Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2020 – 06:20 AM BST

PDB ID	:	4XEQ
Title	:	CRYSTAL STRUCTURE OF A TRAP PERIPLASMIC SOLUTE BINDING PROTEIN FROM DESULFOVIBRIO VULGARIS (Deval_0042, TARGET EFI-510114) BOUND TO COPURIFIED (R)-PANTOIC ACID
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Deposited on	:	2014-12-24
Resolution	:	1.70 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 following versions of software and data (see references (1)) were used in the production of this report:

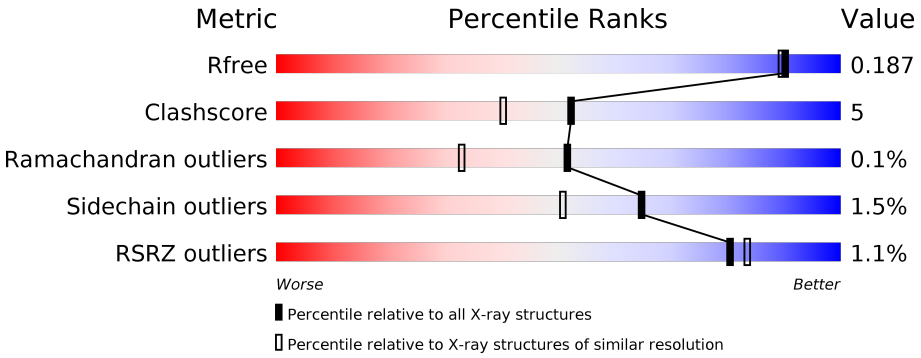
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance

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

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 on 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	82% 11% 8%
1	B	328	79% 13% • 7%
1	C	328	2% 80% 12% 8%
1	D	328	2% 81% 11% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19785 atoms, of which 9494 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
1	A	303	Total	C	H	N	O	S	Se	0	0	0
			4762	1502	2376	432	442	2	8			
1	B	304	Total	C	H	N	O	S	Se	0	0	0
			4772	1505	2381	433	443	2	8			
1	C	302	Total	C	H	N	O	S	Se	0	0	0
			4737	1496	2360	430	441	2	8			
1	D	302	Total	C	H	N	O	S	Se	0	2	0
			4764	1502	2377	432	443	2	8			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MSE	-	initiating methionine	UNP E3ILJ0
A	15	HIS	-	expression tag	UNP E3ILJ0
A	16	HIS	-	expression tag	UNP E3ILJ0
A	17	HIS	-	expression tag	UNP E3ILJ0
A	18	HIS	-	expression tag	UNP E3ILJ0
A	19	HIS	-	expression tag	UNP E3ILJ0
A	20	HIS	-	expression tag	UNP E3ILJ0
A	21	SER	-	expression tag	UNP E3ILJ0
A	22	SER	-	expression tag	UNP E3ILJ0
A	23	GLY	-	expression tag	UNP E3ILJ0
A	24	VAL	-	expression tag	UNP E3ILJ0
A	25	ASP	-	expression tag	UNP E3ILJ0
A	26	LEU	-	expression tag	UNP E3ILJ0
A	27	GLY	-	expression tag	UNP E3ILJ0
A	28	THR	-	expression tag	UNP E3ILJ0
A	29	GLU	-	expression tag	UNP E3ILJ0
A	30	ASN	-	expression tag	UNP E3ILJ0
A	31	LEU	-	expression tag	UNP E3ILJ0
A	32	TYR	-	expression tag	UNP E3ILJ0
A	33	PHE	-	expression tag	UNP E3ILJ0
A	34	GLN	-	expression tag	UNP E3ILJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	35	SER	-	expression tag	UNP E3ILJ0
A	36	MSE	-	expression tag	UNP E3ILJ0
B	14	MSE	-	initiating methionine	UNP E3ILJ0
B	15	HIS	-	expression tag	UNP E3ILJ0
B	16	HIS	-	expression tag	UNP E3ILJ0
B	17	HIS	-	expression tag	UNP E3ILJ0
B	18	HIS	-	expression tag	UNP E3ILJ0
B	19	HIS	-	expression tag	UNP E3ILJ0
B	20	HIS	-	expression tag	UNP E3ILJ0
B	21	SER	-	expression tag	UNP E3ILJ0
B	22	SER	-	expression tag	UNP E3ILJ0
B	23	GLY	-	expression tag	UNP E3ILJ0
B	24	VAL	-	expression tag	UNP E3ILJ0
B	25	ASP	-	expression tag	UNP E3ILJ0
B	26	LEU	-	expression tag	UNP E3ILJ0
B	27	GLY	-	expression tag	UNP E3ILJ0
B	28	THR	-	expression tag	UNP E3ILJ0
B	29	GLU	-	expression tag	UNP E3ILJ0
B	30	ASN	-	expression tag	UNP E3ILJ0
B	31	LEU	-	expression tag	UNP E3ILJ0
B	32	TYR	-	expression tag	UNP E3ILJ0
B	33	PHE	-	expression tag	UNP E3ILJ0
B	34	GLN	-	expression tag	UNP E3ILJ0
B	35	SER	-	expression tag	UNP E3ILJ0
B	36	MSE	-	expression tag	UNP E3ILJ0
C	14	MSE	-	initiating methionine	UNP E3ILJ0
C	15	HIS	-	expression tag	UNP E3ILJ0
C	16	HIS	-	expression tag	UNP E3ILJ0
C	17	HIS	-	expression tag	UNP E3ILJ0
C	18	HIS	-	expression tag	UNP E3ILJ0
C	19	HIS	-	expression tag	UNP E3ILJ0
C	20	HIS	-	expression tag	UNP E3ILJ0
C	21	SER	-	expression tag	UNP E3ILJ0
C	22	SER	-	expression tag	UNP E3ILJ0
C	23	GLY	-	expression tag	UNP E3ILJ0
C	24	VAL	-	expression tag	UNP E3ILJ0
C	25	ASP	-	expression tag	UNP E3ILJ0
C	26	LEU	-	expression tag	UNP E3ILJ0
C	27	GLY	-	expression tag	UNP E3ILJ0
C	28	THR	-	expression tag	UNP E3ILJ0
C	29	GLU	-	expression tag	UNP E3ILJ0
C	30	ASN	-	expression tag	UNP E3ILJ0

