



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 02:51 am GMT

PDB ID : 1RDF
Title : G50P mutant of phosphonoacetaldehyde hydrolase in complex with substrate analogue vinyl sulfonate
Authors : Lahiri, S.D.; Zhang, G.; Dunaway-Mariano, D.; Allen, K.N.
Deposited on : 2003-11-05
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

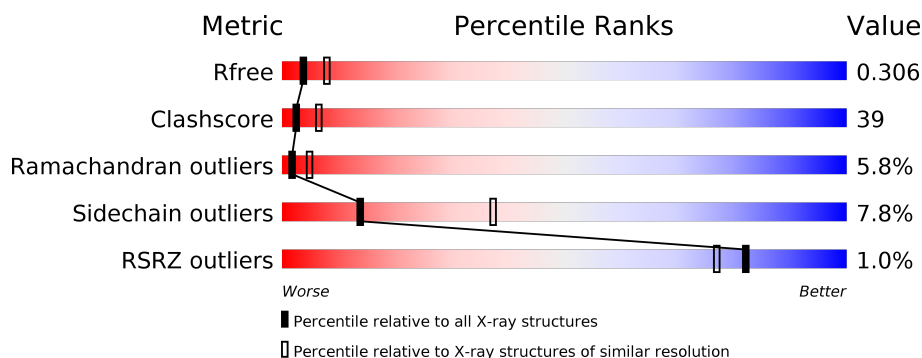
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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. 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	267	
1	B	267	
1	C	267	
1	D	267	
1	E	267	
1	F	267	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12927 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 phosphonoacetaldehyde hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2101	1337	348	399	17			
1	B	263	Total	C	N	O	S	0	0	0
			2098	1335	348	398	17			
1	C	263	Total	C	N	O	S	0	0	0
			2100	1337	348	398	17			
1	D	263	Total	C	N	O	S	0	0	0
			2100	1337	348	398	17			
1	E	263	Total	C	N	O	S	0	0	0
			2100	1337	348	398	17			
1	F	263	Total	C	N	O	S	0	0	0
			2100	1337	348	398	17			

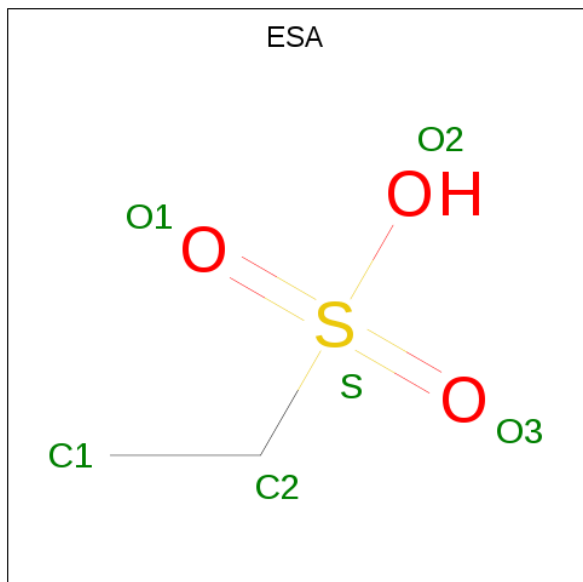
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	PRO	GLY	ENGINEERED	UNP O31156
A	107	ALA	GLY	CONFLICT	UNP O31156
B	50	PRO	GLY	ENGINEERED	UNP O31156
B	107	ALA	GLY	CONFLICT	UNP O31156
C	50	PRO	GLY	ENGINEERED	UNP O31156
C	107	ALA	GLY	CONFLICT	UNP O31156
D	50	PRO	GLY	ENGINEERED	UNP O31156
D	107	ALA	GLY	CONFLICT	UNP O31156
E	50	PRO	GLY	ENGINEERED	UNP O31156
E	107	ALA	GLY	CONFLICT	UNP O31156
F	50	PRO	GLY	ENGINEERED	UNP O31156
F	107	ALA	GLY	CONFLICT	UNP O31156

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is ETHANESULFONIC ACID (three-letter code: ESA) (formula: $C_2H_6O_3S$).

