



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:14 PM UTC

PDB ID : 4PGP / pdb_00004pgp
Title : CRYSTAL STRUCTURE OF A TRAP PERIPLASMIC SOLUTE BINDING PROTEIN FROM DESULFOVIBRIO ALASKENSIS G20 (Dde_0634, TARGET EFI-510120) WITH BOUND 3-INDOLE ACETIC ACID
Authors : Vetting, M.W.; Al Obaidi, N.F.; Morisco, L.L.; Wasserman, S.R.; Stead, M.; Attonito, J.D.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hillerich, B.; Love, J.; Seidel, R.D.; Whalen, K.L.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on : 2014-05-02
Resolution : 2.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)

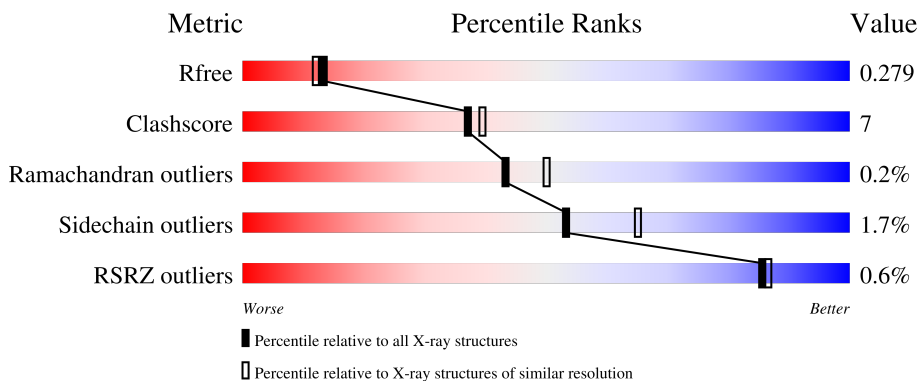
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


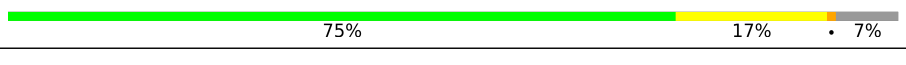
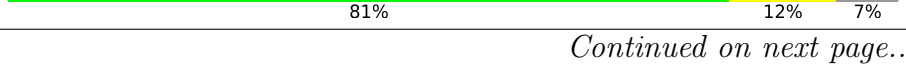
The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

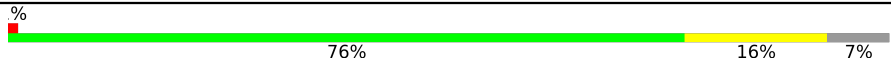
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	334	 79% 13% • 8%
1	B	334	 75% 17% • 7%
1	C	334	 81% 12% 7%

Continued on next page...

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	D	334	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a green segment representing 76%, a yellow segment representing 16%, and a grey segment representing 7%. A small red square is located at the beginning of the bar, followed by a percentage sign (%).</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18869 atoms, of which 8931 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 Extracellular solute-binding protein, family 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	308	4582	1498	2219	412	435	18	0	0	0
1	B	309	4619	1504	2245	413	439	18	0	0	0
1	C	310	4585	1497	2222	407	441	18	0	0	0
1	D	310	4573	1494	2213	407	441	18	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	expression tag	UNP Q315G1
A	9	HIS	-	expression tag	UNP Q315G1
A	10	HIS	-	expression tag	UNP Q315G1
A	11	HIS	-	expression tag	UNP Q315G1
A	12	HIS	-	expression tag	UNP Q315G1
A	13	HIS	-	expression tag	UNP Q315G1
A	14	HIS	-	expression tag	UNP Q315G1
A	15	SER	-	expression tag	UNP Q315G1
A	16	SER	-	expression tag	UNP Q315G1
A	17	GLY	-	expression tag	UNP Q315G1
A	18	VAL	-	expression tag	UNP Q315G1
A	19	ASP	-	expression tag	UNP Q315G1
A	20	LEU	-	expression tag	UNP Q315G1
A	21	GLY	-	expression tag	UNP Q315G1
A	22	THR	-	expression tag	UNP Q315G1
A	23	GLU	-	expression tag	UNP Q315G1
A	24	ASN	-	expression tag	UNP Q315G1
A	25	LEU	-	expression tag	UNP Q315G1
A	26	TYR	-	expression tag	UNP Q315G1
A	27	PHE	-	expression tag	UNP Q315G1
A	28	GLN	-	expression tag	UNP Q315G1

Continued on next page...

Continued from previous page...

