



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 02:08 PM BST

PDB ID : 6VDF
Title : Structure of the periplasmic domain of YejM from *Salmonella typhimurium* (twinned)
Authors : Gabale, U.; Ressler, S.
Deposited on : 2019-12-25
Resolution : 1.92 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 following versions of software and data (see [references ⓘ](#)) 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
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

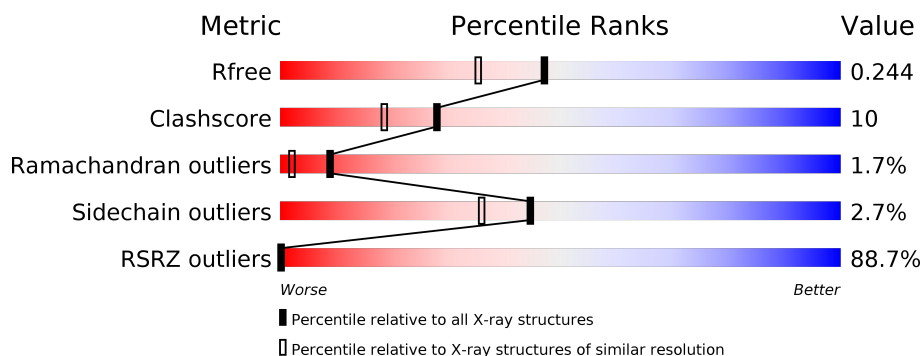
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 $\leq 5\%$. 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	368	<div> <div>80%</div> <div> <div>72%</div> <div>20%</div> <div>7%</div> </div> </div>
1	B	368	<div> <div>87%</div> <div> <div>71%</div> <div>21%</div> <div>7%</div> </div> </div>
1	C	368	<div> <div>83%</div> <div> <div>73%</div> <div>19%</div> <div>7%</div> </div> </div>
1	D	368	<div> <div>80%</div> <div> <div>71%</div> <div>21%</div> <div>7%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PGE	A	601	-	-	-	X
3	PEG	A	602	-	-	-	X
5	MN	B	602	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22294 atoms, of which 10549 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 Periplasmic domain of the cardiolipin transporter protein YejM/PbgA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	H	N	O	S	0	0	0
			5341	1712	2623	476	522	8			
1	B	343	Total	C	H	N	O	S	0	0	0
			5342	1712	2624	476	522	8			
1	C	343	Total	C	H	N	O	S	0	0	0
			5341	1712	2623	476	522	8			
1	D	343	Total	C	H	N	O	S	0	0	0
			5341	1712	2623	476	522	8			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	MET	-	expression tag	UNP A0A5K1U4E1
A	220	SER	-	expression tag	UNP A0A5K1U4E1
A	221	GLY	-	expression tag	UNP A0A5K1U4E1
A	222	HIS	-	expression tag	UNP A0A5K1U4E1
A	223	HIS	-	expression tag	UNP A0A5K1U4E1
A	224	HIS	-	expression tag	UNP A0A5K1U4E1
A	225	HIS	-	expression tag	UNP A0A5K1U4E1
A	226	HIS	-	expression tag	UNP A0A5K1U4E1
A	227	HIS	-	expression tag	UNP A0A5K1U4E1
A	228	SER	-	expression tag	UNP A0A5K1U4E1
A	229	SER	-	expression tag	UNP A0A5K1U4E1
A	230	GLY	-	expression tag	UNP A0A5K1U4E1
A	231	LEU	-	expression tag	UNP A0A5K1U4E1
A	232	VAL	-	expression tag	UNP A0A5K1U4E1
A	233	PRO	-	expression tag	UNP A0A5K1U4E1
A	234	ARG	-	expression tag	UNP A0A5K1U4E1
A	235	GLY	-	expression tag	UNP A0A5K1U4E1
A	236	SER	-	expression tag	UNP A0A5K1U4E1
A	237	HIS	-	expression tag	UNP A0A5K1U4E1
A	238	MET	-	expression tag	UNP A0A5K1U4E1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	ALA	-	expression tag	UNP A0A5K1U4E1
A	240	SER	-	expression tag	UNP A0A5K1U4E1
B	219	MET	-	expression tag	UNP A0A5K1U4E1
B	220	SER	-	expression tag	UNP A0A5K1U4E1
B	221	GLY	-	expression tag	UNP A0A5K1U4E1
B	222	HIS	-	expression tag	UNP A0A5K1U4E1
B	223	HIS	-	expression tag	UNP A0A5K1U4E1
B	224	HIS	-	expression tag	UNP A0A5K1U4E1
B	225	HIS	-	expression tag	UNP A0A5K1U4E1
B	226	HIS	-	expression tag	UNP A0A5K1U4E1
B	227	HIS	-	expression tag	UNP A0A5K1U4E1
B	228	SER	-	expression tag	UNP A0A5K1U4E1
B	229	SER	-	expression tag	UNP A0A5K1U4E1
B	230	GLY	-	expression tag	UNP A0A5K1U4E1
B	231	LEU	-	expression tag	UNP A0A5K1U4E1
B	232	VAL	-	expression tag	UNP A0A5K1U4E1
B	233	PRO	-	expression tag	UNP A0A5K1U4E1
B	234	ARG	-	expression tag	UNP A0A5K1U4E1
B	235	GLY	-	expression tag	UNP A0A5K1U4E1
B	236	SER	-	expression tag	UNP A0A5K1U4E1
B	237	HIS	-	expression tag	UNP A0A5K1U4E1
B	238	MET	-	expression tag	UNP A0A5K1U4E1
B	239	ALA	-	expression tag	UNP A0A5K1U4E1
B	240	SER	-	expression tag	UNP A0A5K1U4E1
C	219	MET	-	expression tag	UNP A0A5K1U4E1
C	220	SER	-	expression tag	UNP A0A5K1U4E1
C	221	GLY	-	expression tag	UNP A0A5K1U4E1
C	222	HIS	-	expression tag	UNP A0A5K1U4E1
C	223	HIS	-	expression tag	UNP A0A5K1U4E1
C	224	HIS	-	expression tag	UNP A0A5K1U4E1
C	225	HIS	-	expression tag	UNP A0A5K1U4E1
C	226	HIS	-	expression tag	UNP A0A5K1U4E1
C	227	HIS	-	expression tag	UNP A0A5K1U4E1
C	228	SER	-	expression tag	UNP A0A5K1U4E1
C	229	SER	-	expression tag	UNP A0A5K1U4E1
C	230	GLY	-	expression tag	UNP A0A5K1U4E1
C	231	LEU	-	expression tag	UNP A0A5K1U4E1
C	232	VAL	-	expression tag	UNP A0A5K1U4E1
C	233	PRO	-	expression tag	UNP A0A5K1U4E1
C	234	ARG	-	expression tag	UNP A0A5K1U4E1
C	235	GLY	-	expression tag	UNP A0A5K1U4E1
C	236	SER	-	expression tag	UNP A0A5K1U4E1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	237	HIS	-	expression tag	UNP A0A5K1U4E1
C	238	MET	-	expression tag	UNP A0A5K1U4E1
C	239	ALA	-	expression tag	UNP A0A5K1U4E1
C	240	SER	-	expression tag	UNP A0A5K1U4E1
D	219	MET	-	expression tag	UNP A0A5K1U4E1
D	220	SER	-	expression tag	UNP A0A5K1U4E1
D	221	GLY	-	expression tag	UNP A0A5K1U4E1
D	222	HIS	-	expression tag	UNP A0A5K1U4E1
D	223	HIS	-	expression tag	UNP A0A5K1U4E1
D	224	HIS	-	expression tag	UNP A0A5K1U4E1
D	225	HIS	-	expression tag	UNP A0A5K1U4E1
D	226	HIS	-	expression tag	UNP A0A5K1U4E1
D	227	HIS	-	expression tag	UNP A0A5K1U4E1
D	228	SER	-	expression tag	UNP A0A5K1U4E1
D	229	SER	-	expression tag	UNP A0A5K1U4E1
D	230	GLY	-	expression tag	UNP A0A5K1U4E1
D	231	LEU	-	expression tag	UNP A0A5K1U4E1
D	232	VAL	-	expression tag	UNP A0A5K1U4E1
D	233	PRO	-	expression tag	UNP A0A5K1U4E1
D	234	ARG	-	expression tag	UNP A0A5K1U4E1
D	235	GLY	-	expression tag	UNP A0A5K1U4E1
D	236	SER	-	expression tag	UNP A0A5K1U4E1
D	237	HIS	-	expression tag	UNP A0A5K1U4E1
D	238	MET	-	expression tag	UNP A0A5K1U4E1
D	239	ALA	-	expression tag	UNP A0A5K1U4E1
D	240	SER	-	expression tag	UNP A0A5K1U4E1

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



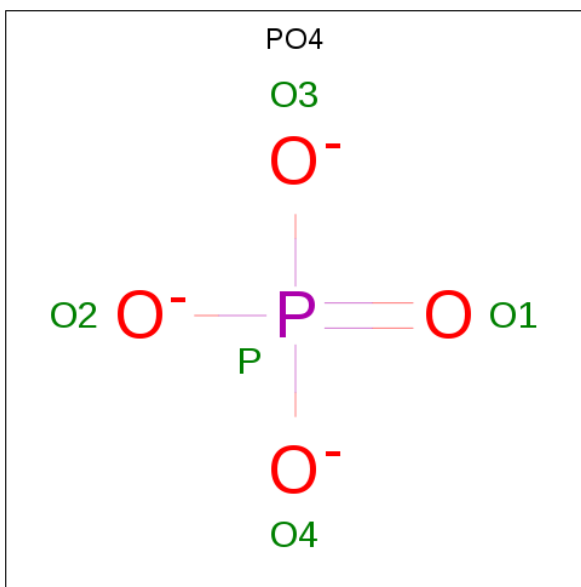
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

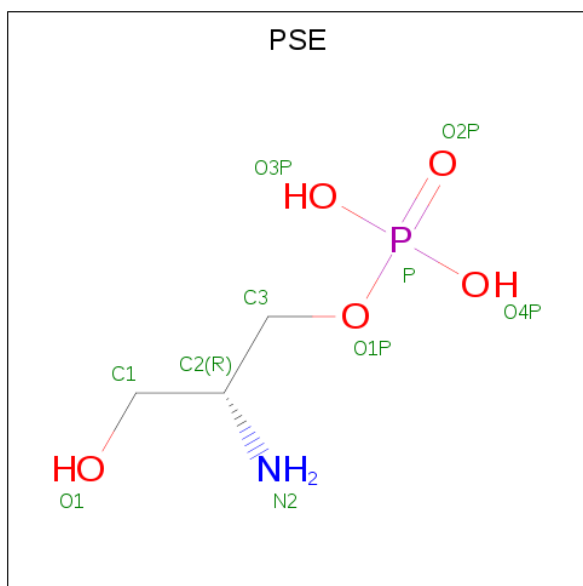
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mn	0	0
			1	1		
5	A	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 7 is O-PHOSPHOETHANOLAMINE (three-letter code: PSE) (formula: $C_3H_{10}NO_5P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	C	1	Total	C	H	N	O	P	0	0
			18	3	8	1	5	1		
7	D	1	Total	C	H	N	O	P	0	0
			18	3	8	1	5	1		

