Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 10:48 AM BST

PDB ID	:	2HV2
Title	:	Crystal Structure of Conserved Protein of Unknown Function from Enterococcus faecalis V583 at 2.4 A Resolution, Probable N-Acyltransferase
Authors	:	Tereshko, V.A.; Qiu, Y.; Kossiakoff, A.A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2006-07-27
Resolution	:	2.40 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:

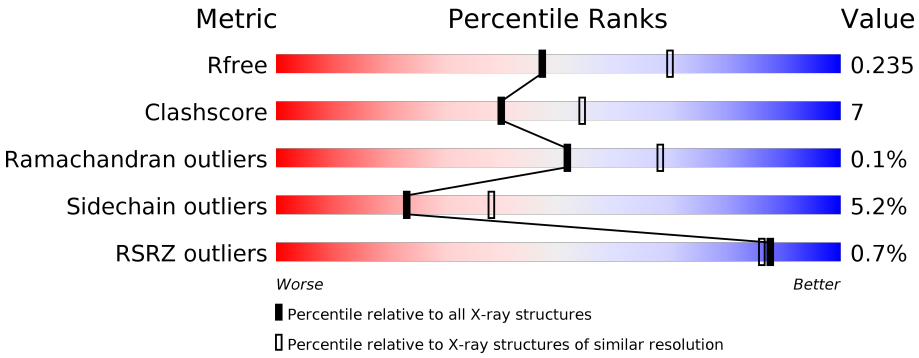
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	400	2% 77% 20%
1	B	400	79% 19%
1	C	400	80% 17%
1	D	400	78% 18%
1	E	400	82% 15%
1	F	400	82% 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19692 atoms, of which 0 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 Hypothetical protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	Se	0	0	0
			3167	2040	522	594	11			
1	B	393	Total	C	N	O	Se	0	0	0
			3175	2045	523	595	12			
1	C	391	Total	C	N	O	Se	0	0	0
			3163	2038	521	592	12			
1	D	390	Total	C	N	O	Se	0	0	0
			3155	2033	520	591	11			
1	E	391	Total	C	N	O	Se	0	0	0
			3163	2038	521	592	12			
1	F	392	Total	C	N	O	Se	0	0	0
			3170	2042	522	594	12			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	CLONING ARTIFACT	UNP Q836T6
A	-1	ASN	-	CLONING ARTIFACT	UNP Q836T6
A	0	ALA	-	CLONING ARTIFACT	UNP Q836T6
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
A	9	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
A	14	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
A	17	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
A	60	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
A	75	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
A	97	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
A	100	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
A	268	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
A	281	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
A	282	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
A	390	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
B	-2	SER	-	CLONING ARTIFACT	UNP Q836T6
B	-1	ASN	-	CLONING ARTIFACT	UNP Q836T6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	CLONING ARTIFACT	UNP Q836T6
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
B	9	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
B	14	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
B	17	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
B	60	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
B	75	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
B	97	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
B	100	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
B	268	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
B	281	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
B	282	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
B	390	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
C	-2	SER	-	CLONING ARTIFACT	UNP Q836T6
C	-1	ASN	-	CLONING ARTIFACT	UNP Q836T6
C	0	ALA	-	CLONING ARTIFACT	UNP Q836T6
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
C	9	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
C	14	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
C	17	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
C	60	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
C	75	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
C	97	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
C	100	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
C	268	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
C	281	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
C	282	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
C	390	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
D	-2	SER	-	CLONING ARTIFACT	UNP Q836T6
D	-1	ASN	-	CLONING ARTIFACT	UNP Q836T6
D	0	ALA	-	CLONING ARTIFACT	UNP Q836T6
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
D	9	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
D	14	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
D	17	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
D	60	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
D	75	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
D	97	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
D	100	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
D	268	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
D	281	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
D	282	MSE	MET	MODIFIED RESIDUE	UNP Q836T6

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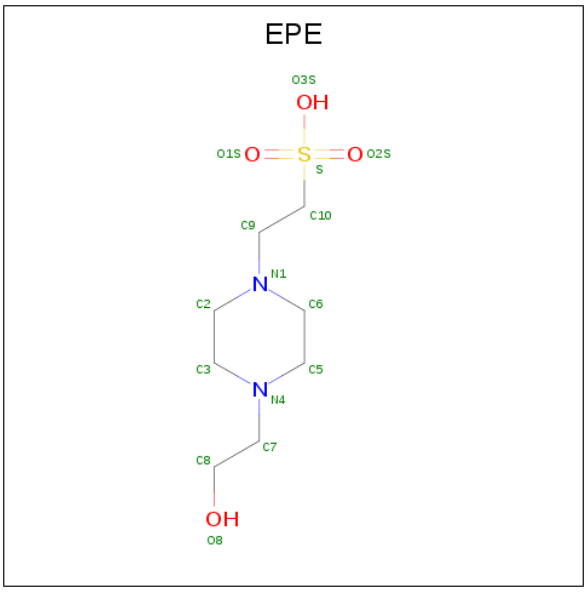
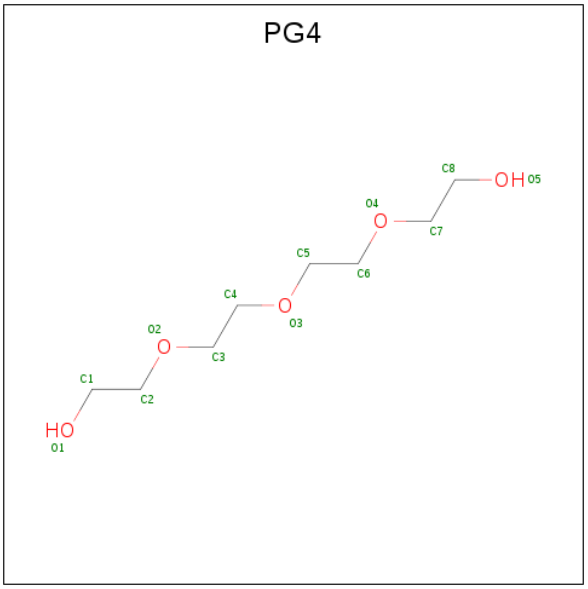
Chain	Residue	Modelled	Actual	Comment	Reference
D	390	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
E	-2	SER	-	CLONING ARTIFACT	UNP Q836T6
E	-1	ASN	-	CLONING ARTIFACT	UNP Q836T6
E	0	ALA	-	CLONING ARTIFACT	UNP Q836T6
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
E	9	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
E	14	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
E	17	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
E	60	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
E	75	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
E	97	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
E	100	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
E	268	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
E	281	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
E	282	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
E	390	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
F	-2	SER	-	CLONING ARTIFACT	UNP Q836T6
F	-1	ASN	-	CLONING ARTIFACT	UNP Q836T6
F	0	ALA	-	CLONING ARTIFACT	UNP Q836T6
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
F	9	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
F	14	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
F	17	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
F	60	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
F	75	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
F	97	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
F	100	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
F	268	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
F	281	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
F	282	MSE	MET	MODIFIED RESIDUE	UNP Q836T6
F	390	MSE	MET	MODIFIED RESIDUE	UNP Q836T6

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 8 5	0	0
3	B	1	Total C O 13 8 5	0	0
3	C	1	Total C O 13 8 5	0	0
3	D	1	Total C O 13 8 5	0	0
3	E	1	Total C O 13 8 5	0	0
3	F	1	Total C O 13 8 5	0	0

- Molecule 4 is water.