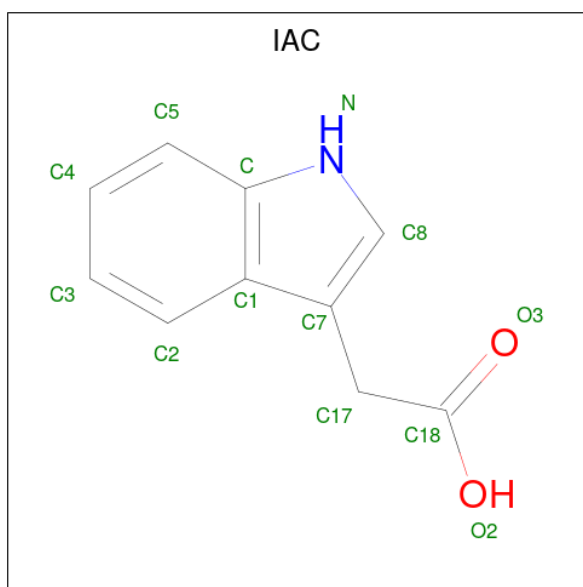
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	SER	-	expression tag	UNP Q315G1
A	30	MET	-	expression tag	UNP Q315G1
B	8	MET	-	expression tag	UNP Q315G1
B	9	HIS	-	expression tag	UNP Q315G1
B	10	HIS	-	expression tag	UNP Q315G1
B	11	HIS	-	expression tag	UNP Q315G1
B	12	HIS	-	expression tag	UNP Q315G1
B	13	HIS	-	expression tag	UNP Q315G1
B	14	HIS	-	expression tag	UNP Q315G1
B	15	SER	-	expression tag	UNP Q315G1
B	16	SER	-	expression tag	UNP Q315G1
B	17	GLY	-	expression tag	UNP Q315G1
B	18	VAL	-	expression tag	UNP Q315G1
B	19	ASP	-	expression tag	UNP Q315G1
B	20	LEU	-	expression tag	UNP Q315G1
B	21	GLY	-	expression tag	UNP Q315G1
B	22	THR	-	expression tag	UNP Q315G1
B	23	GLU	-	expression tag	UNP Q315G1
B	24	ASN	-	expression tag	UNP Q315G1
B	25	LEU	-	expression tag	UNP Q315G1
B	26	TYR	-	expression tag	UNP Q315G1
B	27	PHE	-	expression tag	UNP Q315G1
B	28	GLN	-	expression tag	UNP Q315G1
B	29	SER	-	expression tag	UNP Q315G1
B	30	MET	-	expression tag	UNP Q315G1
C	8	MET	-	expression tag	UNP Q315G1
C	9	HIS	-	expression tag	UNP Q315G1
C	10	HIS	-	expression tag	UNP Q315G1
C	11	HIS	-	expression tag	UNP Q315G1
C	12	HIS	-	expression tag	UNP Q315G1
C	13	HIS	-	expression tag	UNP Q315G1
C	14	HIS	-	expression tag	UNP Q315G1
C	15	SER	-	expression tag	UNP Q315G1
C	16	SER	-	expression tag	UNP Q315G1
C	17	GLY	-	expression tag	UNP Q315G1
C	18	VAL	-	expression tag	UNP Q315G1
C	19	ASP	-	expression tag	UNP Q315G1
C	20	LEU	-	expression tag	UNP Q315G1
C	21	GLY	-	expression tag	UNP Q315G1
C	22	THR	-	expression tag	UNP Q315G1
C	23	GLU	-	expression tag	UNP Q315G1
C	24	ASN	-	expression tag	UNP Q315G1

Continued on next page...

Continued from previous page...