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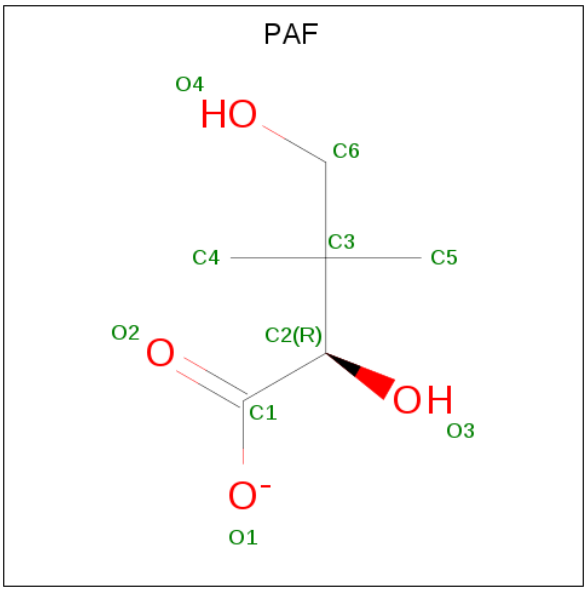
Chain	Residue	Modelled	Actual	Comment	Reference
C	31	LEU	-	expression tag	UNP E3ILJ0
C	32	TYR	-	expression tag	UNP E3ILJ0
C	33	PHE	-	expression tag	UNP E3ILJ0
C	34	GLN	-	expression tag	UNP E3ILJ0
C	35	SER	-	expression tag	UNP E3ILJ0
C	36	MSE	-	expression tag	UNP E3ILJ0
D	14	MSE	-	initiating methionine	UNP E3ILJ0
D	15	HIS	-	expression tag	UNP E3ILJ0
D	16	HIS	-	expression tag	UNP E3ILJ0
D	17	HIS	-	expression tag	UNP E3ILJ0
D	18	HIS	-	expression tag	UNP E3ILJ0
D	19	HIS	-	expression tag	UNP E3ILJ0
D	20	HIS	-	expression tag	UNP E3ILJ0
D	21	SER	-	expression tag	UNP E3ILJ0
D	22	SER	-	expression tag	UNP E3ILJ0
D	23	GLY	-	expression tag	UNP E3ILJ0
D	24	VAL	-	expression tag	UNP E3ILJ0
D	25	ASP	-	expression tag	UNP E3ILJ0
D	26	LEU	-	expression tag	UNP E3ILJ0
D	27	GLY	-	expression tag	UNP E3ILJ0
D	28	THR	-	expression tag	UNP E3ILJ0
D	29	GLU	-	expression tag	UNP E3ILJ0
D	30	ASN	-	expression tag	UNP E3ILJ0
D	31	LEU	-	expression tag	UNP E3ILJ0
D	32	TYR	-	expression tag	UNP E3ILJ0
D	33	PHE	-	expression tag	UNP E3ILJ0
D	34	GLN	-	expression tag	UNP E3ILJ0
D	35	SER	-	expression tag	UNP E3ILJ0
D	36	MSE	-	expression tag	UNP E3ILJ0