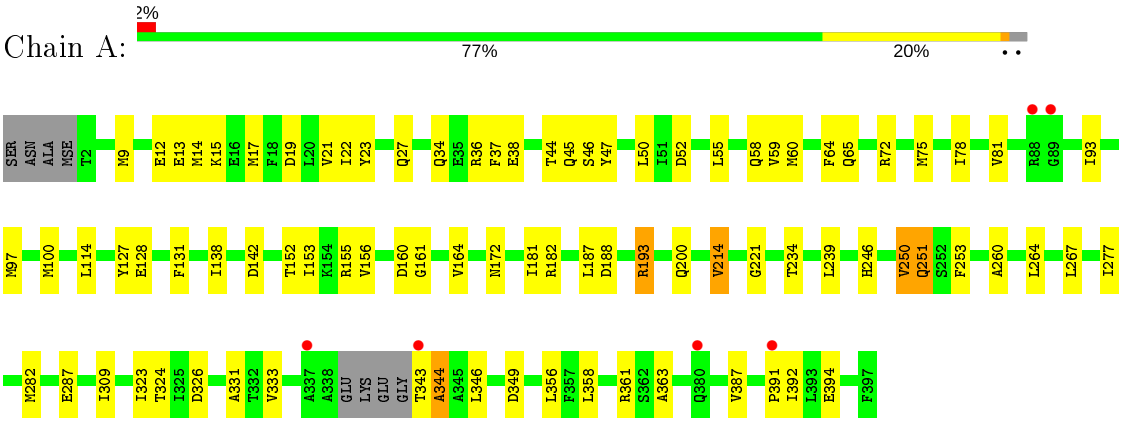
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	85	Total O 85 85	0	0
4	B	94	Total O 96 96	0	2
4	C	98	Total O 98 98	0	0
4	D	77	Total O 78 78	0	1
4	E	99	Total O 101 101	0	2
4	F	88	Total O 88 88	0	0

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.

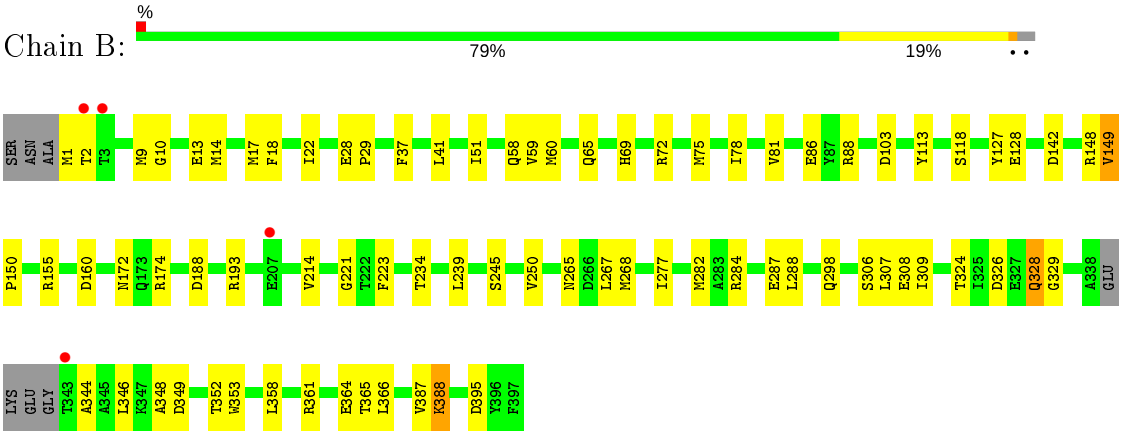
- Molecule 1: Hypothetical protein

Chain A:



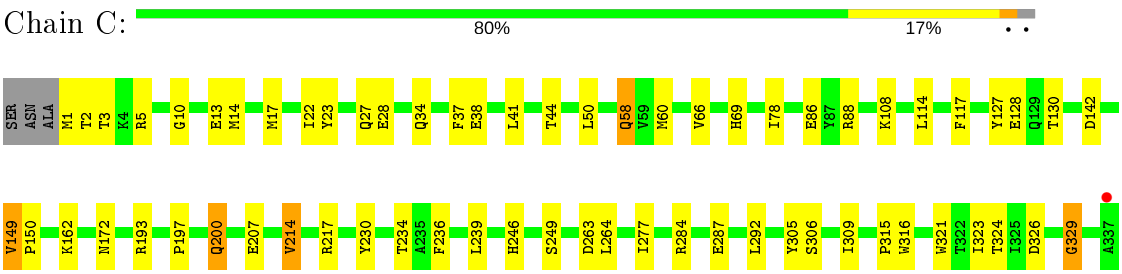
- Molecule 1: Hypothetical protein

Chain B:



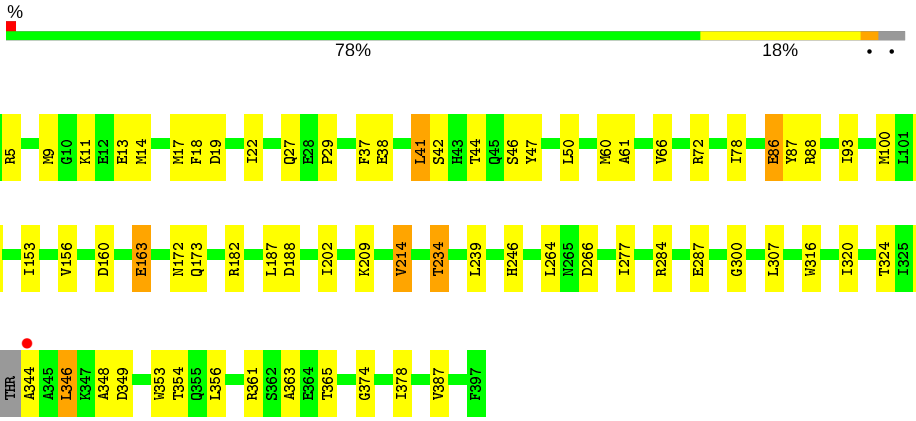
- Molecule 1: Hypothetical protein

Chain C:



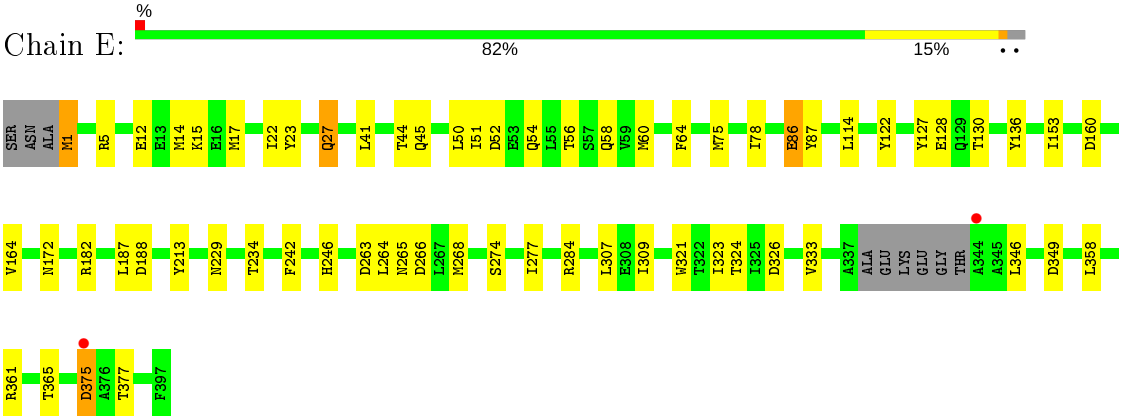
• Molecule 1: Hypothetical protein

Chain D:



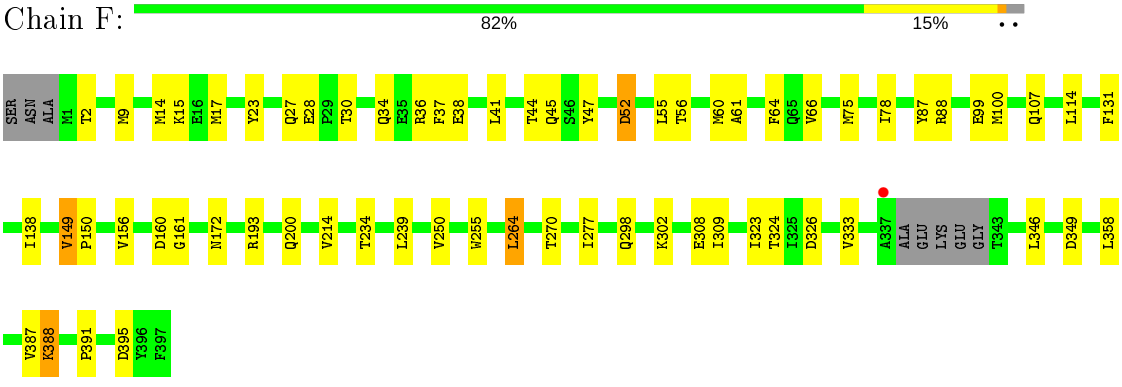
• Molecule 1: Hypothetical protein

Chain E:



• Molecule 1: Hypothetical protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	189.63Å 104.28Å 152.28Å 90.00° 98.26° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 50.23 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.9 (20.00-2.40) 97.9 (50.23-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.233 0.190 , 0.235	Depositor DCC
R_{free} test set	5621 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	42.2	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19692	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, EPE

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	0.57	0/3237	0.93	8/4361 (0.2%)
1	B	0.59	0/3245	0.95	8/4371 (0.2%)
1	C	0.62	0/3233	0.94	4/4354 (0.1%)
1	D	0.57	0/3225	0.93	6/4344 (0.1%)
1	E	0.62	0/3233	0.96	8/4354 (0.2%)
1	F	0.60	0/3240	0.94	5/4364 (0.1%)
All	All	0.60	0/19413	0.94	39/26148 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	349	ASP	CB-CG-OD2	8.15	125.63	118.30
1	D	160	ASP	CB-CG-OD2	7.60	125.14	118.30
1	A	326	ASP	CB-CG-OD2	7.52	125.07	118.30
1	F	326	ASP	CB-CG-OD2	7.51	125.06	118.30
1	C	349	ASP	CB-CG-OD2	7.44	125.00	118.30
1	B	188	ASP	CB-CG-OD2	7.44	125.00	118.30
1	E	52	ASP	CB-CG-OD2	7.35	124.92	118.30
1	D	19	ASP	CB-CG-OD2	7.31	124.88	118.30
1	B	349	ASP	CB-CG-OD2	7.16	124.74	118.30
1	D	326	ASP	CB-CG-OD2	7.14	124.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	326	ASP	CB-CG-OD2	7.14	124.73	118.30
1	C	263	ASP	CB-CG-OD2	7.07	124.67	118.30
1	F	160	ASP	CB-CG-OD2	6.92	124.53	118.30
1	F	349	ASP	CB-CG-OD2	6.91	124.52	118.30
1	A	349	ASP	CB-CG-OD2	6.87	124.48	118.30
1	E	263	ASP	CB-CG-OD2	6.71	124.34	118.30
1	B	103	ASP	CB-CG-OD2	6.46	124.11	118.30
1	D	266	ASP	CB-CG-OD2	6.38	124.04	118.30
1	F	395	ASP	CB-CG-OD2	6.36	124.03	118.30
1	A	188	ASP	CB-CG-OD2	6.30	123.97	118.30
1	E	375	ASP	CB-CG-OD2	6.22	123.90	118.30
1	E	349	ASP	CB-CG-OD2	6.22	123.89	118.30
1	C	326	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	160	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	142	ASP	CB-CG-OD2	5.54	123.29	118.30
1	E	266	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	142	ASP	CB-CG-OD2	5.42	123.18	118.30
1	F	52	ASP	CB-CG-OD2	5.32	123.09	118.30
1	E	188	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	19	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	326	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	284	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	D	188	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	155	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	E	160	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	160	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	395	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	142	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	52	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	329	GLY	Peptide

