0.0%)
1	C	0.47	0/2512	0.58	0/3385
1	D	0.51	0/2517	0.62	0/3390
All	All	0.49	0/10063	0.60	1/13554 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	260	ARG	NE-CZ-NH2	-5.37	117.61	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	2437	2440	2417	19	0
1	B	2457	2457	2420	9	0
1	C	2437	2442	2413	16	0
1	D	2429	2427	2390	19	0
2	A	8	4	4	0	0
2	B	8	4	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	8	4	4	0	0
2	D	8	4	4	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	508	0	0	8	1
4	B	502	0	0	4	1
4	C	496	0	0	8	1
4	D	540	0	0	4	1
All	All	11847	9782	9656	62	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 3.

All (62) 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:D:186:GLN:HG3	1:D:312:MSE:SE	2.15	0.96
1:C:119:LYS:NZ	4:C:950:HOH:O	1.97	0.95
1:D:115:PRO:HB3	1:D:312:MSE:SE	2.16	0.94
1:D:115:PRO:HG2	1:D:312:MSE:HG2	1.62	0.79
1:B:126:ARG:NH2	1:B:334[A]:SER:O	2.22	0.72
1:C:143:LYS:NZ	4:C:613:HOH:O	2.14	0.72
1:B:126:ARG:NH2	1:B:334[B]:SER:O	2.22	0.72
1:D:228:GLU:OE1	4:D:857:HOH:O	2.07	0.71
1:D:115:PRO:CB	1:D:312:MSE:SE	2.88	0.71
1:A:313:LYS:N	1:A:314:PRO:HD2	2.06	0.71
1:C:310:ASN:OD1	4:C:958:HOH:O	2.08	0.71
1:D:115:PRO:CG	1:D:312:MSE:HG2	2.21	0.70
1:A:126[B]:ARG:NH2	4:A:649:HOH:O	2.18	0.69
1:A:295:SER:O	4:A:729:HOH:O	2.13	0.66
1:A:162:SER:OG	1:A:173:LYS:HE2	1.98	0.63
1:D:119:LYS:H	1:D:335:ASN:HD21	1.48	0.61
1:C:286:LYS:NZ	4:C:782:HOH:O	2.32	0.61
1:D:206:LEU:HD23	1:D:211:ILE:HG13	1.83	0.60
1:D:318:GLN:OE1	4:D:810:HOH:O	2.16	0.60
1:B:305[B]:ARG:NH2	4:B:715:HOH:O	2.34	0.59
1:B:313:LYS:N	1:B:314:PRO:CD	2.69	0.55
1:A:296:GLU:HG2	4:A:1000:HOH:O	2.07	0.55
1:D:186:GLN:CG	1:D:312:MSE:SE	3.00	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLU:CB	1:C:104:ARG:HH12	2.21	0.54
1:C:38:PHE:CZ	1:C:51:MSE:HE1	2.43	0.54
1:D:119:LYS:H	1:D:335:ASN:ND2	2.05	0.54
1:A:135[B]:GLN:HG2	4:A:759:HOH:O	2.10	0.52
1:B:305[B]:ARG:HD2	4:B:643:HOH:O	2.09	0.51
1:D:273:TYR:CE2	1:D:277:ILE:HD11	2.46	0.51
1:A:33:PRO:O	4:A:892:HOH:O	2.20	0.49
1:A:126[B]:ARG:NH1	1:A:336:GLU:O	2.46	0.49
1:A:313:LYS:N	1:A:314:PRO:CD	2.75	0.49
1:B:142:ARG:HB2	4:B:769:HOH:O	2.13	0.48
1:B:320:GLU:OE1	4:B:809:HOH:O	2.20	0.48
1:C:51:MSE:HE2	1:C:151:LEU:HD22	1.97	0.47
1:C:119:LYS:HD3	4:C:912:HOH:O	2.15	0.47
1:C:313:LYS:N	1:C:314:PRO:CD	2.78	0.47
1:D:250[B]:THR:HG23	4:D:559:HOH:O	2.13	0.47
1:D:313:LYS:N	1:D:314:PRO:CD	2.78	0.47
1:D:115:PRO:CG	1:D:312:MSE:CG	2.93	0.47
1:A:38:PHE:CZ	1:A:51:MSE:HE1	2.50	0.46
1:D:115:PRO:CB	1:D:312:MSE:HG2	2.45	0.46
1:C:318:GLN:OE1	4:C:712:HOH:O	2.21	0.46
1:A:309:VAL:O	1:A:313:LYS:HB2	2.15	0.46
1:C:206:LEU:HD23	1:C:211[B]:ILE:HG13	1.97	0.45
1:D:142:ARG:NH2	4:D:863:HOH:O	2.48	0.45
1:A:73:PRO:O	1:A:76[A]:GLN:HG2	2.18	0.44
1:C:138:ASN:O	1:C:141:LYS:HG2	2.18	0.44
1:A:46:THR:HB	1:A:47:PRO:HD2	2.00	0.43
1:B:241:LEU:HD21	2:B:401:SIN:H31	2.01	0.43
1:B:153:ASN:HB3	1:B:241:LEU:O	2.19	0.43
1:D:51:MSE:HE2	1:D:151:LEU:HD22	2.01	0.43
1:C:276:GLU:OE1	4:C:873:HOH:O	2.22	0.42
1:A:188:GLN:HG2	4:A:844:HOH:O	2.20	0.42
1:C:313:LYS:N	1:C:314:PRO:HD2	2.36	0.41
1:A:35:GLU:HG2	4:A:802:HOH:O	2.21	0.41
1:A:103:GLU:OE2	1:A:181:ASP:OD2	2.39	0.41
1:A:51:MSE:HE2	1:A:151:LEU:HD22	2.03	0.41
1:A:293:LYS:HE3	4:A:949:HOH:O	2.20	0.41
1:C:276:GLU:HB2	4:C:873:HOH:O	2.21	0.41
1:D:153:ASN:HB3	1:D:241:LEU:O	2.20	0.40
1:C:153:ASN:HB3	1:C:241:LEU:O	2.21	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)
4:A:748:HOH:O	4:C:607:HOH:O[2_757]	2.06	0.14
4:B:814:HOH:O	4:D:859:HOH:O[2_656]	2.11	0.09