- Molecule 2 is PANTOATE (three-letter code: PAF) (formula: $C_6H_{11}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 6 4	0	0
2	B	1	Total C O 10 6 4	0	0
2	C	1	Total C O 10 6 4	0	0
2	D	1	Total C O 10 6 4	0	0

- Molecule 3 is water.

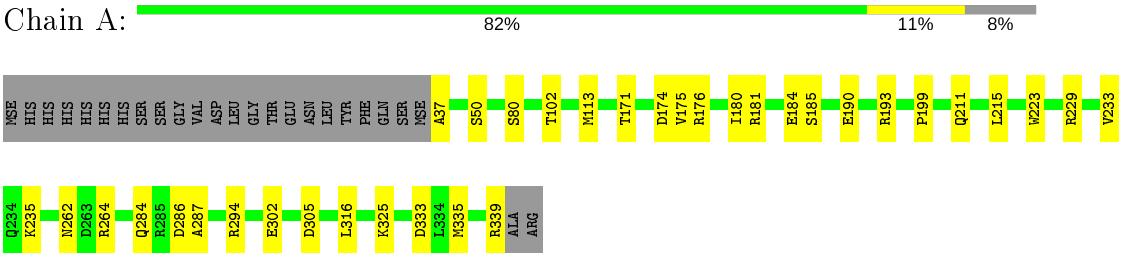
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	225	Total O 225 225	0	0
3	B	192	Total O 192 192	0	0
3	C	156	Total O 156 156	0	0
3	D	137	Total O 137 137	0	0

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.

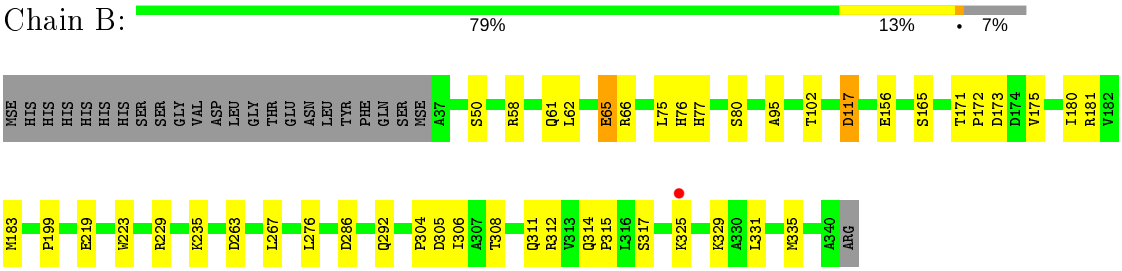
- Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain A:



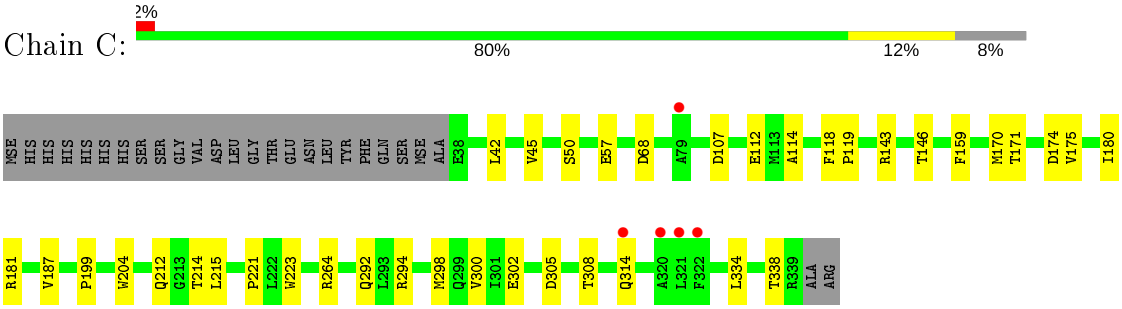
- Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain B:



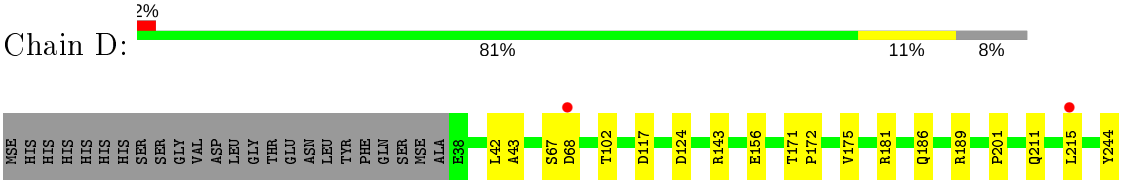
- Molecule 1: TRAP dicarboxylate transporter, DctP subunit

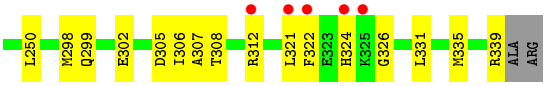
Chain C:



- Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain D:




L250
M298
Q299
E302
D305
I306
A307
T308
R312
L321
F322
E323
H324
K325
G326
L331
M335
R339
ALA
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.75Å 73.60Å 100.21Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	25.25 – 1.70 25.25 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (25.25-1.70) 98.2 (25.25-1.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.157 , 0.185 0.159 , 0.187	Depositor DCC
R_{free} test set	6655 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	17.2	Xtriage
Anisotropy	0.629	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 28.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.386 for h,-k,-l	Xtriage
Reported twinning fraction	0.400 for h,-k,-l	Depositor
Outliers	1 of 131825 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	19785	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.2594e-03.*

[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: PAF

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	0.61	0/2428	0.72	1/3286 (0.0%)
1	B	0.61	0/2433	0.72	0/3293
1	C	0.58	0/2419	0.69	1/3275 (0.0%)
1	D	0.57	0/2436	0.67	0/3297
All	All	0.59	0/9716	0.70	2/13151 (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	264	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	C	264	ARG	NE-CZ-NH1	5.89	123.25	120.30

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	2386	2376	2367	23	2
1	B	2391	2381	2372	31	1
1	C	2377	2360	2351	25	1
1	D	2387	2377	2360	25	0
2	A	10	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	11	0	0
2	C	10	0	11	0	0
2	D	10	0	11	0	0
3	A	225	0	0	14	2
3	B	192	0	0	8	2
3	C	156	0	0	6	1
3	D	137	0	0	6	1
All	All	10291	9494	9494	104	5

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 5.