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	3167	0	3090	55	0
1	B	3175	0	3102	48	0
1	C	3163	0	3090	53	0
1	D	3155	0	3078	57	0
1	E	3163	0	3090	39	0
1	F	3170	0	3097	38	0
2	A	15	0	17	0	0
2	B	15	0	17	0	0
2	C	15	0	17	1	0
2	D	15	0	17	0	0
2	E	15	0	17	0	0
3	A	13	0	18	0	0
3	B	13	0	18	0	0
3	C	13	0	18	0	0
3	D	13	0	18	0	0
3	E	13	0	18	0	0
3	F	13	0	18	0	0
4	A	85	0	0	1	0
4	B	96	0	0	1	0
4	C	98	0	0	4	0
4	D	78	0	0	0	0
4	E	101	0	0	3	0
4	F	88	0	0	1	0
All	All	19692	0	18740	278	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 (278) 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:1:MSE:CE	1:C:2:THR:HG23	1.62	1.30
1:A:277:ILE:HD11	1:B:277:ILE:HD11	1.32	1.08
1:B:214:VAL:HG23	1:B:239:LEU:HD22	1.42	1.01
1:C:1:MSE:HE2	1:C:2:THR:CG2	1.90	1.01
1:C:1:MSE:HE2	1:C:2:THR:HG23	1.00	0.99
1:F:214:VAL:HG23	1:F:239:LEU:HD22	1.45	0.98
1:F:14:MSE:HE2	1:F:37:PHE:HD2	1.28	0.95
1:D:14:MSE:HE2	1:D:37:PHE:HD2	1.42	0.84
1:A:323:ILE:CD1	1:A:333:VAL:HG22	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:MSE:HE3	1:F:38:GLU:HG3	1.60	0.83
1:F:14:MSE:HE2	1:F:37:PHE:CD2	2.15	0.82
1:C:1:MSE:CE	1:C:2:THR:CG2	2.51	0.81
1:A:221:GLY:O	1:A:250:VAL:HG22	1.81	0.80
1:B:214:VAL:CG2	1:B:239:LEU:HD22	2.10	0.80
1:A:277:ILE:CD1	1:B:277:ILE:HD11	2.15	0.76
1:C:1:MSE:HE3	1:C:2:THR:HG23	1.65	0.76
1:C:375:ASP:OD1	1:C:377:THR:HG22	1.86	0.75
1:A:14:MSE:HE2	1:A:37:PHE:HD2	1.50	0.75
1:D:344:ALA:HB1	1:D:378:ILE:HD12	1.68	0.75
1:D:14:MSE:HE3	1:D:38:GLU:HG3	1.69	0.75
1:D:14:MSE:HE3	1:D:38:GLU:CG	2.17	0.74
1:F:9:MSE:HE1	1:F:55:LEU:HD22	1.70	0.73
1:D:214:VAL:HG22	1:D:239:LEU:HD22	1.71	0.73
1:D:14:MSE:HA	1:D:17:MSE:HE3	1.68	0.73
1:A:251:GLN:HA	1:A:251:GLN:HE21	1.54	0.71
1:B:14:MSE:HA	1:B:17:MSE:HE3	1.73	0.71
1:B:78:ILE:HD12	1:B:127:TYR:OH	1.92	0.70
1:D:121:PHE:O	1:D:124:GLN:HG2	1.92	0.70
1:F:44:THR:HG21	1:F:60:MSE:HB3	1.75	0.69
1:C:149:VAL:HG22	1:C:150:PRO:HD2	1.75	0.69
1:B:298:GLN:HE22	1:B:388:LYS:HG3	1.59	0.68
1:C:13:GLU:HB2	1:C:17:MSE:HE2	1.74	0.68
1:D:320:ILE:HG21	1:D:337:ALA:HB2	1.76	0.68
1:A:323:ILE:HD12	1:A:333:VAL:HG22	1.76	0.67
1:E:22:ILE:HG23	1:E:27:GLN:O	1.94	0.67
1:B:221:GLY:O	1:B:250:VAL:HG22	1.94	0.67
1:B:2:THR:HG21	1:B:51:ILE:HG23	1.77	0.66
1:A:214:VAL:CG2	1:A:239:LEU:HD22	2.26	0.66
1:C:14:MSE:HE1	1:C:34:GLN:HG3	1.76	0.66
1:A:14:MSE:HE2	1:A:37:PHE:CD2	2.32	0.65
1:D:22:ILE:HD13	1:D:29:PRO:HB3	1.77	0.65
1:E:14:MSE:HA	1:E:17:MSE:HE3	1.78	0.65
1:F:214:VAL:CG2	1:F:239:LEU:HD22	2.22	0.64
1:D:18:PHE:CE2	1:D:22:ILE:HD11	2.33	0.63
1:E:41:LEU:HD23	1:E:60:MSE:HE2	1.79	0.62
1:B:18:PHE:CE2	1:B:22:ILE:HD11	2.34	0.62
1:C:214:VAL:CG2	1:C:239:LEU:HD22	2.30	0.62
1:D:78:ILE:HD12	1:D:127:TYR:OH	1.99	0.62
1:F:9:MSE:HE1	1:F:55:LEU:CD2	2.29	0.61
1:C:13:GLU:CB	1:C:17:MSE:HE2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:GLU:HG3	1:F:30:THR:HG23	1.82	0.60
1:A:156:VAL:HG11	1:A:161:GLY:HA3	1.83	0.60
1:E:277:ILE:HD11	1:F:277:ILE:HD12	1.83	0.60
1:A:22:ILE:HG23	1:A:27:GLN:O	2.02	0.59
1:B:298:GLN:NE2	1:B:388:LYS:HG3	2.17	0.59
1:C:37:PHE:CZ	1:C:60:MSE:HE1	2.38	0.59
1:D:14:MSE:HE2	1:D:37:PHE:CD2	2.31	0.59
1:F:36:ARG:NH2	1:F:193:ARG:NH2	2.51	0.59
1:B:13:GLU:HB2	1:B:17:MSE:HE2	1.84	0.59
1:D:22:ILE:CD1	1:D:29:PRO:HB3	2.33	0.59
1:A:323:ILE:HD11	1:A:331:ALA:HB1	1.86	0.58
1:C:305:TYR:O	1:C:323:ILE:HG22	2.03	0.58
1:E:182:ARG:HD3	1:E:187:LEU:HD13	1.83	0.58
1:A:23:TYR:OH	1:C:246:HIS:HE1	1.87	0.58
1:E:164:VAL:HG23	4:E:877:HOH:O	2.03	0.58
1:E:265:ASN:OD1	1:E:268:MSE:CE	2.52	0.58
1:D:320:ILE:CG2	1:D:337:ALA:HB2	2.34	0.57
1:B:245:SER:OG	1:D:88:ARG:HD3	2.04	0.57
1:D:78:ILE:CD1	1:D:100:MSE:HE1	2.35	0.57
1:C:214:VAL:HG23	1:C:239:LEU:HD22	1.87	0.57
1:B:78:ILE:CD1	1:B:127:TYR:OH	2.53	0.57
1:D:44:THR:HG21	1:D:60:MSE:HB3	1.87	0.57
1:B:149:VAL:HG22	1:B:150:PRO:HD2	1.86	0.56
4:E:867:HOH:O	1:F:270:THR:HG23	2.04	0.56
1:C:309:ILE:HD13	1:C:321:TRP:CD1	2.40	0.56
1:C:14:MSE:HE2	1:C:37:PHE:HD2	1.70	0.56
1:C:14:MSE:HA	1:C:17:MSE:HE3	1.87	0.56
1:A:138:ILE:HG22	1:A:253:PHE:HB2	1.87	0.56
1:B:10:GLY:O	1:B:17:MSE:HE1	2.06	0.56
1:D:246:HIS:HE1	1:F:23:TYR:OH	1.89	0.56
1:C:375:ASP:CG	1:C:377:THR:HG22	2.25	0.55
1:A:182:ARG:HD3	1:A:187:LEU:HD13	1.88	0.55
1:D:14:MSE:HE3	1:D:38:GLU:HG2	1.86	0.55
1:E:41:LEU:CD2	1:E:60:MSE:HE2	2.36	0.55
1:A:14:MSE:HA	1:A:17:MSE:HE3	1.88	0.55
1:D:356:LEU:HD11	1:D:363:ALA:HB2	1.89	0.55
1:F:298:GLN:HE22	1:F:388:LYS:HE3	1.71	0.55