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	308/328 (94%)	303 (98%)	5 (2%)	0	100	100
1	B	314/328 (96%)	310 (99%)	4 (1%)	0	100	100
1	C	311/328 (95%)	306 (98%)	5 (2%)	0	100	100
1	D	311/328 (95%)	307 (99%)	4 (1%)	0	100	100
All	All	1244/1312 (95%)	1226 (99%)	18 (1%)	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	266/274 (97%)	262 (98%)	4 (2%)	65	44
1	B	269/274 (98%)	266 (99%)	3 (1%)	73	57
1	C	268/274 (98%)	267 (100%)	1 (0%)	91	84
1	D	269/274 (98%)	266 (99%)	3 (1%)	73	57
All	All	1072/1096 (98%)	1061 (99%)	11 (1%)	73	61

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	38	PHE
1	A	216	ASN
1	A	313	LYS
1	B	38	PHE
1	B	216	ASN
1	B	241	LEU
1	C	216	ASN
1	D	38	PHE
1	D	216	ASN
1	D	313	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	318	GLN
1	D	249	ASN
1	D	318	GLN
1	D	335	ASN

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, 9 are monoatomic - leaving 4 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	SIN	A	401	-	7,7,7	1.05	0	8,8,8	1.69	2 (25%)
2	SIN	C	401	-	7,7,7	1.22	0	8,8,8	1.50	1 (12%)
2	SIN	D	401	-	7,7,7	0.96	0	8,8,8	1.49	2 (25%)
2	SIN	B	401	-	7,7,7	0.93	0	8,8,8	1.65	2 (25%)

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
2	SIN	A	401	-	-	4/5/5/5	-
2	SIN	C	401	-	-	4/5/5/5	-
2	SIN	D	401	-	-	4/5/5/5	-
2	SIN	B	401	-	-	4/5/5/5	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	SIN	O4-C4-C3	2.88	123.11	114.00
2	D	401	SIN	C3-C2-C1	-2.56	106.86	113.67
2	B	401	SIN	O2-C1-C2	2.31	121.31	114.00
2	C	401	SIN	C2-C3-C4	-2.24	107.73	113.67
2	B	401	SIN	O4-C4-C3	2.07	120.55	114.00
2	D	401	SIN	O4-C4-C3	2.03	120.43	114.00
2	A	401	SIN	C3-C2-C1	-2.01	108.33	113.67

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	SIN	C2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
2	A	401	SIN	O1-C1-C2-C3
2	B	401	SIN	C2-C3-C4-O3
2	D	401	SIN	C2-C3-C4-O3
2	C	401	SIN	C2-C3-C4-O4
2	A	401	SIN	C2-C3-C4-O4
2	A	401	SIN	O2-C1-C2-C3
2	B	401	SIN	C2-C3-C4-O4
2	C	401	SIN	O2-C1-C2-C3
2	D	401	SIN	O2-C1-C2-C3
2	D	401	SIN	C2-C3-C4-O4
2	B	401	SIN	O2-C1-C2-C3
2	C	401	SIN	O1-C1-C2-C3
2	D	401	SIN	O1-C1-C2-C3
2	B	401	SIN	O1-C1-C2-C3
2	C	401	SIN	C2-C3-C4-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	SIN	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	297/328 (90%)	-0.53	2 (0%)	87	87	8, 14, 29, 40	0
1	B	298/328 (90%)	-0.42	5 (1%)	70	69	10, 17, 29, 44	0
1	C	298/328 (90%)	-0.39	4 (1%)	77	77	10, 18, 31, 40	0
1	D	296/328 (90%)	-0.54	1 (0%)	94	93	9, 15, 29, 38	0
All	All	1189/1312 (90%)	-0.47	12 (1%)	82	82	8, 16, 29, 44	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	32	ALA	6.2
1	B	32	ALA	4.8
1	D	142	ARG	2.7
1	A	142	ARG	2.7
1	B	142	ARG	2.6
1	B	104	ARG	2.4
1	B	336	GLU	2.4
1	C	336	GLU	2.3
1	B	33	PRO	2.3
1	C	142	ARG	2.2
1	C	209	ARG	2.1
1	A	33	PRO	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SIN	C	401	8/8	0.97	0.08	10,12,14,14	0
2	SIN	B	401	8/8	0.98	0.09	9,11,13,13	0
2	SIN	A	401	8/8	0.98	0.09	7,9,10,10	0
2	SIN	D	401	8/8	0.99	0.09	8,10,12,12	0
3	CL	A	403	1/1	0.99	0.04	18,18,18,18	0
3	CL	B	402	1/1	0.99	0.05	15,15,15,15	0
3	CL	C	403	1/1	0.99	0.06	16,16,16,16	0
3	CL	D	403	1/1	0.99	0.05	15,15,15,15	0
3	CL	B	403	1/1	1.00	0.03	16,16,16,16	0
3	CL	C	402	1/1	1.00	0.03	20,20,20,20	0
3	CL	A	404	1/1	1.00	0.10	16,16,16,16	0
3	CL	D	402	1/1	1.00	0.03	17,17,17,17	0
3	CL	A	402	1/1	1.00	0.05	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.