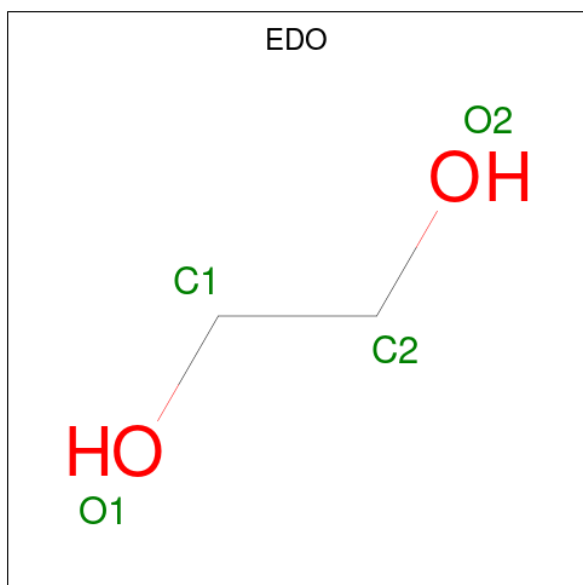
Chain	Residue	Modelled	Actual	Comment	Reference
C	25	LEU	-	expression tag	UNP Q315G1
C	26	TYR	-	expression tag	UNP Q315G1
C	27	PHE	-	expression tag	UNP Q315G1
C	28	GLN	-	expression tag	UNP Q315G1
C	29	SER	-	expression tag	UNP Q315G1
C	30	MET	-	expression tag	UNP Q315G1
D	8	MET	-	expression tag	UNP Q315G1
D	9	HIS	-	expression tag	UNP Q315G1
D	10	HIS	-	expression tag	UNP Q315G1
D	11	HIS	-	expression tag	UNP Q315G1
D	12	HIS	-	expression tag	UNP Q315G1
D	13	HIS	-	expression tag	UNP Q315G1
D	14	HIS	-	expression tag	UNP Q315G1
D	15	SER	-	expression tag	UNP Q315G1
D	16	SER	-	expression tag	UNP Q315G1
D	17	GLY	-	expression tag	UNP Q315G1
D	18	VAL	-	expression tag	UNP Q315G1
D	19	ASP	-	expression tag	UNP Q315G1
D	20	LEU	-	expression tag	UNP Q315G1
D	21	GLY	-	expression tag	UNP Q315G1
D	22	THR	-	expression tag	UNP Q315G1
D	23	GLU	-	expression tag	UNP Q315G1
D	24	ASN	-	expression tag	UNP Q315G1
D	25	LEU	-	expression tag	UNP Q315G1
D	26	TYR	-	expression tag	UNP Q315G1
D	27	PHE	-	expression tag	UNP Q315G1
D	28	GLN	-	expression tag	UNP Q315G1
D	29	SER	-	expression tag	UNP Q315G1
D	30	MET	-	expression tag	UNP Q315G1

- Molecule 2 is 1H-INDOL-3-YLACETIC ACID (CCD ID: IAC) (formula: C₁₀H₉NO₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	Total	C	H	N	O	0	0
			21	10	8	1	2		
2	B	1	Total	C	H	N	O	0	0
			21	10	8	1	2		
2	C	1	Total	C	H	N	O	0	0
			21	10	8	1	2		
2	D	1	Total	C	H	N	O	0	0
			21	10	8	1	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		

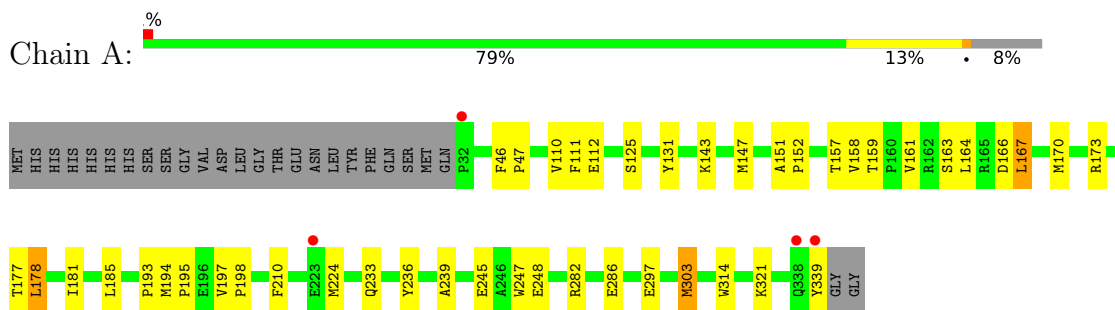
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	B	103	Total	O	0	0
			103	103		
4	C	94	Total	O	0	0
			94	94		
4	D	120	Total	O	0	0
			120	120		