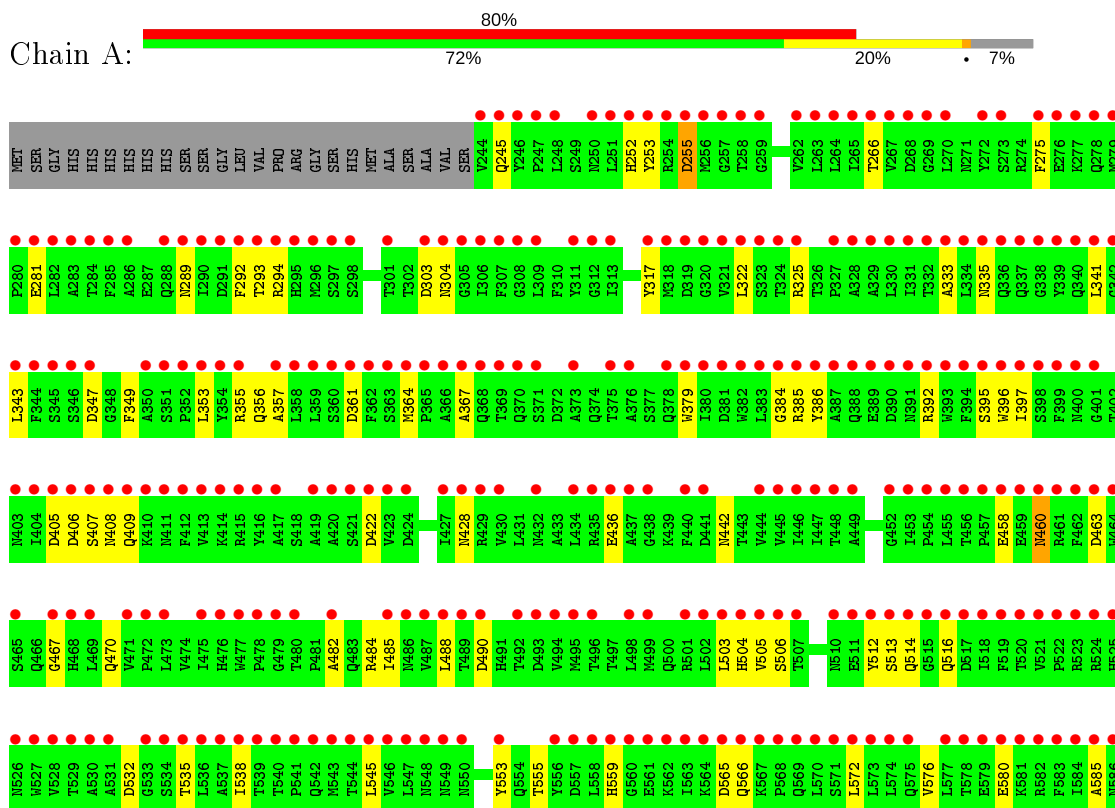
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	183	Total 183	O 183	0	0
8	B	199	Total 199	O 199	0	0
8	C	194	Total 194	O 194	0	0
8	D	236	Total 236	O 236	0	0

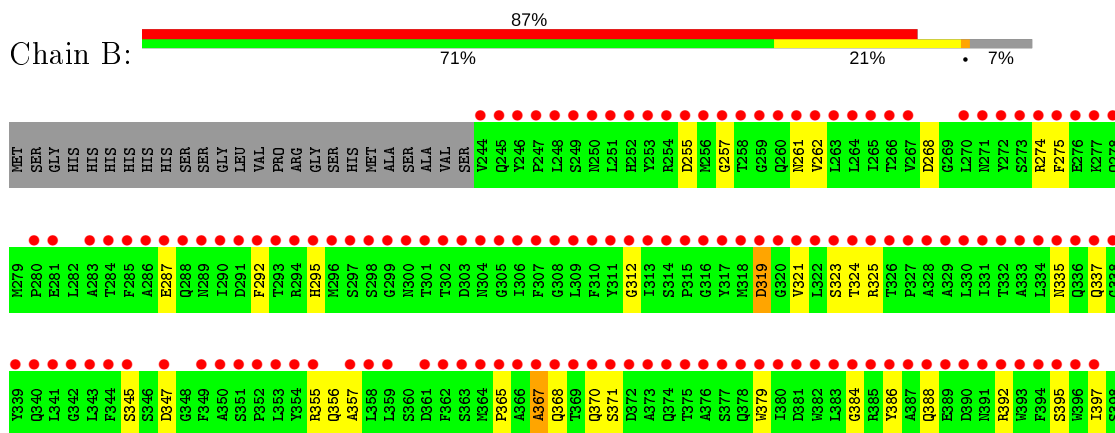
3 Residue-property plots

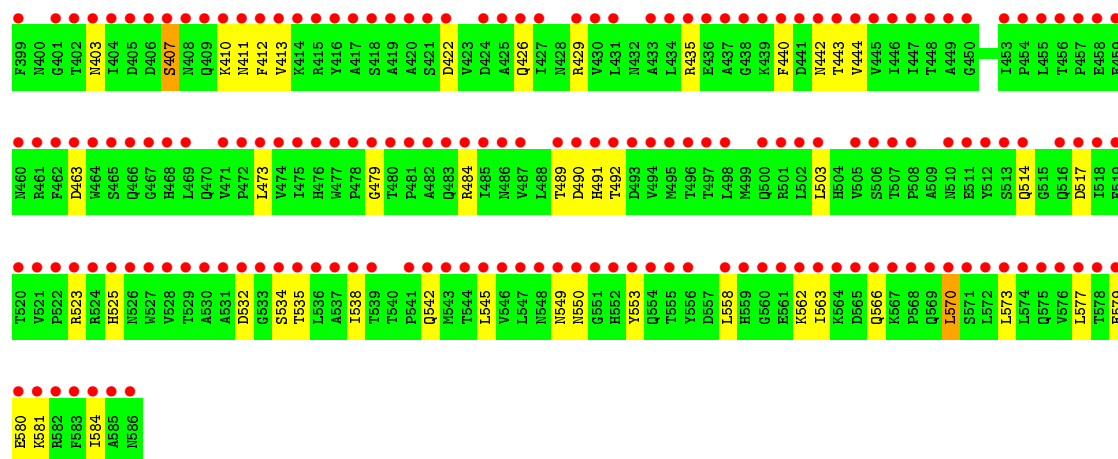
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA

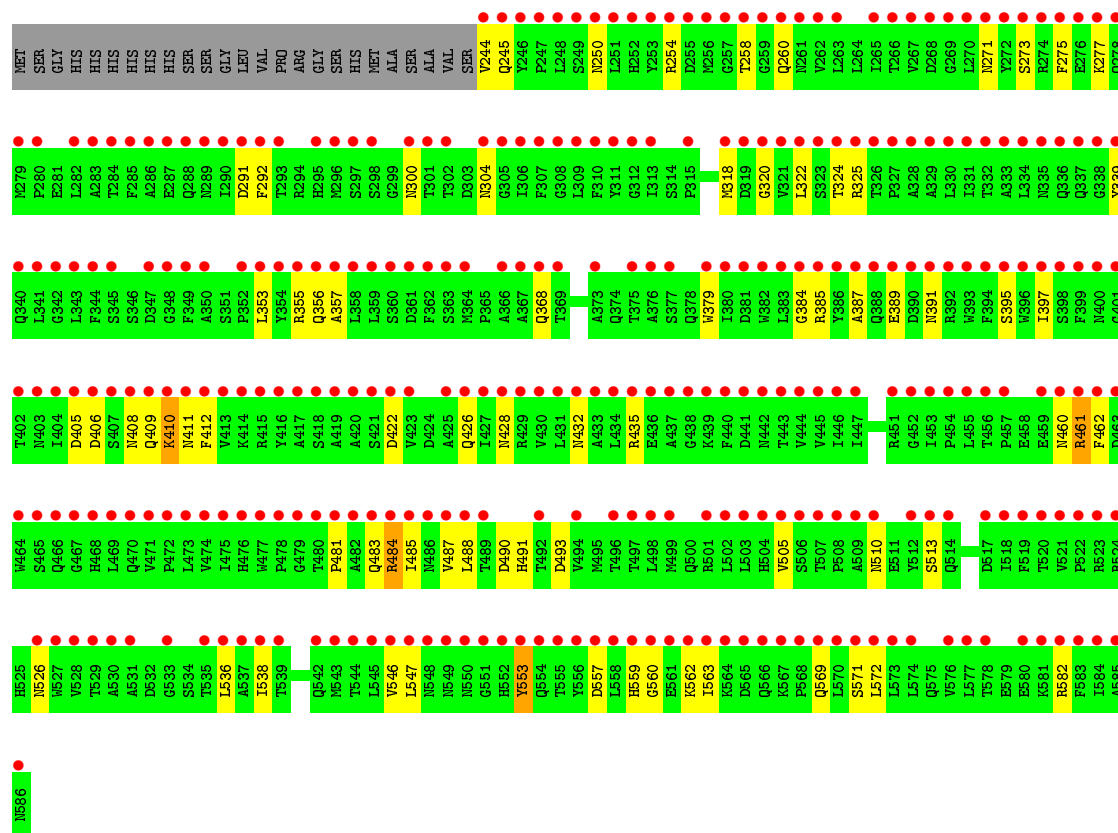
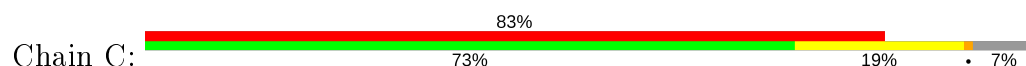


- Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA

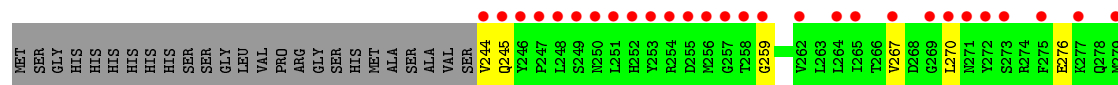
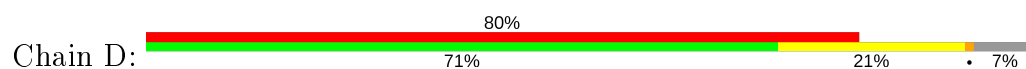