All (104) 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:294:ARG:NH2	1:A:302:GLU:OE1	1.78	1.15
1:A:339:ARG:NH1	3:A:693:HOH:O	2.02	0.93
1:A:284:GLN:OE1	3:A:699:HOH:O	1.93	0.86
1:C:314:GLN:OE1	3:C:626:HOH:O	1.99	0.81
1:B:95:ALA:O	3:B:595:HOH:O	2.00	0.80
1:C:212:GLN:OE1	3:C:501:HOH:O	2.03	0.76
1:A:174:ASP:OD1	3:A:501:HOH:O	2.06	0.72
1:A:181:ARG:HB2	1:A:215:LEU:HD13	1.75	0.69
1:B:286:ASP:OD1	3:B:558:HOH:O	2.12	0.68
1:C:292:GLN:OE1	3:C:577:HOH:O	2.12	0.67
1:A:113:MSE:O	3:A:665:HOH:O	2.13	0.66
1:A:184:GLU:OE2	3:A:502:HOH:O	2.13	0.64
1:D:172:PRO:HG2	1:D:312:ARG:HG3	1.83	0.61
1:A:262:ASN:ND2	3:A:661:HOH:O	2.30	0.60
1:A:211:GLN:HB2	1:A:233:VAL:HG11	1.84	0.60
1:A:37:ALA:N	3:A:707:HOH:O	2.34	0.60
1:B:311:GLN:O	1:B:314:GLN:HG2	2.01	0.60
1:D:189:ARG:NH1	1:D:201:PRO:HD3	2.17	0.60
1:D:181:ARG:HB2	1:D:215:LEU:HD13	1.83	0.59
1:C:214:THR:O	1:C:215:LEU:HD23	2.03	0.58
1:A:171:THR:HG22	1:A:305:ASP:HB3	1.87	0.56
1:D:67:SER:O	1:D:68:ASP:HB2	2.05	0.56
1:C:107:ASP:OD1	3:C:561:HOH:O	2.18	0.56
1:D:339:ARG:NE	3:D:581:HOH:O	2.40	0.55
1:B:325:LYS:O	1:B:329:LYS:HG3	2.06	0.54
1:B:172:PRO:HD2	1:B:308:THR:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:LEU:HD11	1:D:335:MSE:HE3	1.89	0.54
1:B:325:LYS:HG2	1:B:329:LYS:HD2	1.90	0.53
1:D:156:GLU:OE1	1:D:244:TYR:OH	2.18	0.53
1:B:77:HIS:O	1:B:80:SER:OG	2.19	0.53
1:B:305:ASP:OD2	1:B:308:THR:OG1	2.20	0.53
1:B:235:LYS:HG3	3:B:686:HOH:O	2.08	0.52
1:B:117:ASP:OD1	3:B:654:HOH:O	2.19	0.52
1:D:186:GLN:NE2	1:D:321:LEU:HB2	2.25	0.52
1:D:171:THR:HB	1:D:172:PRO:HD2	1.92	0.52
1:D:339:ARG:HG3	3:D:581:HOH:O	2.09	0.51
1:C:42:LEU:C	1:C:42:LEU:HD23	2.31	0.51
1:D:322:PHE:CE1	1:D:331:LEU:HD22	2.44	0.51
1:A:171:THR:HG22	1:A:305:ASP:CB	2.40	0.51
1:C:204:TRP:O	3:C:580:HOH:O	2.20	0.50
1:D:299:GLN:OE1	3:D:501:HOH:O	2.19	0.50
1:B:180:ILE:O	1:B:199:PRO:HA	2.12	0.50
1:D:305:ASP:OD2	1:D:308:THR:OG1	2.16	0.50
1:A:80:SER:HB2	3:A:638:HOH:O	2.14	0.48
1:A:50:SER:HB2	1:A:223:TRP:CZ3	2.48	0.48
1:B:314:GLN:CG	1:B:315:PRO:HD3	2.44	0.47
1:C:57:GLU:HG3	3:C:511:HOH:O	2.13	0.47
1:A:185:SER:HA	3:A:579:HOH:O	2.13	0.47
1:B:172:PRO:HG2	1:B:308:THR:HG22	1.97	0.47
1:C:181:ARG:HD3	1:C:181:ARG:C	2.35	0.47
1:C:305:ASP:OD2	1:C:308:THR:OG1	2.24	0.47