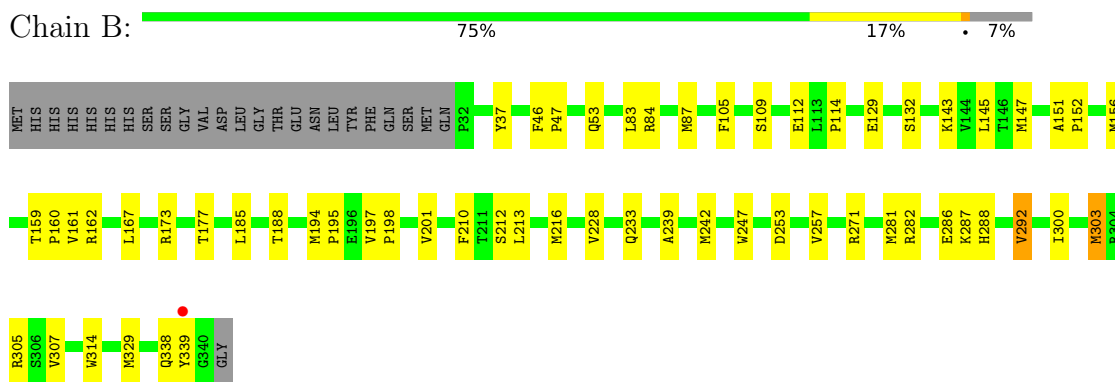
3 Residue-property plots [i](#)

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.

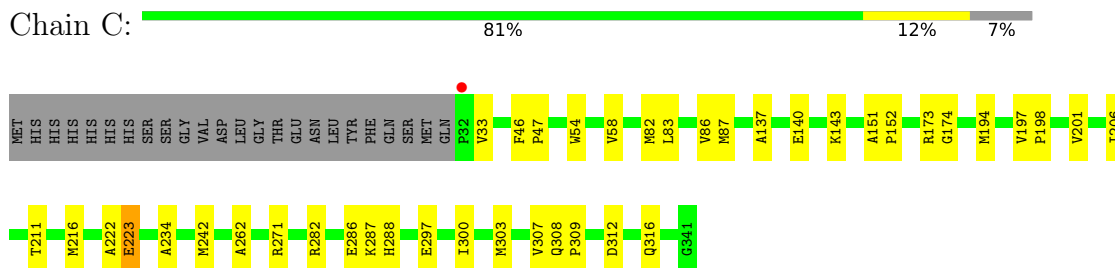
- Molecule 1: Extracellular solute-binding protein, family 7



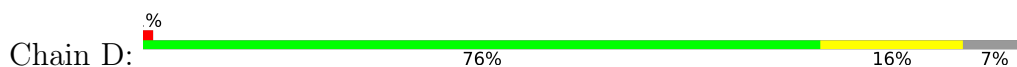
- Molecule 1: Extracellular solute-binding protein, family 7

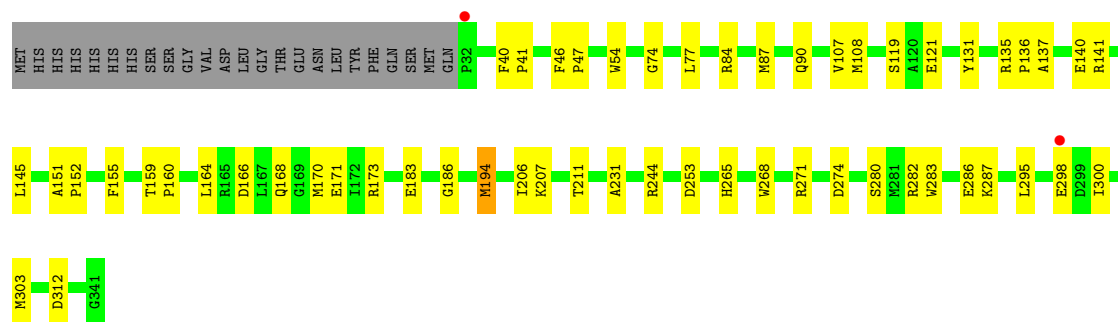


- Molecule 1: Extracellular solute-binding protein, family 7



- Molecule 1: Extracellular solute-binding protein, family 7





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.29Å 145.54Å 97.92Å 90.00° 92.19° 90.00°	Depositor
Resolution (Å)	35.74 – 2.25 35.74 – 2.25	Depositor EDS
% Data completeness (in resolution range)	92.3 (35.74-2.25) 92.4 (35.74-2.25)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.24Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.202 , 0.262 (Not available) , 0.279	Depositor DCC
R_{free} test set	3133 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtrriage
Anisotropy	0.283	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18869	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.03 % 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 2.9018e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: IAC, EDO