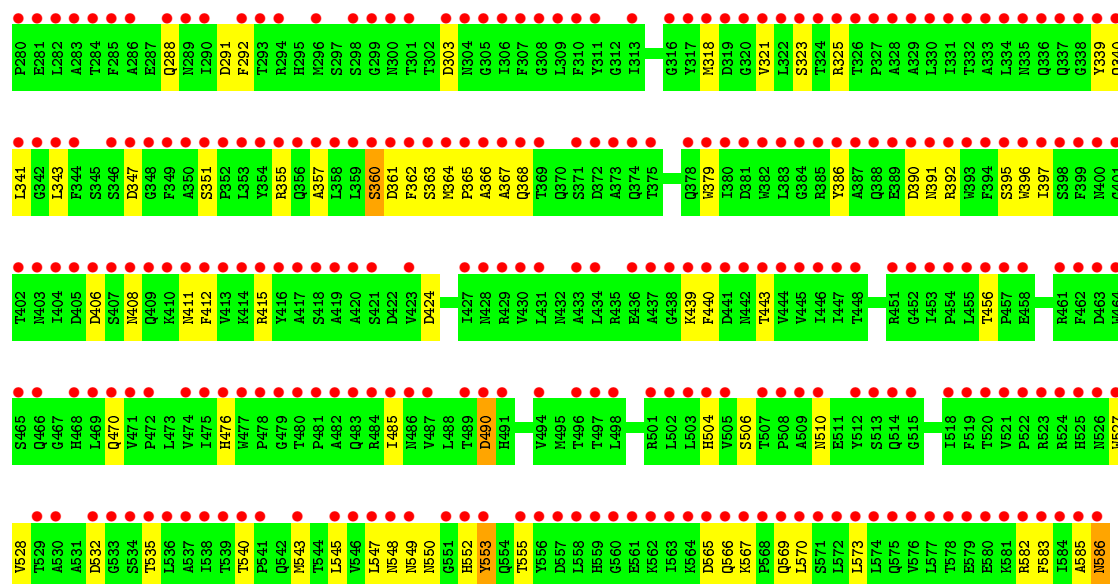


- Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA



- Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.95Å 42.96Å 181.21Å 94.28° 94.02° 111.78°	Depositor
Resolution (Å)	59.90 – 1.92 59.90 – 1.92	Depositor EDS
% Data completeness (in resolution range)	77.2 (59.90-1.92) 76.1 (59.90-1.92)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	15.55 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.211 , 0.261 0.198 , 0.244	Depositor DCC
R_{free} test set	3268 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.428 for k,h,-h-k-l 0.388 for -k,-h,l 0.387 for -h,-k,h+k+l	Xtriage
Reported twinning fraction	0.450 for -h,-k,h+k+l	Depositor
Outliers	0 of 70265 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22294	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 8.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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: PGE, PO4, MN, EDO, PSE, PEG

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	0.24	0/2782	0.43	0/3790
1	B	0.24	0/2782	0.43	0/3790
1	C	0.24	0/2782	0.42	0/3790
1	D	0.24	0/2782	0.42	0/3790
All	All	0.24	0/11128	0.42	0/15160

There are no bond length outliers.

There are no bond angle outliers.

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	2718	2623	2623	52	1
1	B	2718	2624	2623	55	2
1	C	2718	2623	2623	52	3
1	D	2718	2623	2623	55	0
2	A	10	14	14	0	0
3	A	7	10	10	0	0
3	D	7	10	10	0	0
4	A	5	0	0	0	0
4	D	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	4	6	6	0	0
7	C	10	8	8	0	0
7	D	10	8	8	0	0
8	A	183	0	0	31	2
8	B	199	0	0	29	4
8	C	194	0	0	26	3
8	D	236	0	0	25	6
All	All	11745	10549	10548	212	17

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 10.

All (212) 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:C:526:ASN:OD1	8:C:701:HOH:O	1.93	0.86
1:C:462:PHE:O	8:C:702:HOH:O	1.97	0.82
1:A:513:SER:N	8:A:709:HOH:O	2.11	0.82
1:B:484:ARG:NH2	8:B:710:HOH:O	2.11	0.81
1:A:303:ASP:OD2	8:A:701:HOH:O	1.99	0.80
1:D:406:ASP:OD1	8:D:802:HOH:O	1.99	0.80
1:B:514:GLN:OE1	8:B:702:HOH:O	2.01	0.79
1:C:488:LEU:O	8:C:703:HOH:O	2.00	0.79
1:B:443:THR:O	8:B:703:HOH:O	2.01	0.78
1:B:379:TRP:O	8:B:701:HOH:O	2.00	0.78
1:A:514:GLN:OE1	8:A:702:HOH:O	2.02	0.78
1:C:271:ASN:OD1	1:C:273:SER:OG	2.02	0.76
1:D:391:ASN:O	8:D:803:HOH:O	2.01	0.76
1:C:368:GLN:O	8:C:707:HOH:O	2.03	0.76
1:A:294:ARG:NH1	8:A:715:HOH:O	2.19	0.76
1:A:405:ASP:OD1	1:A:408:ASN:ND2	2.18	0.76
1:C:291:ASP:OD1	8:C:708:HOH:O	2.04	0.76
1:A:436:GLU:OE1	8:A:705:HOH:O	2.04	0.75
1:A:281:GLU:OE2	8:A:704:HOH:O	2.03	0.75
1:A:304:ASN:OD1	8:A:703:HOH:O	2.03	0.75
1:B:444:VAL:N	8:B:711:HOH:O	2.12	0.75
1:D:291:ASP:OD1	8:D:805:HOH:O	2.05	0.74
1:B:422:ASP:OD1	8:B:705:HOH:O	2.05	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:GLN:HB2	1:D:585:ALA:HB2	1.68	0.74
1:B:384:GLY:O	8:B:704:HOH:O	2.04	0.74
1:A:355:ARG:NH1	8:A:716:HOH:O	2.20	0.73
1:C:300:ASN:ND2	8:C:720:HOH:O	2.20	0.73
1:D:339:TYR:O	8:D:804:HOH:O	2.04	0.73
1:D:347:ASP:OD1	8:D:806:HOH:O	2.06	0.73
1:B:580:GLU:OE2	8:B:702:HOH:O	2.06	0.73
1:C:254:ARG:NH2	8:C:715:HOH:O	2.21	0.73
1:D:303:ASP:OD1	1:D:351:SER:OG	2.06	0.73
1:A:566:GLN:NE2	8:A:720:HOH:O	2.21	0.73
1:B:357:ALA:O	8:B:707:HOH:O	2.08	0.72
1:A:516:GLN:OE1	8:A:708:HOH:O	2.07	0.72
1:B:407:SER:O	8:B:706:HOH:O	2.07	0.72
1:C:428:ASN:OD1	8:C:710:HOH:O	2.08	0.72
1:A:565:ASP:OD2	8:A:706:HOH:O	2.06	0.71
1:A:463:ASP:OD2	8:A:707:HOH:O	2.06	0.71
1:C:322:LEU:HD21	1:C:353:LEU:HA	1.72	0.70
1:C:510:ASN:O	8:C:709:HOH:O	2.08	0.70
1:D:552:HIS:O	8:D:807:HOH:O	2.09	0.69
1:B:287:GLU:OE2	8:B:708:HOH:O	2.08	0.69
1:B:335:ASN:OD1	8:B:709:HOH:O	2.10	0.69
1:C:493:ASP:OD2	8:C:711:HOH:O	2.09	0.69
1:B:355:ARG:NH1	8:B:717:HOH:O	2.25	0.69
1:D:549:ASN:O	8:D:808:HOH:O	2.10	0.68
1:A:545:LEU:HG	1:A:555:THR:HG22	1.74	0.68
1:A:484:ARG:NH2	8:A:724:HOH:O	2.25	0.68
1:D:456:THR:O	8:D:809:HOH:O	2.11	0.68
1:D:325:ARG:O	8:D:811:HOH:O	2.12	0.68
1:B:484:ARG:NH2	8:B:719:HOH:O	2.27	0.68
1:D:424:ASP:OD2	8:D:810:HOH:O	2.12	0.68
1:C:422:ASP:OD2	8:C:712:HOH:O	2.11	0.67
1:C:389:GLU:OE2	8:C:714:HOH:O	2.12	0.67
1:C:505:VAL:O	8:C:715:HOH:O	2.13	0.67
1:C:384:GLY:O	8:C:713:HOH:O	2.12	0.67
1:B:440:PHE:O	8:B:703:HOH:O	2.12	0.66
1:D:365:PRO:O	8:D:812:HOH:O	2.12	0.66
1:C:538:ILE:HG21	1:C:572:LEU:HD21	1.77	0.66
1:A:428:ASN:ND2	8:A:728:HOH:O	2.28	0.66
1:B:479:GLY:O	8:B:712:HOH:O	2.13	0.66
1:C:559:HIS:NE2	8:C:728:HOH:O	2.28	0.66
1:A:361:ASP:OD1	8:A:710:HOH:O	2.12	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:ASP:OD2	8:C:716:HOH:O	2.13	0.66
1:A:335:ASN:OD1	8:A:711:HOH:O	2.13	0.65
1:B:525:HIS:NE2	1:B:579:GLU:OE1	2.30	0.65
1:B:388:GLN:NE2	8:B:721:HOH:O	2.28	0.65
1:B:411:ASN:O	1:B:413:VAL:N	2.30	0.65
1:D:540:THR:OG1	8:D:814:HOH:O	2.15	0.65
1:C:426:GLN:NE2	8:C:712:HOH:O	2.25	0.65
1:A:482:ALA:O	8:A:712:HOH:O	2.14	0.65
1:B:321:VAL:O	1:B:325:ARG:N	2.29	0.65
1:C:244:VAL:HG23	1:C:324:THR:HG21	1.76	0.65
1:D:259:GLY:O	8:D:813:HOH:O	2.14	0.65
1:B:268:ASP:OD2	1:B:403:ASN:ND2	2.29	0.64
1:A:512:TYR:N	8:A:709:HOH:O	2.31	0.64
1:B:388:GLN:NE2	8:B:722:HOH:O	2.31	0.63
1:A:317:TYR:OH	1:A:580:GLU:O	2.11	0.62
1:D:244:VAL:N	1:D:583:PHE:O	2.33	0.62
1:A:379:TRP:CG	1:A:397:ILE:HD11	2.36	0.61
1:A:253:TYR:N	1:A:506:SER:OG	2.34	0.61
1:A:293:THR:O	1:A:470:GLN:NE2	2.33	0.61
1:D:276:GLU:OE2	8:D:815:HOH:O	2.16	0.61
1:B:345:SER:OG	1:B:347:ASP:OD1	2.19	0.61
1:C:320:GLY:O	1:C:324:THR:HG23	2.00	0.60
1:A:555:THR:HG23	1:A:566:GLN:OE1	2.02	0.60
1:C:560:GLY:O	1:C:562:LYS:NZ	2.33	0.60
1:A:458:GLU:O	8:A:713:HOH:O	2.17	0.59
1:A:252:HIS:HB2	1:A:506:SER:OG	2.02	0.59
1:D:504:HIS:O	8:D:816:HOH:O	2.17	0.59
1:D:470:GLN:NE2	8:D:828:HOH:O	2.35	0.59
1:B:274:ARG:NE	8:B:720:HOH:O	2.27	0.59
1:A:405:ASP:N	8:A:735:HOH:O	2.35	0.58
1:C:318:MET:SD	1:C:353:LEU:HD13	2.44	0.58
1:C:461:ARG:O	8:C:717:HOH:O	2.17	0.58
1:D:548:ASN:ND2	8:D:807:HOH:O	2.36	0.58
1:B:426:GLN:OE1	1:B:429:ARG:NH1	2.36	0.58
1:C:379:TRP:CG	1:C:397:ILE:HD11	2.39	0.57
1:D:547:LEU:HD13	1:D:573:LEU:HD11	1.85	0.57
1:C:571:SER:OG	1:D:550:ASN:O	2.21	0.57
1:A:538:ILE:N	8:A:736:HOH:O	2.36	0.57
1:C:410:LYS:O	1:C:412:PHE:N	2.38	0.57
1:C:481:PRO:O	1:C:483:GLN:NE2	2.36	0.57
1:D:527:TRP:HB3	1:D:540:THR:HG22	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:510:ASN:O	1:D:582:ARG:NH1	2.36	0.56
1:B:337:GLN:O	1:B:392:ARG:NH1	2.37	0.56
1:D:318:MET:O	1:D:321:VAL:N	2.39	0.55
1:A:347:ASP:OD2	1:A:349:PHE:N	2.39	0.55
1:C:582:ARG:NH1	8:C:709:HOH:O	2.37	0.55
1:D:379:TRP:HE1	1:D:395:SER:HG	1.55	0.55
1:D:343:LEU:HD22	1:D:396:TRP:HB3	1.89	0.55
1:B:443:THR:HG23	8:B:711:HOH:O	2.06	0.55
1:A:322:LEU:HD21	1:A:353:LEU:HA	1.89	0.54
1:C:245:GLN:N	8:C:738:HOH:O	2.40	0.54
1:A:460:ASN:ND2	1:A:460:ASN:O	2.37	0.54
1:D:547:LEU:HD12	1:D:553:TYR:HB3	1.89	0.54
1:C:379:TRP:HE1	1:C:395:SER:HG	1.54	0.54
1:A:255:ASP:OD1	1:A:504:HIS:ND1	2.38	0.54
1:B:538:ILE:HD12	1:B:545:LEU:HD22	1.90	0.53
1:A:292:PHE:CE2	1:A:485:ILE:HD13	2.43	0.53
1:C:485:ILE:CG2	1:C:487:VAL:HG22	2.38	0.53
1:D:408:ASN:O	1:D:412:PHE:N	2.42	0.52
1:D:411:ASN:ND2	8:D:834:HOH:O	2.39	0.52
1:A:245:GLN:HB2	1:A:585:ALA:HB2	1.90	0.52
1:B:514:GLN:HB2	8:B:713:HOH:O	2.09	0.52
1:B:255:ASP:OD1	1:B:257:GLY:N	2.42	0.52
1:B:325:ARG:NE	1:B:356:GLN:O	2.40	0.52
1:C:339:TYR:OH	8:C:704:HOH:O	2.00	0.51
1:B:312:GLY:O	8:B:713:HOH:O	2.18	0.51
1:B:295:HIS:CE1	1:B:473:LEU:HD22	2.45	0.51
1:D:361:ASP:O	8:D:817:HOH:O	2.19	0.51
1:C:322:LEU:HD22	1:C:356:GLN:HB2	1.92	0.51
1:C:460:ASN:O	8:C:719:HOH:O	2.20	0.51
1:D:379:TRP:CG	1:D:397:ILE:HD11	2.46	0.50
1:C:258:THR:OG1	1:C:260:GLN:OE1	2.23	0.50
1:D:440:PHE:O	1:D:476:HIS:NE2	2.43	0.50
1:A:422:ASP:OD1	8:A:714:HOH:O	2.18	0.50
1:B:370:GLN:OE1	8:B:714:HOH:O	2.20	0.50
1:C:304:ASN:OD1	8:C:718:HOH:O	2.19	0.49
1:D:340:GLN:O	1:D:341:LEU:HD12	2.12	0.49
1:A:467:GLY:O	8:A:717:HOH:O	2.20	0.49
1:B:323:SER:OG	1:B:324:THR:HG23	2.13	0.49
1:B:492:THR:HG21	8:B:713:HOH:O	2.12	0.49
1:A:532:ASP:OD1	1:A:535:THR:N	2.45	0.48
1:B:379:TRP:CG	1:B:397:ILE:HD11	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ASP:O	1:B:523:ARG:NH1	2.38	0.48
1:D:325:ARG:NE	8:D:846:HOH:O	2.47	0.48
1:D:366:ALA:O	1:D:368:GLN:N	2.47	0.47
1:D:439:LYS:O	1:D:443:THR:OG1	2.25	0.47
1:C:292:PHE:O	8:C:721:HOH:O	2.21	0.47
1:C:244:VAL:HG13	1:C:244:VAL:O	2.16	0.46
1:A:341:LEU:HD23	1:A:343:LEU:HD11	1.97	0.46
1:D:362:PHE:N	8:D:845:HOH:O	2.46	0.46
1:B:573:LEU:HD23	1:B:577:LEU:HD12	1.97	0.46
1:A:392:ARG:NH2	8:A:733:HOH:O	2.33	0.46
1:B:345:SER:N	8:B:739:HOH:O	2.46	0.46
1:D:532:ASP:OD1	1:D:535:THR:N	2.49	0.45
1:B:563:ILE:O	1:B:566:GLN:NE2	2.48	0.45
1:A:347:ASP:OD1	8:A:718:HOH:O	2.21	0.45
1:C:379:TRP:NE1	1:C:395:SER:OG	2.50	0.45
1:D:386:TYR:N	8:D:850:HOH:O	2.49	0.45
1:C:569:GLN:O	8:C:722:HOH:O	2.21	0.45
1:C:513:SER:O	1:C:582:ARG:NH2	2.50	0.44
1:D:363:SER:O	1:D:364:MET:HG2	2.17	0.44
1:B:319:ASP:O	1:B:323:SER:HB3	2.17	0.44
1:A:356:GLN:NE2	8:A:754:HOH:O	2.49	0.43
1:B:355:ARG:HH21	1:B:367:ALA:HB2	1.83	0.43
1:B:534:SER:O	1:B:549:ASN:N	2.46	0.43
1:B:570:LEU:HD23	1:B:573:LEU:HD22	2.00	0.43
1:D:259:GLY:HA2	1:D:392:ARG:HE	1.83	0.43
1:C:553:TYR:CD2	1:D:570:LEU:HD22	2.53	0.43
1:A:572:LEU:O	1:A:576:VAL:HG23	2.17	0.43
1:A:406:ASP:OD1	1:A:406:ASP:N	2.49	0.43
1:B:532:ASP:OD1	1:B:535:THR:N	2.48	0.43
1:C:546:VAL:O	1:C:553:TYR:HB2	2.18	0.42
1:C:547:LEU:HD12	1:C:553:TYR:HB3	2.00	0.42
1:D:411:ASN:O	1:D:415:ARG:N	2.52	0.42
1:C:432:ASN:O	1:C:435:ARG:N	2.53	0.42
1:D:361:ASP:N	8:D:845:HOH:O	2.53	0.42
1:D:411:ASN:OD1	8:D:819:HOH:O	2.21	0.42
1:A:442:ASN:ND2	8:A:745:HOH:O	2.43	0.42
1:B:489:THR:HG22	8:B:751:HOH:O	2.20	0.42
1:A:253:TYR:CE2	1:A:505:VAL:HG22	2.55	0.42
1:B:323:SER:OG	1:B:324:THR:N	2.52	0.42
1:D:267:VAL:HG21	1:D:270:LEU:HD11	2.02	0.41
1:D:543:MET:SD	1:D:555:THR:HB	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:GLN:HA	1:B:558:LEU:HD11	2.01	0.41
1:D:360:SER:OG	1:D:360:SER:O	2.30	0.41
1:D:586:ASN:HD22	1:D:586:ASN:HA	1.72	0.41
1:B:463:ASP:OD2	8:B:715:HOH:O	2.21	0.41
1:D:288:GLN:OE1	8:D:818:HOH:O	2.21	0.41
1:D:490:ASP:OD1	1:D:528:VAL:HB	2.20	0.41
1:B:292:PHE:O	8:B:716:HOH:O	2.22	0.41
1:C:406:ASP:OD1	1:C:406:ASP:N	2.53	0.41
1:B:323:SER:HG	1:B:324:THR:N	2.18	0.41
1:A:488:LEU:N	8:A:755:HOH:O	2.50	0.41
1:B:262:VAL:HA	8:B:711:HOH:O	2.20	0.41
1:C:385:ARG:O	1:C:387:ALA:N	2.50	0.41
1:A:364:MET:O	8:A:716:HOH:O	2.22	0.41
1:C:355:ARG:NE	8:C:750:HOH:O	2.53	0.41
1:D:545:LEU:HD21	1:D:553:TYR:HD1	1.86	0.41
1:B:337:GLN:NE2	1:B:503:LEU:O	2.53	0.41
1:B:581:LYS:HB3	1:B:584:ILE:HD12	2.02	0.40
1:C:536:LEU:N	1:C:547:LEU:O	2.45	0.40
1:A:407:SER:O	8:A:719:HOH:O	2.21	0.40
1:C:408:ASN:OD1	1:C:409:GLN:N	2.54	0.40
1:D:292:PHE:CE2	1:D:485:ILE:HD13	2.55	0.40
1:A:266:THR:OG1	1:A:396:TRP:NE1	2.44	0.40
1:A:333:ALA:CB	1:A:503:LEU:HD13	2.52	0.40
1:A:559:HIS:O	8:A:722:HOH:O	2.22	0.40
1:D:567:LYS:O	1:D:569:GLN:HG2	2.22	0.40