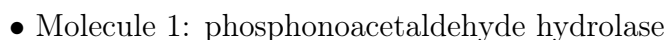
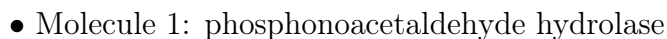


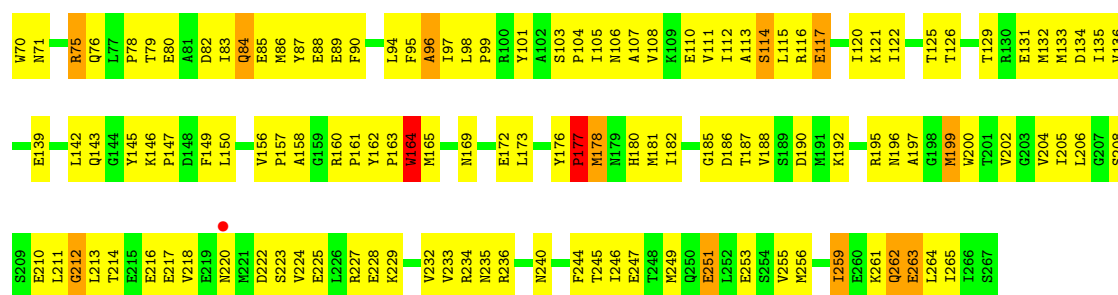
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O S 6 2 3 1	0	0
3	B	1	Total C O S 6 2 3 1	0	0
3	C	1	Total C O S 6 2 3 1	0	0
3	D	1	Total C O S 6 2 3 1	0	0
3	E	1	Total C O S 6 2 3 1	0	0
3	F	1	Total C O S 6 2 3 1	0	0

- Molecule 4 is water.

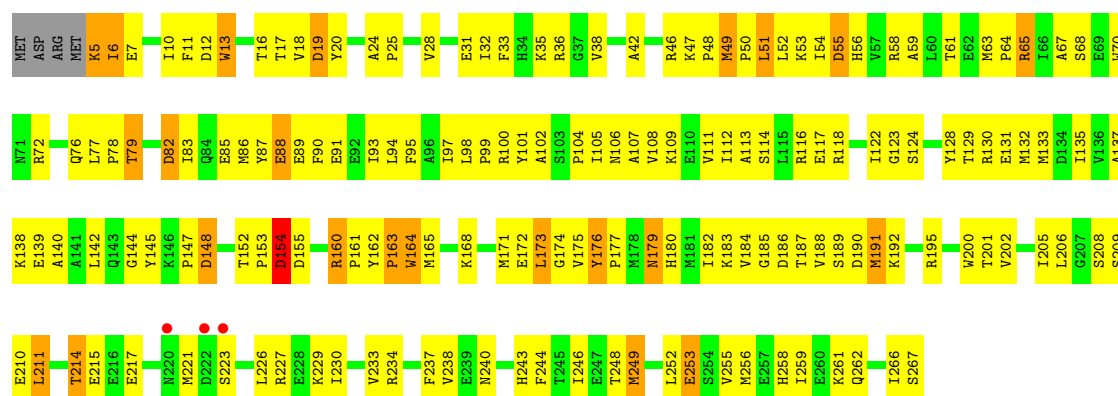
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total 52	O 52	0	0
4	B	57	Total 57	O 57	0	0
4	C	43	Total 43	O 43	0	0
4	D	50	Total 50	O 50	0	0
4	E	49	Total 49	O 49	0	0
4	F	35	Total 35	O 35	0	0