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	0.88	0/2420	0.95	0/3294
1	B	1.00	0/2431	1.06	4/3307 (0.1%)
1	C	0.78	1/2420 (0.0%)	0.94	1/3294 (0.0%)
1	D	0.91	0/2417	1.05	6/3290 (0.2%)
All	All	0.90	1/9688 (0.0%)	1.00	11/13185 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	307	VAL	CA-CB	5.02	1.60	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	135	ARG	CA-C-N	6.96	126.88	119.85
1	D	135	ARG	C-N-CA	6.96	126.88	119.85
1	D	194	MET	CA-C-N	-6.54	113.41	119.82
1	D	194	MET	C-N-CA	-6.54	113.41	119.82
1	B	300	ILE	CB-CA-C	-6.23	103.99	111.97
1	D	295	LEU	CA-C-N	5.51	125.51	119.89
1	D	295	LEU	C-N-CA	5.51	125.51	119.89
1	B	303	MET	N-CA-C	-5.39	104.28	112.04
1	B	188	THR	CA-C-N	5.38	125.14	119.76
1	B	188	THR	C-N-CA	5.38	125.14	119.76
1	C	262	ALA	N-CA-C	5.02	116.44	110.97

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	2363	2219	2329	34	0
1	B	2374	2245	2343	39	0
1	C	2363	2222	2313	26	0
1	D	2360	2213	2304	35	0
2	A	13	8	8	0	0
2	B	13	8	8	0	0
2	C	13	8	8	0	0
2	D	13	8	8	0	0
3	B	4	0	6	1	0
4	A	105	0	0	2	0
4	B	103	0	0	3	0
4	C	94	0	0	1	0
4	D	120	0	0	3	0
All	All	9938	8931	9327	133	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 7.