All (17) 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:B:407:SER:OG	1:B:435:ARG:O[1_655]	1.90	0.30
1:C:322:LEU:O	1:C:484:ARG:NH2[1_655]	1.98	0.22
8:D:979:HOH:O	8:D:983:HOH:O[1_665]	2.04	0.16
8:B:852:HOH:O	8:B:878:HOH:O[1_445]	2.05	0.15
8:B:888:HOH:O	8:B:897:HOH:O[1_445]	2.06	0.14
8:B:880:HOH:O	8:B:895:HOH:O[1_565]	2.08	0.12
8:C:894:HOH:O	8:D:1031:HOH:O[1_455]	2.08	0.12
8:C:845:HOH:O	8:C:849:HOH:O[1_565]	2.08	0.12
8:B:838:HOH:O	8:B:846:HOH:O[1_545]	2.09	0.11
1:A:289:ASN:O	1:A:325:ARG:NH1[1_655]	2.09	0.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:893:HOH:O	8:D:906:HOH:O[1_455]	2.12	0.08
1:B:368:GLN:NE2	8:C:713:HOH:O[1_545]	2.12	0.08
8:A:823:HOH:O	8:D:856:HOH:O[1_556]	2.13	0.07
8:D:879:HOH:O	8:D:881:HOH:O[1_655]	2.13	0.07
1:C:250:ASN:ND2	1:C:557:ASP:OD1[1_665]	2.14	0.06
8:A:801:HOH:O	8:D:950:HOH:O[1_556]	2.18	0.02
1:C:250:ASN:HD22	1:C:557:ASP:OD1[1_665]	1.59	0.01

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	341/368 (93%)	308 (90%)	29 (8%)	4 (1%)	13	4
1	B	341/368 (93%)	302 (89%)	31 (9%)	8 (2%)	6	1
1	C	341/368 (93%)	307 (90%)	27 (8%)	7 (2%)	7	1
1	D	341/368 (93%)	317 (93%)	20 (6%)	4 (1%)	13	4
All	All	1364/1472 (93%)	1234 (90%)	107 (8%)	23 (2%)	9	2

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	409	GLN
1	B	407	SER
1	B	410	LYS
1	C	410	LYS
1	D	367	ALA
1	A	367	ALA
1	B	367	ALA
1	C	391	ASN
1	C	405	ASP
1	C	411	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	365	PRO
1	B	412	PHE
1	C	357	ALA
1	D	357	ALA
1	D	390	ASP
1	D	566	GLN
1	A	384	GLY
1	B	319	ASP
1	B	386	TYR
1	C	563	ILE
1	A	357	ALA
1	B	261	ASN
1	C	325	ARG