1:A:9:MSE:HE3	1:A:13:GLU:HB3	1.89	0.55
1:D:17:MSE:HE1	1:D:41:LEU:HD11	1.87	0.55
1:B:155:ARG:NE	1:D:86:GLU:OE2	2.37	0.55
1:D:2:THR:HG22	1:D:3:THR:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ARG:NH2	1:B:267:LEU:HD21	2.21	0.55
1:D:78:ILE:HD13	1:D:100:MSE:HE1	1.89	0.55
1:E:309:ILE:HD13	1:E:321:TRP:CD1	2.41	0.54
1:F:56:THR:HG22	1:F:87:TYR:CE1	2.43	0.54
1:A:22:ILE:HD13	1:A:27:GLN:HE21	1.73	0.54
1:B:18:PHE:CZ	1:B:22:ILE:HD11	2.42	0.54
1:D:163:GLU:CD	1:D:163:GLU:H	2.11	0.54
1:A:44:THR:HG21	1:A:60:MSE:HB3	1.90	0.54
1:A:22:ILE:HD13	1:A:27:GLN:HB2	1.90	0.53
1:B:309:ILE:N	1:B:309:ILE:CD1	2.71	0.53
1:C:149:VAL:HG22	1:C:150:PRO:CD	2.38	0.53
1:D:214:VAL:CG2	1:D:239:LEU:HD22	2.37	0.53
1:A:131:PHE:CE2	1:A:391:PRO:HB2	2.43	0.53
1:B:65:GLN:HE22	1:B:72:ARG:HD3	1.72	0.53
1:B:22:ILE:CD1	1:B:29:PRO:HB3	2.38	0.53
1:C:23:TYR:OH	1:E:246:HIS:HE1	1.91	0.53
1:C:22:ILE:HD13	1:C:27:GLN:HG3	1.91	0.52
1:A:343:THR:O	1:A:344:ALA:HB3	2.09	0.52
1:E:22:ILE:HD13	1:E:27:GLN:HG3	1.91	0.52
1:F:47:TYR:CE1	1:F:100:MSE:HG3	2.45	0.52
1:B:22:ILE:HD13	1:B:29:PRO:HB3	1.92	0.52
1:D:9:MSE:HB2	1:D:46:SER:HB3	1.92	0.51
1:B:309:ILE:N	1:B:309:ILE:HD12	2.25	0.51
1:D:307:LEU:HD22	1:D:353:TRP:CH2	2.45	0.51
1:D:11:LYS:HG2	1:D:41:LEU:HD13	1.91	0.51
1:F:78:ILE:HB	1:F:114:LEU:HB3	1.93	0.51
1:C:14:MSE:HE2	1:C:37:PHE:CD2	2.45	0.51
1:B:348:ALA:HB1	1:B:352:THR:HB	1.93	0.51
1:E:323:ILE:HG22	1:E:333:VAL:HG13	1.93	0.50
1:F:14:MSE:HE1	1:F:34:GLN:HG3	1.94	0.50
1:A:214:VAL:HG22	1:A:239:LEU:HD22	1.92	0.50
1:B:308:GLU:C	1:B:309:ILE:HD12	2.32	0.50
1:C:127:TYR:CE2	1:C:284:ARG:HG2	2.46	0.50
1:C:14:MSE:HE1	1:C:34:GLN:CG	2.41	0.50
1:A:251:GLN:CA	1:A:251:GLN:HE21	2.23	0.49
1:A:246:HIS:HE1	1:E:23:TYR:OH	1.95	0.49
1:F:149:VAL:HG22	1:F:150:PRO:HD2	1.94	0.49
1:F:255:TRP:CZ3	1:F:264:LEU:HD23	2.46	0.49
1:C:306:SER:OG	1:C:344:ALA:HA	2.13	0.49
1:D:78:ILE:CD1	1:D:127:TYR:OH	2.59	0.49
1:A:21:VAL:HG23	1:A:58:GLN:HE22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:ILE:HD11	1:D:277:ILE:HD12	1.94	0.49
1:C:292:LEU:HD13	1:C:323:ILE:HD12	1.94	0.49
1:F:14:MSE:HE3	1:F:38:GLU:CG	2.36	0.49
1:C:44:THR:HG21	1:C:60:MSE:HB3	1.94	0.49
1:D:93:ILE:HD12	1:D:93:ILE:H	1.77	0.49
1:F:131:PHE:CE2	1:F:391:PRO:HB2	2.48	0.49
1:A:9:MSE:HE3	1:A:13:GLU:CB	2.44	0.48
1:A:50:LEU:HD23	1:A:55:LEU:HA	1.95	0.48
1:E:58:GLN:HE22	1:E:60:MSE:SE	2.47	0.48
1:A:13:GLU:HB2	1:A:17:MSE:HE2	1.96	0.48
1:A:164:VAL:HG23	4:A:877:HOH:O	2.13	0.48
1:E:136:TYR:OH	1:E:264:LEU:HD22	2.14	0.48
1:E:50:LEU:HA	1:E:54:GLN:O	2.13	0.48
1:F:14:MSE:HA	1:F:17:MSE:HE3	1.95	0.48
1:A:114:LEU:HD12	1:A:114:LEU:C	2.35	0.47
1:D:22:ILE:HG23	1:D:27:GLN:O	2.15	0.47
1:E:44:THR:HG21	1:E:60:MSE:HB3	1.97	0.47
1:C:128:GLU:O	1:C:130:THR:HG23	2.14	0.47
1:C:348:ALA:HB3	1:C:353:TRP:CE2	2.50	0.47
1:C:37:PHE:HZ	1:C:60:MSE:HE1	1.79	0.47
1:C:309:ILE:HD13	1:C:321:TRP:HD1	1.77	0.47
1:A:81:VAL:HG13	1:A:93:ILE:HD12	1.97	0.47
1:B:9:MSE:HE3	1:B:13:GLU:CB	2.45	0.47
1:B:223:PHE:N	1:B:250:VAL:HG21	2.30	0.47
1:A:97:MSE:HE1	1:A:127:TYR:HE1	1.80	0.46
1:A:9:MSE:HE2	1:A:55:LEU:HD22	1.98	0.46
1:E:128:GLU:O	1:E:130:THR:HG23	2.15	0.46
1:E:182:ARG:HD3	1:E:187:LEU:CD1	2.46	0.46
1:B:387:VAL:HG22	1:B:388:LYS:NZ	2.30	0.46
1:C:305:TYR:HB2	1:C:323:ILE:CG2	2.46	0.46
1:B:59:VAL:HG13	1:B:81:VAL:HG22	1.97	0.46
1:A:343:THR:O	1:A:344:ALA:CB	2.63	0.46
1:E:361:ARG:HH21	1:E:365:THR:HG21	1.81	0.46
1:F:45:GLN:HE22	1:F:107:GLN:HE22	1.63	0.46
1:A:44:THR:HG22	1:A:45:GLN:N	2.30	0.46
1:F:37:PHE:CZ	1:F:60:MSE:HE1	2.50	0.46
1:C:108:LYS:HE3	4:C:814:HOH:O	2.15	0.46
1:F:78:ILE:O	4:F:850:HOH:O	2.21	0.46
1:A:260:ALA:HB2	1:A:392:ILE:HD11	1.96	0.46
1:E:44:THR:HG22	1:E:45:GLN:N	2.31	0.45
1:E:64:PHE:HB2	1:E:75:MSE:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:LEU:HD11	1:E:323:ILE:HD13	1.99	0.45
4:C:898:HOH:O	1:D:234:THR:CG2	2.65	0.45
1:D:361:ARG:HH21	1:D:365:THR:HG21	1.81	0.45
1:A:182:ARG:HD3	1:A:187:LEU:CD1	2.45	0.45
1:B:361:ARG:HH21	1:B:365:THR:HG21	1.82	0.45
1:F:298:GLN:HE22	1:F:388:LYS:CE	2.29	0.45
1:A:309:ILE:HD12	1:A:309:ILE:N	2.32	0.45
1:A:59:VAL:HG13	1:A:81:VAL:HG22	1.99	0.45
1:A:214:VAL:HG23	1:A:239:LEU:HD22	1.96	0.45
1:D:346:LEU:HD12	1:D:374:GLY:HA3	1.99	0.45
1:C:117:PHE:CE2	2:C:703:EPE:H92	2.52	0.44
1:C:69:HIS:NE2	1:C:387:VAL:HG11	2.32	0.44
1:A:356:LEU:HD11	1:A:363:ALA:HB2	1.99	0.44
1:B:307:LEU:HD22	1:B:353:TRP:CH2	2.53	0.44
1:E:41:LEU:CD2	1:E:60:MSE:CE	2.96	0.44