1:B:331:LEU:O	1:B:335:MSE:HG3	2.14	0.47
1:C:171:THR:HG22	1:C:305:ASP:HB3	1.96	0.47
1:A:80:SER:CB	3:A:638:HOH:O	2.62	0.46
1:B:62:LEU:O	1:B:66:ARG:HG3	2.14	0.46
1:D:171:THR:HG22	1:D:305:ASP:HB3	1.97	0.46
1:A:287:ALA:HB3	3:A:624:HOH:O	2.16	0.46
3:A:683:HOH:O	1:C:146:THR:HG22	2.15	0.46
1:B:314:GLN:HG3	1:B:315:PRO:HD3	1.97	0.46
1:B:58:ARG:NH1	1:B:61:GLN:OE1	2.47	0.46
1:B:62:LEU:O	1:B:65:GLU:HB2	2.16	0.46
1:C:112:GLU:OE2	1:C:143:ARG:HD2	2.16	0.45
1:A:193:ARG:HG3	1:A:199:PRO:HG3	1.99	0.45
1:A:180:ILE:O	1:A:199:PRO:HA	2.16	0.45
1:C:112:GLU:OE2	1:C:143:ARG:CD	2.65	0.45
1:D:298:MSE:HG2	3:D:595:HOH:O	2.17	0.45
1:C:334:LEU:O	1:C:338:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:PRO:O	1:B:175:VAL:HG22	2.17	0.44
1:C:50:SER:HB2	1:C:223:TRP:CH2	2.52	0.44
1:B:292:GLN:OE1	3:B:501:HOH:O	2.21	0.44
1:B:171:THR:HG22	1:B:305:ASP:HB3	1.99	0.44
1:C:171:THR:HG22	1:C:305:ASP:CB	2.48	0.44
1:C:50:SER:HB2	1:C:223:TRP:CZ3	2.52	0.44
1:D:324:HIS:CE1	1:D:326:GLY:H	2.35	0.44
1:B:304:PRO:O	1:B:306:ILE:N	2.51	0.44
1:A:325:LYS:HE2	3:A:519:HOH:O	2.18	0.43
1:B:172:PRO:HG2	1:B:312:ARG:HG3	1.99	0.43
1:D:42:LEU:HD23	1:D:43:ALA:N	2.33	0.43
1:C:118:PHE:CG	1:C:119:PRO:HD2	2.54	0.43
1:C:159:PHE:O	1:C:221:PRO:HA	2.18	0.43
1:D:339:ARG:CG	3:D:581:HOH:O	2.66	0.43
1:B:335:MSE:HE1	3:B:535:HOH:O	2.17	0.43
1:C:114:ALA:HB1	1:C:187:VAL:HB	2.00	0.43
1:A:335:MSE:HB3	1:A:339:ARG:HH12	1.83	0.43
1:D:124:ASP:HB2	3:D:570:HOH:O	2.19	0.43
1:B:165:SER:OG	3:B:557:HOH:O	2.14	0.43
1:C:294:ARG:NH2	1:C:302:GLU:OE1	2.48	0.43
1:B:75:LEU:HD12	1:B:76:HIS:N	2.34	0.42
1:D:306:ILE:O	1:D:307:ALA:C	2.55	0.42
1:B:263:ASP:O	1:B:267:LEU:HD13	2.19	0.42
1:C:300:VAL:HG12	1:C:302:GLU:HG3	2.01	0.42
1:B:102:THR:HG21	1:B:183:MSE:SE	2.70	0.41
1:D:211:GLN:O	1:D:211:GLN:HG2	2.19	0.41
1:C:170:MSE:HB2	1:C:174:ASP:OD2	2.20	0.41
1:D:181:ARG:C	1:D:181:ARG:HD3	2.40	0.41
1:D:172:PRO:O	1:D:175:VAL:HG22	2.21	0.41
1:C:180:ILE:O	1:C:199:PRO:HA	2.21	0.41
1:A:190:GLU:HG3	1:A:316:LEU:CD1	2.51	0.41
1:D:250:LEU:HD12	1:D:250:LEU:C	2.42	0.41
1:B:317:SER:O	3:B:582:HOH:O	2.22	0.40
1:B:50:SER:HB2	1:B:223:TRP:CH2	2.56	0.40
1:A:235:LYS:HE2	3:A:528:HOH:O	2.19	0.40
1:B:181:ARG:HD3	1:B:181:ARG:C	2.42	0.40