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	295/315 (94%)	287 (97%)	8 (3%)	44	36
1	B	295/315 (94%)	285 (97%)	10 (3%)	37	27
1	C	295/315 (94%)	289 (98%)	6 (2%)	55	49
1	D	295/315 (94%)	287 (97%)	8 (3%)	44	36
All	All	1180/1260 (94%)	1148 (97%)	32 (3%)	44	36

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	ASP
1	A	275	PHE
1	A	385	ARG
1	A	386	TYR
1	A	395	SER
1	A	460	ASN
1	A	490	ASP
1	A	553	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	275	PHE
1	B	371	SER
1	B	395	SER
1	B	442	ASN
1	B	490	ASP
1	B	491	HIS
1	B	550	ASN
1	B	553	TYR
1	B	562	LYS
1	B	570	LEU
1	C	275	PHE
1	C	277	LYS
1	C	461	ARG
1	C	484	ARG
1	C	491	HIS
1	C	553	TYR
1	D	323	SER
1	D	355	ARG
1	D	360	SER
1	D	490	ASP
1	D	506	SER
1	D	553	TYR
1	D	565	ASP
1	D	586	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	HIS
1	A	304	ASN
1	A	408	ASN
1	B	260	GLN
1	B	370	GLN
1	B	391	ASN
1	C	428	ASN
1	C	468	HIS
1	D	559	HIS
1	D	586	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	PEG	A	602	-	6,6,6	0.48	0	5,5,5	0.43	0
6	EDO	B	601	-	3,3,3	0.76	0	2,2,2	0.55	0
7	PSE	C	601	-	9,9,9	0.85	0	9,12,12	0.68	0
3	PEG	D	702	-	6,6,6	0.49	0	5,5,5	0.47	0
4	PO4	A	603	-	4,4,4	0.91	0	6,6,6	0.43	0
7	PSE	D	701	-	9,9,9	0.84	0	9,12,12	0.68	0
2	PGE	A	601	-	9,9,9	0.31	0	8,8,8	0.35	0
4	PO4	D	703	-	4,4,4	0.93	0	6,6,6	0.44	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	PEG	A	602	-	-	2/4/4/4	-
6	EDO	B	601	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PSE	C	601	-	-	5/8/8/8	-
3	PEG	D	702	-	-	1/4/4/4	-
7	PSE	D	701	-	-	4/8/8/8	-
2	PGE	A	601	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	601	EDO	O1-C1-C2-O2
7	C	601	PSE	O1-C1-C2-N2
7	C	601	PSE	O1-C1-C2-C3
7	C	601	PSE	C3-O1P-P-O3P
7	C	601	PSE	C3-O1P-P-O4P
7	D	701	PSE	C3-O1P-P-O3P
7	C	601	PSE	C3-O1P-P-O2P
3	A	602	PEG	O2-C3-C4-O4
2	A	601	PGE	O1-C1-C2-O2
7	D	701	PSE	O1-C1-C2-C3
2	A	601	PGE	C3-C4-O3-C5
7	D	701	PSE	N2-C2-C3-O1P
7	D	701	PSE	O1-C1-C2-N2
3	A	602	PEG	O1-C1-C2-O2
2	A	601	PGE	O2-C3-C4-O3
3	D	702	PEG	C4-C3-O2-C2

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

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, 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	343/368 (93%)	3.76	295 (86%) 0 0	9, 17, 36, 52	0
1	B	343/368 (93%)	4.33	320 (93%) 0 0	11, 19, 34, 64	0
1	C	343/368 (93%)	4.09	307 (89%) 0 0	11, 18, 35, 52	0
1	D	343/368 (93%)	3.84	295 (86%) 0 0	9, 16, 36, 52	0
All	All	1372/1472 (93%)	4.01	1217 (88%) 0 0	9, 18, 36, 64	0