1:A:153:ILE:HD13	1:A:239:LEU:HD23	1.99	0.44
1:C:315:PRO:HD2	1:C:316:TRP:CZ3	2.52	0.44
1:E:1:MSE:HA	1:E:1:MSE:HE2	1.99	0.44
1:A:72:ARG:HG3	1:A:181:ILE:CD1	2.47	0.44
1:B:18:PHE:CE2	1:B:22:ILE:CD1	3.00	0.44
1:D:9:MSE:HE3	1:D:13:GLU:HB3	1.99	0.44
4:C:898:HOH:O	1:D:234:THR:HG22	2.17	0.44
1:C:10:GLY:O	1:C:17:MSE:HE1	2.17	0.44
1:C:5:ARG:NH1	1:C:50:LEU:HD12	2.33	0.44
1:B:2:THR:HG21	1:B:51:ILE:CG2	2.47	0.44
1:C:1:MSE:HE3	1:C:2:THR:CG2	2.37	0.44
1:B:75:MSE:HE2	1:B:113:TYR:CD2	2.53	0.44
1:C:1:MSE:C	1:C:1:MSE:HE3	2.38	0.44
1:E:114:LEU:C	1:E:114:LEU:HD12	2.38	0.44
1:F:309:ILE:N	1:F:309:ILE:HD12	2.33	0.44
1:D:348:ALA:HB3	1:D:353:TRP:CE2	2.53	0.44
1:E:78:ILE:HB	1:E:114:LEU:HB3	1.98	0.44
1:A:97:MSE:HE1	1:A:127:TYR:CE1	2.52	0.43
1:C:58:GLN:OE1	1:C:60:MSE:HE3	2.18	0.43
1:D:344:ALA:CB	1:D:378:ILE:HD12	2.43	0.43
1:A:47:TYR:CE1	1:A:100:MSE:HG3	2.53	0.43
1:D:114:LEU:C	1:D:114:LEU:HD12	2.38	0.43
1:E:234:THR:HG22	4:E:885:HOH:O	2.17	0.43
1:F:64:PHE:HB2	1:F:75:MSE:HE3	2.01	0.43
1:C:348:ALA:HB3	1:C:353:TRP:NE1	2.34	0.43
1:A:264:LEU:HD12	1:A:267:LEU:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:HB	1:A:114:LEU:HB3	2.00	0.43
1:E:153:ILE:HD13	1:E:242:PHE:HB2	1.99	0.43
1:E:56:THR:HG22	1:E:87:TYR:CE1	2.54	0.43
1:C:230:TYR:CD1	1:C:236:PHE:HB2	2.53	0.43
1:F:323:ILE:HG13	1:F:333:VAL:HG22	2.00	0.43
1:B:37:PHE:CZ	1:B:60:MSE:HE1	2.53	0.43
1:C:375:ASP:HB3	1:C:378:ILE:HG12	2.01	0.43
1:F:255:TRP:HZ3	1:F:264:LEU:HD23	1.84	0.43
1:D:114:LEU:HD12	1:D:114:LEU:O	2.19	0.43
1:E:114:LEU:HD21	1:E:122:TYR:CD2	2.53	0.43
1:E:375:ASP:OD1	1:E:377:THR:HG22	2.18	0.43
1:D:5:ARG:NH1	1:D:50:LEU:HD12	2.34	0.43
1:F:308:GLU:C	1:F:309:ILE:HD12	2.39	0.43
1:B:41:LEU:HD21	1:B:60:MSE:HE2	2.01	0.42
1:D:13:GLU:C	1:D:17:MSE:HE2	2.40	0.42
1:C:78:ILE:HB	1:C:114:LEU:HB3	2.01	0.42
1:C:277:ILE:HD11	1:D:277:ILE:CD1	2.49	0.42
1:F:9:MSE:HE3	1:F:17:MSE:HG2	2.00	0.42
1:C:197:PRO:O	1:C:217:ARG:NH1	2.50	0.42
1:D:300:GLY:O	1:D:327:GLU:HA	2.19	0.42
1:D:44:THR:HG23	1:D:61:ALA:C	2.40	0.42
1:E:41:LEU:HD21	1:E:60:MSE:CE	2.49	0.42
1:D:47:TYR:CE1	1:D:100:MSE:HG3	2.55	0.42
1:D:102:ALA:HA	1:D:316:TRP:CH2	2.55	0.42
1:E:309:ILE:HD13	1:E:321:TRP:HD1	1.83	0.42
1:A:114:LEU:O	1:A:114:LEU:HD12	2.20	0.41
1:B:69:HIS:NE2	1:B:387:VAL:HG11	2.35	0.41
1:E:309:ILE:HD12	1:E:309:ILE:N	2.34	0.41
1:B:288:LEU:CD2	1:B:309:ILE:HG12	2.50	0.41
1:D:78:ILE:HD11	1:D:100:MSE:CE	2.49	0.41
1:F:302:LYS:HE2	1:F:324:THR:HG21	2.02	0.41
1:A:128:GLU:HA	1:A:282:MSE:HE2	2.02	0.41
1:C:22:ILE:HD13	1:C:22:ILE:HA	1.94	0.41
1:B:329:GLY:HA3	4:B:845:HOH:O	2.20	0.41
1:E:213:TYR:OH	1:E:229:ASN:ND2	2.45	0.41
1:E:86:GLU:H	1:E:86:GLU:CD	2.23	0.41
1:A:65:GLN:HB3	1:A:181:ILE:HD12	2.01	0.41
1:A:36:ARG:NE	1:A:193:ARG:HD3	2.36	0.41
1:B:128:GLU:HA	1:B:282:MSE:HE2	2.03	0.41
1:E:127:TYR:CE2	1:E:284:ARG:HG2	2.55	0.41
1:E:51:ILE:HD12	1:E:56:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:THR:CG2	1:B:51:ILE:HG23	2.47	0.41
1:D:17:MSE:CE	1:D:41:LEU:HD11	2.51	0.41
1:D:284:ARG:HA	1:D:354:THR:HG21	2.01	0.41
1:A:64:PHE:HB2	1:A:75:MSE:HE3	2.02	0.41
1:C:329:GLY:HA3	4:C:853:HOH:O	2.20	0.41
1:A:46:SER:HB2	1:A:60:MSE:HE2	2.03	0.41
1:C:200:GLN:HB2	1:C:200:GLN:HE21	1.74	0.41
1:D:182:ARG:HD3	1:D:187:LEU:HD13	2.03	0.41
1:F:2:THR:HG23	1:F:52:ASP:OD2	2.21	0.41
1:B:265:ASN:OD1	1:B:268:MSE:CE	2.69	0.40
1:B:352:THR:HG23	1:B:366:LEU:HD22	2.04	0.40
1:B:9:MSE:HE3	1:B:13:GLU:HB3	2.02	0.40
1:C:14:MSE:HE3	1:C:38:GLU:HG3	2.04	0.40
1:D:172:ASN:OD1	1:D:173:GLN:N	2.53	0.40
1:D:86:GLU:OE1	1:D:87:TYR:CE1	2.74	0.40
1:F:156:VAL:HG11	1:F:161:GLY:HA3	2.02	0.40
1:B:14:MSE:CA	1:B:17:MSE:HE3	2.47	0.40
1:B:288:LEU:HD22	1:B:309:ILE:HG12	2.03	0.40
1:F:44:THR:HG23	1:F:61:ALA:O	2.21	0.40
1:F:87:TYR:C	1:F:88:ARG:HG3	2.41	0.40
1:B:75:MSE:HE2	1:B:113:TYR:CE2	2.56	0.40
1:D:11:LYS:HE2	1:D:42:SER:HA	2.04	0.40
1:D:153:ILE:HA	1:D:202:ILE:O	2.22	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	388/400 (97%)	377 (97%)	10 (3%)	1 (0%)	41	55
1	B	389/400 (97%)	377 (97%)	10 (3%)	2 (0%)	29	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	387/400 (97%)	375 (97%)	12 (3%)	0	100	100
1	D	386/400 (96%)	378 (98%)	8 (2%)	0	100	100
1	E	387/400 (97%)	378 (98%)	9 (2%)	0	100	100
1	F	388/400 (97%)	377 (97%)	11 (3%)	0	100	100
All	All	2325/2400 (97%)	2262 (97%)	60 (3%)	3 (0%)	51	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	344	ALA
1	A	344	ALA
1	B	328	GLN