All (133) 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:228:VAL:HG21	1:B:281:MET:HE1	1.58	0.83
1:D:87:MET:HE1	1:D:141:ARG:HE	1.50	0.75
1:D:107:VAL:HG12	1:D:108:MET:HE2	1.72	0.71
1:A:297:GLU:OE2	4:A:551:HOH:O	2.09	0.71
1:B:145:LEU:HD11	1:B:242:MET:HE3	1.74	0.70
1:B:305:ARG:NH1	4:B:543:HOH:O	2.29	0.66
1:A:321:LYS:O	4:A:578:HOH:O	2.13	0.66
3:B:402:EDO:H22	4:B:548:HOH:O	1.94	0.66
1:D:164:LEU:O	1:D:168:GLN:NE2	2.29	0.65
1:B:84:ARG:HD2	1:C:287:LYS:O	1.97	0.65
1:A:185:LEU:CD2	1:A:303:MET:HB2	2.27	0.64
1:B:287:LYS:O	1:B:288:HIS:CD2	2.51	0.63
1:D:108:MET:HE3	1:D:136:PRO:HG3	1.83	0.61
1:A:46:PHE:CD2	1:A:47:PRO:HD3	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:GLU:OE2	1:C:288:HIS:NE2	2.35	0.60
1:D:283:TRP:NE1	1:D:287:LYS:HD3	2.17	0.60
1:B:147:MET:HE3	1:B:239:ALA:HB2	1.83	0.60
1:A:185:LEU:HD22	1:A:303:MET:HB2	1.84	0.59
1:C:83:LEU:O	1:C:87:MET:HG3	2.03	0.59
1:D:283:TRP:CD1	1:D:287:LYS:HD3	2.38	0.57
1:A:233:GLN:HE21	1:A:303:MET:HE3	1.69	0.57
1:B:314:TRP:CZ3	1:B:329:MET:HE2	2.39	0.57
1:B:129:GLU:HG3	1:B:339:TYR:CZ	2.41	0.56
1:D:107:VAL:CG1	1:D:108:MET:HE2	2.35	0.56
1:B:287:LYS:O	1:B:288:HIS:CG	2.59	0.56
1:B:143:LYS:HE2	1:B:247:TRP:CZ2	2.41	0.55
1:A:157:THR:HB	1:A:170:MET:HE1	1.89	0.55
1:B:271:ARG:NH1	4:B:545:HOH:O	2.38	0.55
1:B:213:LEU:HD13	1:B:281:MET:SD	2.46	0.55
1:C:46:PHE:CD2	1:C:47:PRO:HD3	2.42	0.54
1:C:300:ILE:O	1:C:303:MET:HB3	2.08	0.54
1:B:210:PHE:HZ	1:B:233:GLN:HG3	1.73	0.54
1:D:46:PHE:CD2	1:D:47:PRO:HD3	2.43	0.53
1:A:112:GLU:HB3	1:A:177:THR:HB	1.90	0.53
1:D:173:ARG:HD3	1:D:173:ARG:C	2.33	0.52
1:A:161:VAL:HG11	1:A:167:LEU:HD13	1.90	0.52
1:A:143:LYS:HE2	1:A:247:TRP:CZ2	2.43	0.52
1:C:137:ALA:O	1:C:140:GLU:HG2	2.10	0.52
1:D:84:ARG:HG2	4:D:586:HOH:O	2.10	0.52
1:B:197:VAL:O	1:B:201:VAL:HG23	2.09	0.51
1:B:129:GLU:HG3	1:B:339:TYR:OH	2.12	0.50
1:B:129:GLU:HG3	1:B:339:TYR:CE1	2.46	0.50
1:B:83:LEU:HG	1:B:87:MET:HE2	1.92	0.50
1:D:171:GLU:HB3	1:D:206:ILE:HA	1.94	0.49
1:A:210:PHE:HZ	1:A:233:GLN:HG3	1.77	0.49
1:B:161:VAL:HG11	1:B:167:LEU:HD13	1.94	0.49
1:A:147:MET:HE2	1:A:239:ALA:HB2	1.94	0.49
1:D:166:ASP:O	1:D:170:MET:HE3	2.13	0.49
1:B:105:PHE:O	1:B:109:SER:HB3	2.12	0.49
1:B:197:VAL:N	1:B:198:PRO:CD	2.76	0.49
1:D:168:GLN:HA	1:D:186:GLY:O	2.13	0.49
1:A:177:THR:O	1:A:181:ILE:HG13	2.13	0.49
1:B:156:MET:HE2	1:B:213:LEU:HD23	1.95	0.48
1:A:245:GLU:HA	1:A:248:GLU:HG2	1.94	0.48
1:A:151:ALA:HB1	1:A:152:PRO:CD	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:MET:O	1:C:86:VAL:HG23	2.14	0.48
1:C:194:MET:HE1	1:C:211:THR:HG21	1.94	0.48
1:D:137:ALA:HA	1:D:140:GLU:HG3	1.96	0.47
1:C:308:GLN:HB2	1:C:309:PRO:HD3	1.95	0.47
1:B:84:ARG:CD	1:C:287:LYS:O	2.61	0.47
1:A:173:ARG:C	1:A:173:ARG:HD3	2.39	0.47
1:A:143:LYS:HE2	1:A:247:TRP:CH2	2.50	0.47
1:D:74:GLY:HA2	1:D:77:LEU:O	2.15	0.47
1:B:53:GLN:OE1	1:B:53:GLN:HA	2.15	0.46
1:B:194:MET:N	1:B:195:PRO:CD	2.78	0.46
1:C:54:TRP:O	1:C:58:VAL:HG23	2.16	0.46
1:C:271:ARG:NH1	4:C:561:HOH:O	2.38	0.46
1:D:298:GLU:OE2	1:D:298:GLU:O	2.34	0.46
1:B:253:ASP:O	1:B:257:VAL:HG23	2.15	0.46
1:A:198:PRO:HB3	1:A:224:MET:HE1	1.98	0.46