All (1217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	ALA	20.5
1	A	386	TYR	16.9
1	D	391	ASN	14.8
1	C	404	ILE	14.7
1	B	343	LEU	13.4
1	C	386	TYR	13.0
1	B	386	TYR	12.8
1	C	586	ASN	12.6
1	D	386	TYR	12.5
1	A	409	GLN	12.4
1	D	389	GLU	12.1
1	C	391	ASN	11.7
1	D	585	ALA	11.6
1	C	244	VAL	11.6
1	D	406	ASP	11.6
1	C	585	ALA	11.6
1	A	363	SER	11.3
1	B	411	ASN	11.3
1	C	411	ASN	11.1
1	B	456	THR	10.8
1	D	410	LYS	10.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	407	SER	10.7
1	D	586	ASN	10.7
1	C	408	ASN	10.7
1	B	285	PHE	10.6
1	D	405	ASP	10.6
1	C	552	HIS	10.6
1	B	553	TYR	10.5
1	D	565	ASP	10.3
1	C	387	ALA	10.1
1	C	405	ASP	10.1
1	A	553	TYR	10.1
1	B	406	ASP	9.8
1	B	383	LEU	9.8
1	C	568	PRO	9.7
1	D	515	GLY	9.6
1	D	390	ASP	9.6
1	C	553	TYR	9.6
1	B	251	LEU	9.5
1	B	550	ASN	9.5
1	D	486	ASN	9.5
1	B	364	MET	9.4
1	A	387	ALA	9.4
1	C	569	GLN	9.3
1	D	461	ARG	9.3
1	C	406	ASP	9.2
1	B	408	ASN	9.2
1	C	456	THR	9.2
1	B	530	ALA	9.2
1	D	387	ALA	9.1
1	A	568	PRO	9.1
1	D	549	ASN	9.0
1	B	407	SER	9.0
1	A	533	GLY	9.0
1	D	411	ASN	8.9
1	A	244	VAL	8.9
1	B	558	LEU	8.6
1	D	552	HIS	8.5
1	B	485	ILE	8.5
1	C	413	VAL	8.4
1	C	349	PHE	8.4
1	D	570	LEU	8.4
1	A	256	MET	8.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	340	GLN	8.3
1	C	389	GLU	8.2
1	D	367	ALA	8.1
1	C	572	LEU	8.1
1	D	533	GLY	8.0
1	D	564	LYS	8.0
1	C	394	PHE	7.9
1	B	521	VAL	7.9
1	B	404	ILE	7.9
1	B	244	VAL	7.9
1	C	251	LEU	7.8
1	D	502	LEU	7.8
1	A	526	ASN	7.8
1	C	397	ILE	7.8
1	B	454	PRO	7.7
1	B	390	ASP	7.7
1	A	353	LEU	7.6
1	B	585	ALA	7.6
1	B	551	GLY	7.6
1	B	478	PRO	7.5
1	B	275	PHE	7.5
1	D	440	PHE	7.5
1	A	390	ASP	7.4
1	C	362	PHE	7.4
1	D	534	SER	7.3
1	A	570	LEU	7.3
1	C	270	LEU	7.3
1	A	521	VAL	7.3
1	C	548	ASN	7.3
1	A	273	SER	7.3
1	A	461	ARG	7.3
1	D	563	ILE	7.3
1	B	440	PHE	7.2
1	A	408	ASN	7.1
1	B	430	VAL	7.1
1	B	321	VAL	7.1
1	C	409	GLN	7.1
1	A	248	LEU	7.1
1	B	389	GLU	7.1
1	D	366	ALA	7.0
1	C	440	PHE	7.0
1	C	290	ILE	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	399	PHE	6.9
1	C	280	PRO	6.9
1	C	565	ASP	6.9
1	D	457	PRO	6.9
1	B	342	GLY	6.9
1	A	252	HIS	6.8
1	B	247	PRO	6.8
1	B	433	ALA	6.8
1	D	409	GLN	6.8
1	B	391	ASN	6.8
1	B	573	LEU	6.8
1	B	331	ILE	6.8
1	B	312	GLY	6.7
1	C	348	GLY	6.7
1	B	350	ALA	6.7
1	C	334	LEU	6.7
1	B	387	ALA	6.7
1	C	562	LYS	6.7
1	C	494	VAL	6.7
1	D	341	LEU	6.7
1	C	462	PHE	6.7
1	B	460	ASN	6.6
1	A	560	GLY	6.6
1	B	333	ALA	6.6
1	A	407	SER	6.6
1	C	275	PHE	6.6
1	B	435	ARG	6.5
1	D	567	LYS	6.5
1	B	382	TRP	6.5
1	C	393	TRP	6.5
1	B	258	THR	6.5
1	D	507	THR	6.4
1	C	340	GLN	6.4
1	D	407	SER	6.4
1	B	340	GLN	6.4
1	A	385	ARG	6.4
1	B	265	ILE	6.4
1	B	412	PHE	6.4
1	C	519	PHE	6.4
1	C	480	THR	6.4
1	A	277	LYS	6.3
1	A	584	ILE	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	522	PRO	6.3
1	B	519	PHE	6.3
1	D	362	PHE	6.3
1	D	583	PHE	6.2
1	B	416	TYR	6.2
1	C	533	GLY	6.2
1	B	417	ALA	6.2
1	B	453	ILE	6.2
1	B	414	LYS	6.2
1	B	301	THR	6.2
1	A	573	LEU	6.1
1	B	362	PHE	6.1
1	C	396	TRP	6.1
1	A	290	ILE	6.1
1	A	364	MET	6.1
1	B	349	PHE	6.1
1	D	397	ILE	6.1
1	A	422	ASP	6.0
1	D	569	GLN	6.0
1	B	528	VAL	6.0
1	B	409	GLN	6.0
1	A	362	PHE	6.0
1	B	543	MET	5.9
1	C	419	ALA	5.9
1	C	482	ALA	5.9
1	B	392	ARG	5.9
1	B	457	PRO	5.9
1	B	420	ALA	5.9
1	C	344	PHE	5.9
1	D	584	ILE	5.9
1	C	341	LEU	5.9
1	B	261	ASN	5.9
1	D	412	PHE	5.9
1	B	264	LEU	5.9
1	C	381	ASP	5.9
1	D	485	ILE	5.9
1	B	270	LEU	5.9
1	C	434	LEU	5.9
1	A	565	ASP	5.9
1	B	472	PRO	5.9
1	D	259	GLY	5.9
1	C	379	TRP	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	527	TRP	5.8
1	A	330	LEU	5.8
1	D	526	ASN	5.8
1	A	520	THR	5.8
1	D	363	SER	5.8
1	A	550	ASN	5.8
1	C	307	PHE	5.8
1	B	413	VAL	5.8
1	A	456	THR	5.8
1	B	464	TRP	5.8
1	B	276	GLU	5.8
1	C	474	VAL	5.8
1	C	277	LYS	5.7
1	B	366	ALA	5.7
1	C	265	ILE	5.7
1	D	402	THR	5.7
1	B	466	GLN	5.7
1	A	430	VAL	5.7
1	B	526	ASN	5.7
1	C	442	ASN	5.7
1	D	566	GLN	5.7
1	C	339	TYR	5.7
1	C	526	ASN	5.7
1	A	542	GLN	5.7
1	C	463	ASP	5.6
1	A	567	LYS	5.6
1	B	545	LEU	5.6
1	C	332	THR	5.6
1	C	384	GLY	5.6
1	B	272	TYR	5.6
1	A	360	SER	5.6
1	B	262	VAL	5.6
1	B	336	GLN	5.6
1	B	393	TRP	5.5
1	A	352	PRO	5.5
1	B	388	GLN	5.5
1	C	289	ASN	5.5
1	A	396	TRP	5.5
1	A	415	ARG	5.5
1	C	363	SER	5.5
1	C	551	GLY	5.5
1	B	326	THR	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	389	GLU	5.5
1	B	259	GLY	5.5
1	D	334	LEU	5.5
1	D	525	HIS	5.5
1	A	556	TYR	5.5
1	D	275	PHE	5.5
1	C	477	TRP	5.5
1	B	492	THR	5.5
1	D	419	ALA	5.5
1	A	545	LEU	5.5
1	A	515	GLY	5.4
1	B	338	GLY	5.4
1	D	388	GLN	5.4
1	D	414	LYS	5.4
1	D	250	ASN	5.4
1	A	384	GLY	5.4
1	B	455	LEU	5.4
1	C	383	LEU	5.4
1	A	405	ASP	5.4
1	B	462	PHE	5.4
1	B	506	SER	5.4
1	B	487	VAL	5.4
1	A	489	THR	5.4
1	B	486	ASN	5.4
1	B	565	ASP	5.3
1	B	552	HIS	5.3
1	D	408	ASN	5.3
1	B	365	PRO	5.3
1	B	477	TRP	5.3
1	C	286	ALA	5.3
1	A	335	ASN	5.3
1	C	514	GLN	5.3
1	A	460	ASN	5.3
1	B	299	GLY	5.3
1	D	323	SER	5.3
1	D	348	GLY	5.3
1	D	379	TRP	5.2
1	C	531	ALA	5.2
1	D	396	TRP	5.2
1	B	491	HIS	5.2
1	D	427	ILE	5.2
1	A	319	ASP	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	251	LEU	5.2
1	B	246	TYR	5.2
1	B	567	LYS	5.2
1	C	520	THR	5.2
1	C	582	ARG	5.2
1	A	344	PHE	5.1
1	A	246	TYR	5.1
1	D	324	THR	5.1
1	B	419	ALA	5.1
1	B	292	PHE	5.1
1	B	436	GLU	5.1
1	A	549	ASN	5.1
1	D	545	LEU	5.1
1	B	266	THR	5.1
1	C	272	TYR	5.1
1	A	524	ARG	5.1
1	C	521	VAL	5.1
1	C	438	GLY	5.1
1	B	484	ARG	5.1
1	A	263	LEU	5.1
1	A	416	TYR	5.1
1	B	354	TYR	5.1
1	D	439	LYS	5.1
1	A	342	GLY	5.1
1	B	284	THR	5.1
1	B	476	HIS	5.1
1	C	412	PHE	5.1
1	A	368	GLN	5.1
1	D	572	LEU	5.1
1	C	367	ALA	5.0
1	A	569	GLN	5.0
1	B	324	THR	5.0
1	C	410	LYS	5.0
1	C	357	ALA	5.0
1	C	441	ASP	5.0
1	A	574	LEU	5.0
1	B	520	THR	5.0
1	B	252	HIS	5.0
1	A	412	PHE	5.0
1	B	522	PRO	5.0
1	C	245	GLN	5.0
1	D	309	LEU	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	458	GLU	5.0
1	A	365	PRO	4.9
1	D	385	ARG	4.9
1	D	501	ARG	4.9
1	D	365	PRO	4.9
1	D	353	LEU	4.9
1	A	534	SER	4.9
1	B	534	SER	4.9
1	B	586	ASN	4.9
1	A	563	ILE	4.9
1	B	319	ASP	4.9
1	B	422	ASP	4.9
1	C	324	THR	4.9
1	C	555	THR	4.9
1	B	547	LEU	4.9
1	A	512	TYR	4.9
1	A	262	VAL	4.9
1	C	273	SER	4.9
1	D	498	LEU	4.9
1	A	253	TYR	4.8
1	B	421	SER	4.8
1	A	369	THR	4.8
1	C	369	THR	4.8
1	C	392	ARG	4.8
1	C	361	ASP	4.8
1	D	421	SER	4.8
1	C	263	LEU	4.8
1	D	392	ARG	4.8
1	A	437	ALA	4.8
1	A	455	LEU	4.8
1	C	547	LEU	4.8
1	B	583	PHE	4.8
1	C	318	MET	4.8
1	A	487	VAL	4.8
1	A	586	ASN	4.8
1	D	518	ILE	4.8
1	A	527	TRP	4.8
1	B	405	ASP	4.8
1	D	413	VAL	4.8
1	B	531	ALA	4.7
1	D	464	TRP	4.7
1	C	583	PHE	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	416	TYR	4.7
1	C	382	TRP	4.7
1	C	455	LEU	4.7
1	D	264	LEU	4.7
1	D	394	PHE	4.7
1	C	390	ASP	4.7
1	B	563	ILE	4.7
1	A	499	MET	4.7
1	C	377	SER	4.7
1	D	270	LEU	4.7
1	A	376	ALA	4.7
1	B	437	ALA	4.7
1	C	453	ILE	4.7
1	A	264	LEU	4.7
1	C	536	LEU	4.7
1	D	284	THR	4.7
1	B	542	GLN	4.7
1	C	364	MET	4.7
1	A	411	ASN	4.7
1	B	359	LEU	4.6
1	D	547	LEU	4.6
1	C	271	ASN	4.6
1	D	399	PHE	4.6
1	C	475	ILE	4.6
1	D	380	ILE	4.6
1	D	382	TRP	4.6
1	D	423	VAL	4.6
1	B	473	LEU	4.6
1	A	519	PHE	4.6
1	C	246	TYR	4.6
1	D	404	ILE	4.6
1	A	421	SER	4.6
1	A	525	HIS	4.6
1	B	254	ARG	4.6
1	A	305	GLY	4.6
1	D	529	THR	4.5
1	B	415	ARG	4.5
1	B	438	GLY	4.5
1	A	535	THR	4.5
1	C	283	ALA	4.5
1	B	527	TRP	4.5
1	D	248	LEU	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	361	ASP	4.5
1	B	369	THR	4.5
1	C	402	THR	4.5
1	C	460	ASN	4.5
1	A	543	MET	4.5
1	B	467	GLY	4.5
1	C	485	ILE	4.5
1	C	584	ILE	4.5
1	B	523	ARG	4.5
1	A	382	TRP	4.5
1	A	445	VAL	4.5
1	D	344	PHE	4.5
1	D	512	TYR	4.5