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	328/322 (102%)	310 (94%)	18 (6%)	21	35
1	B	329/322 (102%)	309 (94%)	20 (6%)	18	30
1	C	328/322 (102%)	307 (94%)	21 (6%)	17	28
1	D	327/322 (102%)	311 (95%)	16 (5%)	25	40
1	E	328/322 (102%)	317 (97%)	11 (3%)	37	56
1	F	329/322 (102%)	313 (95%)	16 (5%)	25	40
All	All	1969/1932 (102%)	1867 (95%)	102 (5%)	23	38

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	15	LYS
1	A	34	GLN
1	A	38	GLU

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Mol	Chain	Res	Type
1	A	152	THR
1	A	172	ASN
1	A	193	ARG
1	A	200	GLN
1	A	214	VAL
1	A	234	THR
1	A	250	VAL
1	A	251	GLN
1	A	287	GLU
1	A	324	THR
1	A	346	LEU
1	A	358	LEU
1	A	387	VAL
1	A	394	GLU
1	B	1	MSE
1	B	28	GLU
1	B	58	GLN
1	B	86	GLU
1	B	88	ARG
1	B	118	SER
1	B	148	ARG
1	B	149	VAL
1	B	172	ASN
1	B	174	ARG
1	B	193	ARG
1	B	234	THR
1	B	287	GLU
1	B	306	SER
1	B	324	THR
1	B	328	GLN
1	B	346	LEU
1	B	358	LEU
1	B	364	GLU
1	B	388	LYS
1	C	3	THR
1	C	28	GLU
1	C	41	LEU
1	C	58	GLN
1	C	66	VAL
1	C	86	GLU
1	C	88	ARG
1	C	149	VAL

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Mol	Chain	Res	Type
1	C	162	LYS
1	C	172	ASN
1	C	193	ARG
1	C	200	GLN
1	C	207	GLU
1	C	214	VAL
1	C	234	THR
1	C	249	SER
1	C	264	LEU
1	C	287	GLU
1	C	324	THR
1	C	346	LEU
1	C	387	VAL
1	D	41	LEU
1	D	66	VAL
1	D	72	ARG
1	D	86	GLU
1	D	149	VAL
1	D	156	VAL
1	D	163	GLU
1	D	209	LYS
1	D	214	VAL
1	D	234	THR
1	D	264	LEU
1	D	287	GLU
1	D	324	THR
1	D	334	THR
1	D	346	LEU
1	D	387	VAL
1	E	1	MSE
1	E	5	ARG
1	E	12	GLU
1	E	15	LYS
1	E	27	GLN
1	E	86	GLU
1	E	172	ASN
1	E	274	SER
1	E	324	THR
1	E	346	LEU
1	E	358	LEU
1	F	15	LYS
1	F	27	GLN

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Mol	Chain	Res	Type
1	F	41	LEU
1	F	66	VAL
1	F	99	GLU
1	F	138	ILE
1	F	149	VAL
1	F	172	ASN
1	F	200	GLN
1	F	234	THR
1	F	250	VAL
1	F	264	LEU
1	F	346	LEU
1	F	358	LEU
1	F	387	VAL
1	F	388	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	58	GLN
1	A	129	GLN
1	A	173	GLN
1	A	200	GLN
1	A	246	HIS
1	A	251	GLN
1	A	289	GLN
1	A	384	GLN
1	B	27	GLN
1	B	65	GLN
1	B	200	GLN
1	B	246	HIS
1	B	298	GLN
1	C	129	GLN
1	C	200	GLN
1	C	246	HIS
1	C	289	GLN
1	C	384	GLN
1	D	45	GLN
1	D	129	GLN
1	D	173	GLN
1	D	200	GLN
1	D	233	ASN

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Mol	Chain	Res	Type
1	D	246	HIS
1	D	289	GLN
1	E	58	GLN
1	E	65	GLN
1	E	129	GLN
1	E	200	GLN
1	E	246	HIS
1	F	45	GLN
1	F	129	GLN
1	F	200	GLN
1	F	233	ASN
1	F	246	HIS
1	F	298	GLN
1	F	384	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)