1:B:114:PRO:HG3	1:B:307:VAL:HG11	1.97	0.45
1:B:282:ARG:O	1:B:286:GLU:HG2	2.16	0.45
1:A:178:LEU:HD22	1:A:178:LEU:N	2.31	0.45
1:D:131:TYR:CD2	1:D:131:TYR:C	2.95	0.45
1:D:300:ILE:O	1:D:303:MET:HB3	2.17	0.45
1:B:173:ARG:HD3	1:B:173:ARG:C	2.41	0.45
1:B:185:LEU:CD2	1:B:303:MET:HG3	2.46	0.45
1:B:151:ALA:HB1	1:B:152:PRO:HD2	1.99	0.45
1:D:119:SER:HB2	1:D:274:ASP:OD2	2.16	0.45
1:D:155:PHE:CE2	1:D:231:ALA:HB2	2.51	0.45
1:C:46:PHE:N	1:C:47:PRO:CD	2.80	0.45
1:D:159:THR:HB	1:D:160:PRO:CD	2.46	0.45
1:B:228:VAL:HB	1:B:292:VAL:HG13	1.98	0.45
1:C:312:ASP:O	1:C:316:GLN:HG2	2.17	0.45
1:A:282:ARG:O	1:A:286:GLU:HG2	2.16	0.45
1:D:40:PHE:CG	1:D:41:PRO:HD3	2.52	0.45
1:A:131:TYR:CD2	1:A:131:TYR:C	2.94	0.44
1:D:121:GLU:CD	1:D:271:ARG:HB2	2.42	0.44
1:D:282:ARG:O	1:D:286:GLU:HG2	2.17	0.44
1:C:173:ARG:HG3	1:C:197:VAL:HG22	1.98	0.44
1:C:151:ALA:HB1	1:C:152:PRO:CD	2.47	0.44
1:A:314:TRP:CD2	1:A:314:TRP:C	2.94	0.44
1:B:151:ALA:HB1	1:B:152:PRO:CD	2.48	0.44
1:C:173:ARG:HD2	1:C:174:GLY:O	2.17	0.44
1:A:339:TYR:CD1	1:A:339:TYR:N	2.85	0.43
1:B:173:ARG:HG3	1:B:197:VAL:HG22	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:PRO:HB2	1:A:195:PRO:HD2	2.00	0.43
1:B:156:MET:HE1	1:B:212:SER:O	2.18	0.43
1:A:151:ALA:HB1	1:A:152:PRO:HD2	2.00	0.43
1:C:201:VAL:HG23	1:C:206:ILE:HD11	2.01	0.43
1:A:173:ARG:HG3	1:A:197:VAL:HG22	1.99	0.43
1:B:216:MET:HE2	1:B:228:VAL:HG21	2.01	0.43
1:A:125:SER:HB3	1:A:339:TYR:CD2	2.54	0.43
1:A:125:SER:HB3	1:A:339:TYR:HD2	1.83	0.43
1:C:282:ARG:O	1:C:286:GLU:HG2	2.19	0.43
1:C:197:VAL:N	1:C:198:PRO:CD	2.82	0.43
1:D:194:MET:HE1	1:D:211:THR:HG21	2.00	0.43
1:D:159:THR:HB	1:D:160:PRO:HD2	2.00	0.42
1:A:158:VAL:HG23	1:A:159:THR:HG23	2.01	0.42
1:A:194:MET:N	1:A:195:PRO:CD	2.82	0.42
1:D:108:MET:CE	1:D:136:PRO:HG3	2.48	0.42
1:D:145:LEU:HA	1:D:145:LEU:HD23	1.80	0.42
1:C:216:MET:HE3	1:C:222:ALA:HA	2.02	0.42
1:D:183:GLU:OE2	4:D:595:HOH:O	2.22	0.42
1:D:268:TRP:CE3	1:D:268:TRP:C	2.98	0.42
1:B:46:PHE:CD2	1:B:47:PRO:HD3	2.55	0.42
1:D:207:LYS:NZ	4:D:504:HOH:O	2.52	0.41
1:D:244:ARG:HA	1:D:244:ARG:HD3	1.91	0.41
1:A:161:VAL:HG13	1:A:166:ASP:HB2	2.02	0.41
1:A:110:VAL:HB	1:A:314:TRP:CZ2	2.55	0.41
1:C:143:LYS:HB3	1:C:242:MET:HB3	2.02	0.41
1:D:151:ALA:HB1	1:D:152:PRO:CD	2.50	0.41
1:C:151:ALA:HB1	1:C:152:PRO:HD2	2.02	0.41
1:A:339:TYR:N	1:A:339:TYR:HD1	2.18	0.41
1:C:216:MET:CE	1:C:222:ALA:HA	2.50	0.41
1:A:178:LEU:HG	1:A:236:TYR:CZ	2.56	0.41
1:B:112:GLU:HB3	1:B:177:THR:HB	2.02	0.41
1:B:159:THR:HB	1:B:160:PRO:HD2	2.02	0.41
1:C:87:MET:HE2	1:C:87:MET:HB3	1.82	0.41
1:C:46:PHE:CG	1:C:47:PRO:HD3	2.55	0.41
1:D:54:TRP:HB2	1:D:265:HIS:CE1	2.57	0.40
1:B:145:LEU:HD21	1:B:242:MET:HE3	2.03	0.40
1:D:151:ALA:HB1	1:D:152:PRO:HD2	2.03	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	306/334 (92%)	299 (98%)	7 (2%)	0	100	100
1	B	307/334 (92%)	296 (96%)	10 (3%)	1 (0%)	36	40
1	C	308/334 (92%)	302 (98%)	5 (2%)	1 (0%)	36	40
1	D	308/334 (92%)	299 (97%)	9 (3%)	0	100	100
All	All	1229/1336 (92%)	1196 (97%)	31 (2%)	2 (0%)	43	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	338	GLN
1	C	234	ALA