1	C	287	GLU	4.5
1	A	539	THR	4.5
1	C	326	THR	4.5
1	A	477	TRP	4.5
1	B	337	GLN	4.5
1	C	256	MET	4.5
1	A	440	PHE	4.5
1	D	292	PHE	4.5
1	C	454	PRO	4.5
1	B	469	LEU	4.4
1	A	452	GLY	4.4
1	A	391	ASN	4.4
1	C	380	ILE	4.4
1	C	398	SER	4.4
1	A	581	LYS	4.4
1	C	567	LYS	4.4
1	B	361	ASP	4.4
1	C	487	VAL	4.4
1	C	578	THR	4.4
1	A	469	LEU	4.4
1	B	458	GLU	4.4
1	B	490	ASP	4.4
1	A	537	ALA	4.4
1	D	301	THR	4.4
1	B	384	GLY	4.4
1	D	580	GLU	4.4
1	A	333	ALA	4.4
1	B	549	ASN	4.4
1	D	436	GLU	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	338	GLY	4.4
1	D	313	ILE	4.4
1	A	285	PHE	4.4
1	A	585	ALA	4.4
1	C	476	HIS	4.4
1	D	306	ILE	4.3
1	D	310	PHE	4.3
1	C	323	SER	4.3
1	D	244	VAL	4.3
1	D	576	VAL	4.3
1	A	478	PRO	4.3
1	B	541	PRO	4.3
1	C	259	GLY	4.3
1	B	307	PHE	4.3
1	B	352	PRO	4.3
1	B	508	PRO	4.3
1	A	558	LEU	4.3
1	A	572	LEU	4.3
1	D	445	VAL	4.3
1	A	283	ALA	4.3
1	A	350	ALA	4.3
1	B	329	ALA	4.3
1	A	311	TYR	4.3
1	D	256	MET	4.3
1	A	544	THR	4.3
1	D	456	THR	4.3
1	D	535	THR	4.3
1	A	339	TYR	4.2
1	B	253	TYR	4.2
1	B	317	TYR	4.2
1	B	353	LEU	4.2
1	D	556	TYR	4.2
1	C	459	GLU	4.2
1	D	522	PRO	4.2
1	C	322	LEU	4.2
1	C	543	MET	4.2
1	C	570	LEU	4.2
1	D	455	LEU	4.2
1	D	553	TYR	4.2
1	B	310	PHE	4.2
1	C	444	VAL	4.2
1	B	357	ALA	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	254	ARG	4.2
1	A	498	LEU	4.2
1	A	393	TRP	4.2
1	D	568	PRO	4.2
1	C	388	GLN	4.2
1	C	461	ARG	4.2
1	B	447	ILE	4.2
1	B	257	GLY	4.2
1	C	310	PHE	4.2
1	D	279	MET	4.2
1	A	562	LYS	4.2
1	B	320	GLY	4.2
1	B	297	SER	4.2
1	C	558	LEU	4.2
1	D	358	LEU	4.2
1	D	469	LEU	4.2
1	A	267	VAL	4.2
1	D	462	PHE	4.2
1	D	257	GLY	4.1
1	A	383	LEU	4.1
1	B	309	LEU	4.1
1	B	518	ILE	4.1
1	C	331	ILE	4.1
1	D	416	TYR	4.1
1	B	474	VAL	4.1
1	D	321	VAL	4.1
1	B	394	PHE	4.1
1	D	524	ARG	4.1
1	D	360	SER	4.1
1	D	434	LEU	4.1
1	A	331	ILE	4.1
1	A	392	ARG	4.1
1	D	494	VAL	4.1
1	A	566	GLN	4.1
1	B	511	GLU	4.1
1	B	498	LEU	4.1
1	C	423	VAL	4.1
1	D	571	SER	4.1
1	C	385	ARG	4.1
1	C	350	ALA	4.1
1	A	309	LEU	4.1
1	B	323	SER	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	538	ILE	4.1
1	A	259	GLY	4.1
1	C	319	ASP	4.1
1	A	434	LEU	4.0
1	A	488	LEU	4.0
1	B	431	LEU	4.0
1	B	548	ASN	4.0
1	D	477	TRP	4.0
1	C	313	ILE	4.0
1	B	570	LEU	4.0
1	C	472	PRO	4.0
1	B	494	VAL	4.0
1	B	305	GLY	4.0
1	C	581	LYS	4.0
1	A	571	SER	4.0
1	B	482	ALA	4.0
1	C	486	ASN	4.0
1	B	256	MET	4.0
1	A	540	THR	4.0
1	B	332	THR	4.0
1	C	564	LYS	4.0
1	D	332	THR	4.0
1	D	573	LEU	4.0
1	A	413	VAL	4.0
1	C	561	GLU	4.0
1	B	376	ALA	4.0
1	A	463	ASP	4.0
1	D	347	ASP	4.0
1	C	252	HIS	4.0
1	D	258	THR	4.0
1	B	442	ASN	4.0
1	C	353	LEU	4.0
1	B	267	VAL	4.0
1	B	381	ASP	4.0
1	C	262	VAL	4.0
1	D	286	ALA	4.0
1	B	300	ASN	4.0
1	C	507	THR	4.0
1	A	361	ASP	4.0
1	A	254	ARG	4.0
1	A	313	ILE	3.9
1	A	518	ILE	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	258	THR	3.9
1	B	512	TYR	3.9
1	B	410	LYS	3.9
1	A	343	LEU	3.9
1	C	342	GLY	3.9
1	C	452	GLY	3.9
1	A	546	VAL	3.9
1	A	306	ILE	3.9
1	B	375	THR	3.9
1	B	535	THR	3.9
1	C	427	ILE	3.9
1	B	311	TYR	3.9
1	B	510	ASN	3.9
1	C	436	GLU	3.9
1	B	379	TRP	3.9
1	B	358	LEU	3.9
1	B	314	SER	3.9
1	B	318	MET	3.9
1	B	363	SER	3.9
1	C	321	VAL	3.9
1	C	563	ILE	3.9
1	D	557	ASP	3.9
1	A	325	ARG	3.9
1	C	524	ARG	3.9
1	A	337	GLN	3.9
1	C	443	THR	3.9
1	A	321	VAL	3.9
1	D	442	ASN	3.9
1	B	313	ILE	3.9
1	A	410	LYS	3.9
1	C	320	GLY	3.9
1	A	454	PRO	3.9
1	B	249	SER	3.9
1	D	285	PHE	3.8
1	A	266	THR	3.8
1	A	557	ASP	3.8
1	C	415	ARG	3.8
1	C	484	ARG	3.8
1	A	336	GLN	3.8
1	B	536	LEU	3.8
1	A	323	SER	3.8
1	C	354	TYR	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	512	TYR	3.8
1	B	260	GLN	3.8
1	B	399	PHE	3.8
1	C	282	LEU	3.8
1	B	445	VAL	3.8
1	A	447	ILE	3.8
1	C	414	LYS	3.8
1	D	368	GLN	3.8
1	D	428	ASN	3.8
1	A	284	THR	3.8
1	A	480	THR	3.8
1	B	578	THR	3.8
1	A	494	VAL	3.8
1	C	300	ASN	3.8
1	D	327	PRO	3.8
1	D	252	HIS	3.8
1	B	380	ILE	3.8
1	B	475	ILE	3.8
1	C	306	ILE	3.8
1	D	513	SER	3.8
1	B	280	PRO	3.8
1	C	502	LEU	3.8
1	A	528	VAL	3.8
1	A	417	ALA	3.8
1	B	293	THR	3.8
1	B	507	THR	3.8
1	B	538	ILE	3.8
1	D	254	ARG	3.8
1	D	400	ASN	3.8
1	C	504	HIS	3.8
1	A	282	LEU	3.8
1	C	276	GLU	3.8
1	D	543	MET	3.7
1	D	447	ILE	3.7
1	B	339	TYR	3.7
1	D	280	PRO	3.7
1	B	368	GLN	3.7
1	B	560	GLY	3.7
1	B	546	VAL	3.7
1	B	559	HIS	3.7
1	C	446	ILE	3.7
1	B	370	GLN	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	556	TYR	3.7
1	D	354	TYR	3.7
1	C	527	TRP	3.7
1	A	275	PHE	3.7
1	C	298	SER	3.7
1	A	516	GLN	3.7
1	C	356	GLN	3.7
1	B	424	ASP	3.7
1	B	302	THR	3.7
1	A	394	PHE	3.7
1	B	572	LEU	3.7
1	D	343	LEU	3.7
1	D	381	ASP	3.7
1	A	276	GLU	3.7
1	B	308	GLY	3.7
1	B	273	SER	3.7
1	B	367	ALA	3.7
1	D	509	ALA	3.7
1	A	457	PRO	3.7
1	C	577	LEU	3.7
1	A	312	GLY	3.7
1	C	355	ARG	3.7
1	B	514	GLN	3.7
1	A	354	TYR	3.6
1	A	367	ALA	3.6
1	B	322	LEU	3.6
1	C	343	LEU	3.6
1	A	281	GLU	3.6
1	D	505	VAL	3.6
1	B	395	SER	3.6
1	B	289	ASN	3.6
1	C	496	THR	3.6
1	C	538	ILE	3.6
1	D	446	ILE	3.6
1	C	373	ALA	3.6
1	A	381	ASP	3.6
1	C	248	LEU	3.6
1	A	464	TRP	3.6
1	C	292	PHE	3.6
1	D	548	ASN	3.6
1	D	582	ARG	3.6
1	C	327	PRO	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	508	PRO	3.6
1	A	530	ALA	3.6
1	B	524	ARG	3.6
1	C	358	LEU	3.6
1	C	471	VAL	3.6
1	B	532	ASP	3.6
1	C	566	GLN	3.6
1	B	503	LEU	3.6
1	D	319	ASP	3.6
1	B	344	PHE	3.6
1	D	578	THR	3.6
1	B	461	ARG	3.6
1	D	325	ARG	3.6
1	D	463	ASP	3.6
1	D	438	GLY	3.6
1	D	474	VAL	3.6
1	D	300	ASN	3.5
1	A	580	GLU	3.5
1	D	393	TRP	3.5
1	D	317	TYR	3.5
1	D	478	PRO	3.5
1	A	388	GLN	3.5
1	D	375	THR	3.5
1	A	503	LEU	3.5
1	B	574	LEU	3.5
1	B	577	LEU	3.5
1	B	576	VAL	3.5
1	B	579	GLU	3.5
1	C	530	ALA	3.5
1	B	288	GLN	3.5
1	A	257	GLY	3.5
1	B	295	HIS	3.5
1	A	358	LEU	3.5
1	B	283	ALA	3.5
1	B	316	GLY	3.5
1	B	448	THR	3.5
1	C	345	SER	3.5
1	A	523	ARG	3.5
1	B	325	ARG	3.5
1	B	426	GLN	3.5
1	D	378	GLN	3.5
1	D	458	GLU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	432	ASN	3.5
1	C	437	ALA	3.5
1	D	433	ALA	3.5
1	A	247	PRO	3.5
1	A	245	GLN	3.5
1	A	397	ILE	3.5
1	D	514	GLN	3.5
1	A	486	ASN	3.5
1	B	396	TRP	3.5
1	D	322	LEU	3.5
1	D	521	VAL	3.5
1	D	536	LEU	3.5
1	B	355	ARG	3.5
1	C	375	THR	3.5
1	D	490	ASP	3.4
1	D	305	GLY	3.4
1	B	566	GLN	3.4
1	C	368	GLN	3.4
1	B	564	LYS	3.4
1	A	462	PHE	3.4
1	A	453	ILE	3.4
1	A	506	SER	3.4
1	C	376	ALA	3.4
1	C	506	SER	3.4
1	D	383	LEU	3.4
1	D	471	VAL	3.4
1	D	296	MET	3.4
1	B	584	ILE	3.4
1	C	478	PRO	3.4
1	D	481	PRO	3.4
1	A	579	GLU	3.4
1	C	431	LEU	3.4
1	D	430	VAL	3.4
1	A	340	GLN	3.4
1	B	328	ALA	3.4
1	D	480	THR	3.4
1	D	308	GLY	3.4
1	D	364	MET	3.4
1	B	517	ASP	3.4
1	D	298	SER	3.4
1	C	330	LEU	3.4
1	C	422	ASP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	528	VAL	3.4
1	D	339	TYR	3.4
1	A	510	ASN	3.3
1	C	435	ARG	3.3
1	D	333	ALA	3.3
1	D	417	ALA	3.3
1	B	463	ASP	3.3
1	B	569	GLN	3.3
1	C	421	SER	3.3
1	A	357	ALA	3.3
1	C	425	ALA	3.3
1	D	342	GLY	3.3
1	D	357	ALA	3.3
1	C	549	ASN	3.3
1	B	371	SER	3.3
1	A	404	ILE	3.3
1	B	568	PRO	3.3
1	D	574	LEU	3.3
1	A	272	TYR	3.3
1	A	406	ASP	3.3
1	C	333	ALA	3.3
1	C	510	ASN	3.3
1	A	332	THR	3.3
1	D	540	THR	3.3
1	C	352	PRO	3.3
1	C	288	GLN	3.3
1	B	556	TYR	3.3
1	B	385	ARG	3.3
1	D	289	ASN	3.3
1	A	341	LEU	3.3
1	D	359	LEU	3.3
1	B	377	SER	3.3
1	B	439	LYS	3.3
1	D	530	ALA	3.3
1	A	495	MET	3.3
1	B	479	GLY	3.2
1	A	473	LEU	3.2
1	A	378	GLN	3.2
1	D	466	GLN	3.2
1	C	447	ILE	3.2
1	C	420	ALA	3.2
1	D	267	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	282	LEU	3.2
1	C	464	TRP	3.2
1	D	579	GLU	3.2
1	D	479	GLY	3.2
1	D	281	GLU	3.2
1	D	277	LYS	3.2
1	A	269	GLY	3.2
1	B	502	LEU	3.2
1	D	401	GLY	3.2
1	D	431	LEU	3.2
1	D	546	VAL	3.2
1	D	577	LEU	3.2