11 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	EPE	C	703	-	15,15,15	0.98	1 (6%)	18,20,20	1.46	4 (22%)
3	PG4	E	805	-	12,12,12	0.59	0	11,11,11	0.31	0
3	PG4	C	803	-	12,12,12	0.63	0	11,11,11	0.41	0
2	EPE	B	702	-	15,15,15	0.94	1 (6%)	18,20,20	1.32	2 (11%)
2	EPE	E	705	-	15,15,15	0.70	1 (6%)	18,20,20	1.31	2 (11%)
3	PG4	D	804	-	12,12,12	0.66	0	11,11,11	0.42	0
2	EPE	A	701	-	15,15,15	0.87	1 (6%)	18,20,20	1.59	3 (16%)
3	PG4	F	806	-	12,12,12	0.58	0	11,11,11	0.46	0
3	PG4	A	801	-	12,12,12	0.60	0	11,11,11	0.41	0
2	EPE	D	704	-	15,15,15	1.01	1 (6%)	18,20,20	1.53	2 (11%)
3	PG4	B	802	-	12,12,12	0.58	0	11,11,11	0.17	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	EPE	C	703	-	-	2/9/19/19	0/1/1/1
3	PG4	E	805	-	-	4/10/10/10	-
3	PG4	C	803	-	-	3/10/10/10	-
2	EPE	B	702	-	-	3/9/19/19	0/1/1/1
2	EPE	E	705	-	-	4/9/19/19	0/1/1/1
3	PG4	D	804	-	-	7/10/10/10	-
2	EPE	A	701	-	-	6/9/19/19	0/1/1/1
3	PG4	F	806	-	-	3/10/10/10	-
3	PG4	A	801	-	-	5/10/10/10	-
2	EPE	D	704	-	-	7/9/19/19	0/1/1/1
3	PG4	B	802	-	-	4/10/10/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	704	EPE	C10-S	3.63	1.82	1.77
2	B	702	EPE	C10-S	3.33	1.82	1.77
2	A	701	EPE	C10-S	3.02	1.81	1.77
2	C	703	EPE	C10-S	2.92	1.81	1.77
2	E	705	EPE	C10-S	2.49	1.81	1.77

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	704	EPE	O3S-S-C10	3.45	111.35	105.77
2	C	703	EPE	O2S-S-C10	3.36	110.96	106.92
2	B	702	EPE	O2S-S-C10	3.36	110.95	106.92
2	A	701	EPE	O3S-S-C10	3.18	110.91	105.77
2	D	704	EPE	O2S-S-C10	3.15	110.71	106.92
2	A	701	EPE	O2S-S-C10	3.05	110.59	106.92
2	E	705	EPE	O2S-S-C10	2.94	110.45	106.92
2	A	701	EPE	C6-C5-N4	2.88	116.54	110.64
2	E	705	EPE	O3S-S-C10	2.85	110.38	105.77
2	C	703	EPE	C2-C3-N4	2.70	116.19	110.64
2	B	702	EPE	O1S-S-C10	2.52	109.95	106.92
2	C	703	EPE	C3-C2-N1	2.32	115.40	110.64
2	C	703	EPE	C9-N1-C6	-2.16	105.72	111.23

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	703	EPE	N4-C7-C8-O8
2	E	705	EPE	C9-C10-S-O1S
2	A	701	EPE	C9-C10-S-O2S
2	A	701	EPE	C9-C10-S-O3S
2	D	704	EPE	C8-C7-N4-C3
2	D	704	EPE	C9-C10-S-O2S
2	D	704	EPE	C9-C10-S-O3S
3	F	806	PG4	O4-C7-C8-O5
3	C	803	PG4	O3-C5-C6-O4
3	B	802	PG4	O3-C5-C6-O4
3	E	805	PG4	O2-C3-C4-O3
3	E	805	PG4	O1-C1-C2-O2
3	D	804	PG4	O2-C3-C4-O3
3	B	802	PG4	O1-C1-C2-O2
3	C	803	PG4	O2-C3-C4-O3
2	B	702	EPE	C9-C10-S-O3S
3	E	805	PG4	O4-C7-C8-O5
3	A	801	PG4	O2-C3-C4-O3
3	D	804	PG4	O3-C5-C6-O4
3	F	806	PG4	C3-C4-O3-C5
2	A	701	EPE	N4-C7-C8-O8
3	A	801	PG4	O3-C5-C6-O4
2	A	701	EPE	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
3	D	804	PG4	O4-C7-C8-O5
3	A	801	PG4	O4-C7-C8-O5
2	E	705	EPE	C10-C9-N1-C2
2	E	705	EPE	C10-C9-N1-C6
2	A	701	EPE	C8-C7-N4-C3
3	E	805	PG4	C1-C2-O2-C3
2	D	704	EPE	C8-C7-N4-C5
3	D	804	PG4	C4-C3-O2-C2
3	D	804	PG4	C3-C4-O3-C5
3	B	802	PG4	O4-C7-C8-O5
3	B	802	PG4	C5-C6-O4-C7
2	B	702	EPE	C9-C10-S-O1S
2	B	702	EPE	C9-C10-S-O2S
2	E	705	EPE	C9-C10-S-O2S
2	A	701	EPE	C9-C10-S-O1S
2	D	704	EPE	C9-C10-S-O1S
3	A	801	PG4	C3-C4-O3-C5
3	F	806	PG4	O2-C3-C4-O3
3	C	803	PG4	C4-C3-O2-C2
3	A	801	PG4	C6-C5-O3-C4
2	D	704	EPE	C10-C9-N1-C2
2	D	704	EPE	C10-C9-N1-C6
3	D	804	PG4	C5-C6-O4-C7
3	D	804	PG4	C6-C5-O3-C4
2	C	703	EPE	S-C10-C9-N1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	703	EPE	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

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	381/400 (95%)	-0.04	6 (1%)	72 70	28, 39, 50, 55	0
1	B	381/400 (95%)	-0.23	4 (1%)	82 80	29, 39, 51, 68	0
1	C	379/400 (94%)	-0.25	1 (0%)	94 93	30, 39, 50, 65	0
1	D	379/400 (94%)	-0.19	2 (0%)	91 89	29, 39, 50, 55	0
1	E	379/400 (94%)	-0.26	2 (0%)	91 89	29, 39, 50, 61	0
1	F	380/400 (95%)	-0.17	1 (0%)	94 93	29, 39, 50, 58	0
All	All	2279/2400 (94%)	-0.19	16 (0%)	87 86	28, 39, 50, 68	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	337	ALA	5.3
1	D	344	ALA	4.6
1	A	89	GLY	3.4
1	B	3	THR	3.1
1	A	380	GLN	2.5
1	B	207	GLU	2.3
1	E	344	ALA	2.3
1	A	391	PRO	2.3
1	F	337	ALA	2.2
1	B	2	THR	2.2
1	B	343	THR	2.2
1	D	2	THR	2.2
1	A	343	THR	2.2
1	A	88	ARG	2.1
1	E	375	ASP	2.1
1	A	337	ALA	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, 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	EPE	D	704	15/15	0.81	0.22	78,80,86,86	0
2	EPE	E	705	15/15	0.83	0.24	83,86,94,94	0
3	PG4	E	805	13/13	0.84	0.22	73,75,76,77	0
3	PG4	B	802	13/13	0.85	0.45	62,63,65,65	0
3	PG4	A	801	13/13	0.86	0.28	58,60,64,65	0
2	EPE	A	701	15/15	0.87	0.24	65,66,73,73	0
2	EPE	B	702	15/15	0.88	0.17	62,66,73,73	0
3	PG4	C	803	13/13	0.88	0.19	56,60,61,62	0
3	PG4	D	804	13/13	0.90	0.25	56,58,59,59	0
3	PG4	F	806	13/13	0.91	0.26	62,65,66,66	0
2	EPE	C	703	15/15	0.91	0.16	58,61,69,70	0

6.5 Other polymers (i)

There are no such residues in this entry.