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	247/273 (90%)	241 (98%)	6 (2%)	43	54
1	B	249/273 (91%)	245 (98%)	4 (2%)	55	66
1	C	246/273 (90%)	243 (99%)	3 (1%)	63	74
1	D	245/273 (90%)	241 (98%)	4 (2%)	55	66
All	All	987/1092 (90%)	970 (98%)	17 (2%)	53	65

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

Mol	Chain	Res	Type
1	A	111	PHE
1	A	163	SER
1	A	164	LEU
1	A	167	LEU
1	A	178	LEU
1	A	303	MET
1	B	37	TYR
1	B	132	SER
1	B	162	ARG
1	B	292	VAL
1	C	33	VAL
1	C	223	GLU
1	C	297	GLU
1	D	90	GLN
1	D	253	ASP
1	D	280	SER
1	D	312	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	101	HIS
1	A	202	GLN
1	B	36	ASN
1	B	220	ASN
1	B	288	HIS
1	C	36	ASN
1	C	293	HIS
1	D	90	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	IAC	B	401	-	14,14,14	1.77	4 (28%)	19,19,19	0.98	1 (5%)
2	IAC	D	401	-	14,14,14	1.25	1 (7%)	19,19,19	1.61	5 (26%)
2	IAC	A	401	-	14,14,14	1.66	3 (21%)	19,19,19	1.52	2 (10%)
2	IAC	C	401	-	14,14,14	1.26	2 (14%)	19,19,19	1.32	3 (15%)
3	EDO	B	402	-	3,3,3	1.04	0	2,2,2	0.83	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	IAC	B	401	-	-	2/4/4/4	0/2/2/2
2	IAC	D	401	-	-	2/4/4/4	0/2/2/2
2	IAC	A	401	-	-	0/4/4/4	0/2/2/2
2	IAC	C	401	-	-	2/4/4/4	0/2/2/2
3	EDO	B	402	-	-	0/1/1/1	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	IAC	C1-C7	-3.86	1.37	1.44
2	A	401	IAC	C1-C7	-3.61	1.38	1.44
2	B	401	IAC	C-N	-2.88	1.33	1.37
2	A	401	IAC	C-N	-2.82	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	IAC	C1-C	-2.69	1.38	1.41
2	B	401	IAC	C5-C	-2.57	1.35	1.39
2	C	401	IAC	C1-C7	-2.56	1.39	1.44
2	C	401	IAC	C1-C	-2.26	1.38	1.41
2	A	401	IAC	C5-C	-2.18	1.36	1.39
2	B	401	IAC	C1-C	-2.03	1.38	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	IAC	C18-C17-C7	-4.53	107.98	114.93
2	D	401	IAC	C18-C17-C7	-3.66	109.31	114.93
2	C	401	IAC	C7-C8-N	-3.08	106.92	110.31
2	D	401	IAC	O2-C18-C17	2.55	122.40	114.51
2	A	401	IAC	C7-C8-N	-2.43	107.64	110.31
2	C	401	IAC	O2-C18-C17	2.37	121.84	114.51
2	D	401	IAC	C7-C8-N	-2.33	107.75	110.31
2	C	401	IAC	C1-C7-C8	2.29	108.50	106.16
2	D	401	IAC	O2-C18-O3	-2.24	117.58	123.33
2	D	401	IAC	C-N-C8	2.21	111.04	109.08
2	B	401	IAC	C7-C8-N	-2.03	108.08	110.31

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	IAC	C7-C17-C18-O3
2	B	401	IAC	C7-C17-C18-O3
2	C	401	IAC	C7-C17-C18-O2
2	D	401	IAC	C7-C17-C18-O3
2	B	401	IAC	C7-C17-C18-O2
2	D	401	IAC	C7-C17-C18-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	EDO	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	308/334 (92%)	-0.10	4 (1%) 75 76	26, 40, 59, 84	0
1	B	309/334 (92%)	-0.38	1 (0%) 90 90	20, 32, 56, 77	0
1	C	310/334 (92%)	0.01	1 (0%) 90 90	29, 46, 78, 109	0
1	D	310/334 (92%)	-0.20	2 (0%) 85 86	20, 36, 67, 88	0
All	All	1237/1336 (92%)	-0.17	8 (0%) 85 86	20, 39, 68, 109	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	32	PRO	3.1
1	A	339	TYR	3.0
1	B	339	TYR	2.9
1	D	32	PRO	2.8
1	A	338	GLN	2.8
1	A	32	PRO	2.8
1	D	298	GLU	2.1
1	A	223	GLU	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 oligosaccharides 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
3	EDO	B	402	4/4	0.93	0.07	20,20,20,20	0
2	IAC	B	401	13/13	0.96	0.05	14,21,27,32	0
2	IAC	C	401	13/13	0.96	0.06	25,32,37,41	0
2	IAC	A	401	13/13	0.96	0.04	17,24,29,31	0
2	IAC	D	401	13/13	0.97	0.06	17,25,30,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.