1	B	303	ASP	3.2
1	D	249	SER	3.2
1	A	582	ARG	3.2
1	B	489	THR	3.2
1	A	575	GLN	3.2
1	B	250	ASN	3.2
1	A	441	ASP	3.2
1	B	554	GLN	3.2
1	A	419	ALA	3.2
1	B	263	LEU	3.1
1	D	335	ASN	3.2
1	A	278	GLN	3.1
1	C	260	GLN	3.1
1	C	470	GLN	3.1
1	B	480	THR	3.1
1	B	481	PRO	3.1
1	A	482	ALA	3.1
1	C	279	MET	3.1
1	A	423	VAL	3.1
1	B	306	ILE	3.1
1	B	525	HIS	3.1
1	B	575	GLN	3.1
1	C	498	LEU	3.1
1	C	302	THR	3.1
1	D	496	THR	3.1
1	A	548	ASN	3.1
1	C	329	ALA	3.1
1	C	571	SER	3.1
1	D	437	ALA	3.1
1	D	318	MET	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	255	ASP	3.1
1	B	441	ASP	3.1
1	C	505	VAL	3.1
1	D	330	LEU	3.1
1	D	472	PRO	3.1
1	D	476	HIS	3.1
1	A	289	ASN	3.1
1	A	327	PRO	3.1
1	A	485	ILE	3.1
1	B	434	LEU	3.1
1	C	489	THR	3.1
1	A	395	SER	3.1
1	C	249	SER	3.1
1	D	311	TYR	3.1
1	B	403	ASN	3.1
1	C	517	ASP	3.1
1	A	492	THR	3.1
1	B	539	THR	3.1
1	B	544	THR	3.1
1	C	529	THR	3.1
1	D	491	HIS	3.1
1	B	449	ALA	3.1
1	C	499	MET	3.1
1	D	429	ARG	3.1
1	D	487	VAL	3.0
1	A	334	LEU	3.0
1	C	545	LEU	3.0
1	D	336	GLN	3.0
1	A	346	SER	3.0
1	B	351	SER	3.0
1	A	308	GLY	3.0
1	D	262	VAL	3.0
1	A	536	LEU	3.0
1	D	415	ARG	3.0
1	C	284	THR	3.0
1	D	293	THR	3.0
1	C	308	GLY	3.0
1	A	444	VAL	3.0
1	B	278	GLN	3.0
1	C	554	GLN	3.0
1	A	472	PRO	3.0
1	A	547	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	468	HIS	3.0
1	A	583	PHE	3.0
1	B	446	ILE	3.0
1	D	519	PHE	3.0
1	C	296	MET	3.0
1	B	537	ALA	3.0
1	C	400	ASN	3.0
1	D	255	ASP	3.0
1	A	511	GLU	2.9
1	B	443	THR	2.9
1	D	290	ILE	2.9
1	D	316	GLY	2.9
1	A	379	TRP	2.9
1	C	297	SER	2.9
1	C	509	ALA	2.9
1	B	444	VAL	2.9
1	B	341	LEU	2.9
1	B	277	LYS	2.9
1	A	436	GLU	2.9
1	A	459	GLU	2.9
1	D	403	ASN	2.9
1	D	246	TYR	2.9
1	D	581	LYS	2.9
1	B	471	VAL	2.9
1	B	248	LEU	2.9
1	D	272	TYR	2.9
1	D	328	ALA	2.9
1	A	507	THR	2.9
1	D	395	SER	2.9
1	C	285	PHE	2.9
1	B	425	ALA	2.9
1	A	577	LEU	2.9
1	D	294	ARG	2.9
1	D	320	GLY	2.9
1	A	446	ILE	2.9
1	A	564	LYS	2.9
1	A	375	THR	2.8
1	A	578	THR	2.8
1	D	465	SER	2.8
1	B	505	VAL	2.8
1	C	267	VAL	2.8
1	A	359	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	473	LEU	2.8
1	A	380	ILE	2.8
1	C	433	ALA	2.8
1	C	301	THR	2.8
1	D	497	THR	2.8
1	C	253	TYR	2.8
1	C	274	ARG	2.8
1	D	484	ARG	2.8
1	B	581	LYS	2.8
1	B	450	GLY	2.8
1	D	374	GLN	2.8
1	B	334	LEU	2.8
1	A	265	ILE	2.8
1	A	468	HIS	2.8
1	A	501	ARG	2.8
1	D	251	LEU	2.8
1	D	558	LEU	2.8
1	A	329	ALA	2.8
1	B	286	ALA	2.8
1	A	320	GLY	2.8
1	B	495	MET	2.8
1	D	346	SER	2.8
1	A	505	VAL	2.8
1	C	445	VAL	2.8
1	C	309	LEU	2.8
1	A	401	GLY	2.8
1	A	427	ILE	2.8
1	B	429	ARG	2.8
1	C	518	ILE	2.8
1	C	426	GLN	2.8
1	A	373	ALA	2.7
1	D	560	GLY	2.7
1	C	488	LEU	2.7
1	A	476	HIS	2.7
1	D	559	HIS	2.7
1	B	296	MET	2.7
1	A	307	PHE	2.7
1	C	439	LYS	2.7
1	A	449	ALA	2.7
1	C	557	ASP	2.7
1	C	295	HIS	2.7
1	B	397	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	475	ILE	2.7
1	A	301	THR	2.7
1	A	279	MET	2.7
1	C	479	GLY	2.7
1	A	541	PRO	2.7
1	A	303	ASP	2.7
1	B	493	ASP	2.7
1	B	327	PRO	2.7
1	C	457	PRO	2.7
1	A	403	ASN	2.7
1	D	273	SER	2.7
1	D	350	ALA	2.7
1	A	291	ASP	2.7
1	D	245	GLN	2.7
1	A	479	GLY	2.7
1	A	400	ASN	2.7
1	D	247	PRO	2.7
1	B	459	GLU	2.7
1	C	417	ALA	2.6
1	C	257	GLY	2.6
1	C	311	TYR	2.6
1	A	559	HIS	2.6
1	D	468	HIS	2.6
1	C	247	PRO	2.6
1	D	503	LEU	2.6
1	C	465	SER	2.6
1	D	489	THR	2.6
1	C	537	ALA	2.6
1	D	482	ALA	2.6
1	A	438	GLY	2.6
1	D	349	PHE	2.6
1	D	253	TYR	2.6
1	B	345	SER	2.6
1	B	330	LEU	2.6
1	C	258	THR	2.6
1	C	573	LEU	2.6
1	B	561	GLU	2.6
1	C	366	ALA	2.6
1	D	299	GLY	2.6
1	D	444	VAL	2.6
1	C	492	THR	2.6
1	A	414	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	550	ASN	2.6
1	A	286	ALA	2.6
1	D	538	ILE	2.6
1	A	355	ARG	2.6
1	B	274	ARG	2.6
1	A	496	THR	2.6
1	A	428	ASN	2.6
1	D	303	ASP	2.6
1	C	468	HIS	2.6
1	D	561	GLU	2.6
1	D	352	PRO	2.6
1	B	287	GLU	2.6
1	A	297	SER	2.5
1	D	371	SER	2.5
1	A	338	GLY	2.5
1	B	427	ILE	2.5
1	C	293	THR	2.5
1	C	535	THR	2.5
1	D	539	THR	2.5
1	D	504	HIS	2.5
1	A	292	PHE	2.5
1	C	360	SER	2.5
1	A	288	GLN	2.5
1	B	516	GLN	2.5
1	D	532	ASP	2.5
1	C	542	GLN	2.5
1	D	351	SER	2.5
1	A	250	ASN	2.5
1	D	541	PRO	2.5
1	C	429	ARG	2.5
1	D	326	THR	2.5
1	B	290	ILE	2.5
1	D	329	ALA	2.5
1	D	373	ALA	2.5
1	D	537	ALA	2.5
1	D	355	ARG	2.5
1	D	452	GLY	2.5
1	C	466	GLN	2.5
1	D	356	GLN	2.5
1	B	496	THR	2.5
1	A	513	SER	2.5
1	C	401	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	430	VAL	2.5
1	D	562	LYS	2.5
1	B	529	THR	2.5
1	C	544	THR	2.5
1	A	561	GLU	2.5
1	B	298	SER	2.5
1	B	513	SER	2.5
1	B	533	GLY	2.4
1	B	347	ASP	2.4
1	C	428	ASN	2.4
1	D	271	ASN	2.4
1	C	497	THR	2.4
1	C	501	ARG	2.4
1	B	580	GLU	2.4
1	A	420	ALA	2.4
1	C	403	ASN	2.4
1	B	497	THR	2.4
1	B	555	THR	2.4
1	C	278	GLN	2.4
1	D	337	GLN	2.4
1	C	315	PRO	2.4
1	D	307	PHE	2.4
1	D	510	ASN	2.4
1	D	369	THR	2.4
1	D	555	THR	2.4
1	A	268	ASP	2.4
1	D	384	GLY	2.4
1	C	539	THR	2.4
1	C	250	ASN	2.4
1	B	281	GLU	2.4
1	A	371	SER	2.4
1	A	318	MET	2.4
1	A	531	ALA	2.4
1	C	325	ARG	2.4
1	C	451	ARG	2.4
1	C	266	THR	2.4
1	A	467	GLY	2.4
1	B	335	ASN	2.4
1	C	347	ASP	2.3
1	A	435	ARG	2.3
1	B	582	ARG	2.3
1	B	571	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	513	SER	2.3
1	B	374	GLN	2.3
1	C	336	GLN	2.3
1	A	317	TYR	2.3
1	A	324	THR	2.3
1	A	529	THR	2.3
1	B	402	THR	2.3
1	A	490	ASP	2.3
1	C	337	GLN	2.3
1	C	467	GLY	2.3
1	A	432	ASN	2.3
1	B	378	GLN	2.3
1	C	546	VAL	2.3
1	C	576	VAL	2.3
1	A	424	ASP	2.3
1	C	268	ASP	2.3
1	C	291	ASP	2.3
1	C	481	PRO	2.3
1	C	503	LEU	2.3
1	C	395	SER	2.3
1	D	483	GLN	2.3
1	A	370	GLN	2.3
1	A	475	ILE	2.3
1	A	514	GLN	2.3
1	A	399	PHE	2.2
1	C	261	ASN	2.2
1	D	283	ALA	2.2
1	B	418	SER	2.2
1	A	517	ASP	2.2
1	A	322	LEU	2.2
1	A	504	HIS	2.2
1	C	574	LEU	2.2
1	D	288	GLN	2.2
1	B	501	ARG	2.2
1	A	493	ASP	2.2
1	C	312	GLY	2.2
1	C	304	ASN	2.2
1	D	372	ASP	2.2
1	B	562	LYS	2.2
1	C	469	LEU	2.2
1	A	293	THR	2.2
1	B	500	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	483	GLN	2.2
1	A	328	ALA	2.2
1	D	551	GLY	2.2
1	B	271	ASN	2.2
1	B	294	ARG	2.2
1	D	523	ARG	2.2
1	D	453	ILE	2.2
1	A	280	PRO	2.2
1	A	270	LEU	2.2
1	B	245	GLN	2.2
1	D	575	GLN	2.2
1	C	269	GLY	2.2
1	C	255	ASP	2.2
1	B	483	GLN	2.2
1	D	520	THR	2.1
1	A	347	ASP	2.1
1	C	328	ALA	2.1
1	D	420	ALA	2.1
1	A	345	SER	2.1
1	A	465	SER	2.1
1	D	451	ARG	2.1
1	D	331	ILE	2.1
1	D	443	THR	2.1
1	A	298	SER	2.1
1	A	295	HIS	2.1
1	A	522	PRO	2.1
1	C	523	ARG	2.1
1	D	441	ASP	2.1
1	C	338	GLY	2.1
1	C	560	GLY	2.1
1	A	448	THR	2.1
1	D	448	THR	2.1
1	C	580	GLU	2.1
1	D	265	ILE	2.1
1	B	373	ALA	2.1
1	B	465	SER	2.1
1	D	398	SER	2.1
1	B	255	ASP	2.1
1	B	291	ASP	2.1
1	B	315	PRO	2.1
1	D	470	GLN	2.1
1	B	401	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	269	GLY	2.1
1	A	471	VAL	2.1
1	A	429	ARG	2.1
1	A	502	LEU	2.1
1	D	418	SER	2.1
1	B	304	ASN	2.1
1	D	454	PRO	2.1
1	C	305	GLY	2.1
1	B	372	ASP	2.1
1	D	508	PRO	2.1
1	A	296	MET	2.0
1	C	418	SER	2.0
1	D	304	ASN	2.0
1	C	559	HIS	2.0
1	C	335	ASN	2.0
1	A	351	SER	2.0
1	A	398	SER	2.0
1	A	304	ASN	2.0
1	C	359	LEU	2.0
1	A	294	ARG	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(\AA^2)	Q<0.9
2	PGE	A	601	10/10	0.19	0.54	36,43,44,44	0
5	MN	B	602	1/1	0.33	0.42	65,65,65,65	0
5	MN	D	704	1/1	0.34	0.31	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PEG	A	602	7/7	0.36	0.49	43,52,53,53	0
7	PSE	C	601	10/10	0.39	0.38	49,50,59,59	0
6	EDO	B	601	4/4	0.47	0.34	44,53,53,53	0
5	MN	A	604	1/1	0.59	0.19	45,45,45,45	0
4	PO4	A	603	5/5	0.63	0.35	54,54,54,54	0
3	PEG	D	702	7/7	0.66	0.34	43,51,52,52	0
7	PSE	D	701	10/10	0.67	0.32	43,45,54,55	0
4	PO4	D	703	5/5	0.70	0.33	62,64,64,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.