All (5) 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)
3:A:519:HOH:O	3:B:501:HOH:O[2_856]	1.85	0.35
3:B:534:HOH:O	3:D:525:HOH:O[2_747]	2.15	0.05
3:A:512:HOH:O	3:C:503:HOH:O[1_554]	2.16	0.04
1:A:333:ASP:OD1	1:B:229:ARG:HH12[2_856]	1.59	0.01
1:A:176:ARG:HH22	1:C:68:ASP:OD1[2_856]	1.60	0.00

5.3 Torsion angles

5.3.1 Protein backbone

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	301/328 (92%)	295 (98%)	6 (2%)	0	100 100
1	B	302/328 (92%)	297 (98%)	4 (1%)	1 (0%)	41 24
1	C	300/328 (92%)	292 (97%)	8 (3%)	0	100 100
1	D	302/328 (92%)	299 (99%)	3 (1%)	0	100 100
All	All	1205/1312 (92%)	1183 (98%)	21 (2%)	1 (0%)	51 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	65	GLU

5.3.2 Protein sidechains

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	252/264 (96%)	248 (98%)	4 (2%)	62 48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	252/264 (96%)	247 (98%)	5 (2%)	55 38
1	C	251/264 (95%)	248 (99%)	3 (1%)	71 59
1	D	254/264 (96%)	251 (99%)	3 (1%)	71 59
All	All	1009/1056 (96%)	994 (98%)	15 (2%)	65 51

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	THR
1	A	175	VAL
1	A	229	ARG
1	A	286	ASP
1	B	117	ASP
1	B	156	GLU
1	B	173	ASP
1	B	219	GLU
1	B	276	LEU
1	C	45	VAL
1	C	175	VAL
1	C	298	MSE
1	D	102	THR
1	D	117	ASP
1	D	302	GLU

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

Mol	Chain	Res	Type
1	C	212	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)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PAF	C	401	-	6,9,9	1.19	1 (16%)	7,13,13	1.23	1 (14%)
2	PAF	D	401	-	6,9,9	0.92	0	7,13,13	1.02	1 (14%)
2	PAF	A	401	-	6,9,9	0.36	0	7,13,13	1.03	0
2	PAF	B	401	-	6,9,9	0.77	0	7,13,13	0.93	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
2	PAF	C	401	-	-	0/9/13/13	-
2	PAF	D	401	-	-	0/9/13/13	-
2	PAF	A	401	-	-	0/9/13/13	-
2	PAF	B	401	-	-	0/9/13/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	PAF	C6-C3	-2.30	1.52	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	PAF	O4-C6-C3	-2.47	108.53	112.96
2	C	401	PAF	C4-C3-C2	2.04	112.35	108.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	295/328 (89%)	0.12	0 100 100	11, 16, 23, 28	0
1	B	296/328 (90%)	0.14	1 (0%) 94 94	12, 17, 25, 30	0
1	C	294/328 (89%)	0.19	5 (1%) 70 74	12, 18, 26, 32	0
1	D	294/328 (89%)	0.24	7 (2%) 59 63	14, 21, 28, 35	0
All	All	1179/1312 (89%)	0.17	13 (1%) 80 83	11, 18, 27, 35	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	322	PHE	4.1
1	D	325	LYS	3.5
1	D	321	LEU	3.2
1	C	79	ALA	2.9
1	C	320	ALA	2.6
1	D	68	ASP	2.6
1	C	322	PHE	2.5
1	B	325	LYS	2.5
1	D	324	HIS	2.3
1	C	321	LEU	2.2
1	C	314	GLN	2.1
1	D	312	ARG	2.1
1	D	215	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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	PAF	C	401	10/10	0.96	0.13	10,12,13,13	0
2	PAF	B	401	10/10	0.97	0.10	10,12,13,13	0
2	PAF	A	401	10/10	0.98	0.12	9,11,12,13	0
2	PAF	D	401	10/10	0.98	0.10	15,16,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.