- Molecule 1: phosphonoacetaldehyde hydrolase

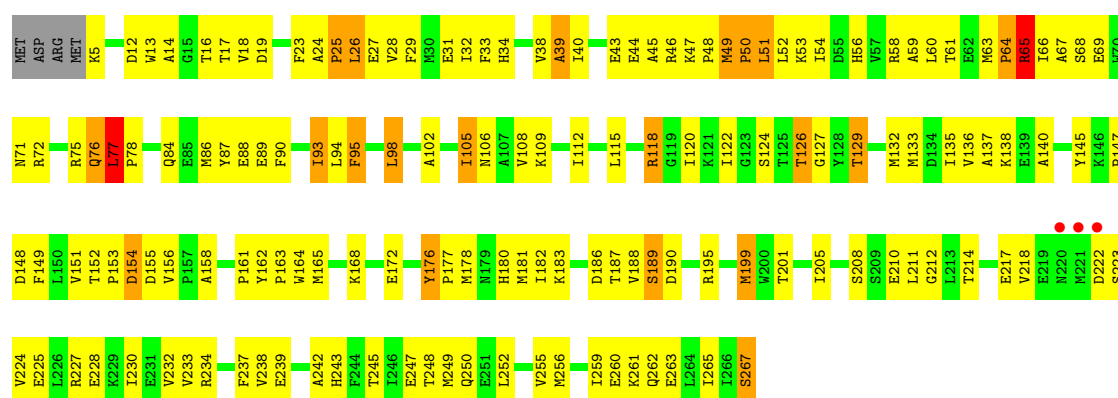




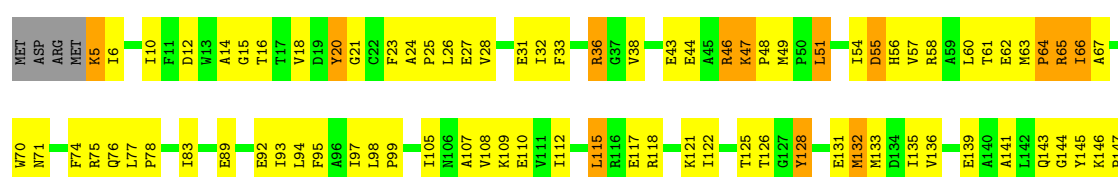
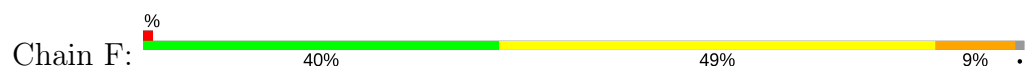
• Molecule 1: phosphonoacetaldehyde hydrolase

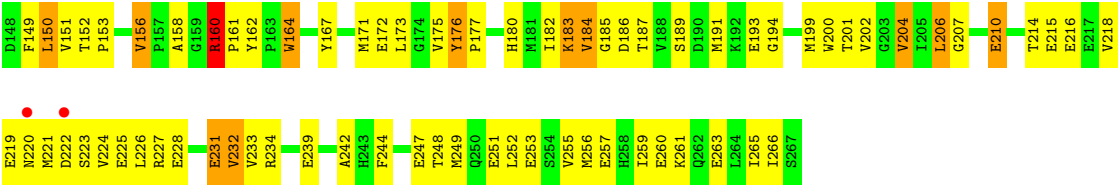


• Molecule 1: phosphonoacetaldehyde hydrolase



• Molecule 1: phosphonoacetaldehyde hydrolase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.71Å 147.35Å 131.31Å 90.00° 125.21° 90.00°	Depositor
Resolution (Å)	34.09 – 2.80 34.09 – 2.70	Depositor EDS
% Data completeness (in resolution range)	77.2 (34.09-2.80) 73.9 (34.09-2.70)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	0.28	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.260 0.248 , 0.306	Depositor DCC
R_{free} test set	5437 reflections (9.49%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12927	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.6614e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.41	0/2144	0.69	2/2898 (0.1%)
1	B	0.42	0/2140	0.73	2/2893 (0.1%)
1	C	0.42	0/2143	0.80	3/2898 (0.1%)
1	D	0.42	0/2143	0.68	0/2898
1	E	0.43	0/2143	0.63	0/2898
1	F	0.42	0/2143	0.65	0/2898
All	All	0.42	0/12856	0.70	7/17383 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	TYR	C-N-CD	-22.46	71.18	120.60
1	B	48	PRO	CA-N-CD	-11.61	95.25	111.50
1	C	176	TYR	C-N-CA	10.42	165.77	122.00
1	B	47	LYS	C-N-CD	-5.47	108.56	120.60
1	C	177	PRO	CA-N-CD	-5.39	103.95	111.50

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	2101	0	2084	165	0
1	B	2098	0	2078	174	0
1	C	2100	0	2084	182	0
1	D	2100	0	2084	162	0
1	E	2100	0	2084	161	0
1	F	2100	0	2084	161	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	6	0	3	0	0
3	B	6	0	3	1	0
3	C	6	0	3	3	0
3	D	6	0	3	0	0
3	E	6	0	3	1	0
3	F	6	0	3	1	0
4	A	52	0	0	20	0
4	B	57	0	0	23	0
4	C	43	0	0	17	0
4	D	50	0	0	20	0
4	E	49	0	0	24	0
4	F	35	0	0	6	0
All	All	12927	0	12516	992	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 39.

The worst 5 of 992 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:TYR:HB3	1:B:177:PRO:HD3	1.24	1.13
1:B:205:ILE:HG21	1:B:230:ILE:HG23	1.41	1.03
1:F:65:ARG:HG2	1:F:66:ILE:H	1.23	1.01
1:E:49:MET:HB3	1:E:50:PRO:HD3	1.44	1.00
1:B:176:TYR:HB3	1:B:177:PRO:CD	1.92	0.98

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	261/267 (98%)	196 (75%)	46 (18%)	19 (7%)	1	2
1	B	261/267 (98%)	201 (77%)	40 (15%)	20 (8%)	1	2
1	C	261/267 (98%)	198 (76%)	48 (18%)	15 (6%)	2	5
1	D	261/267 (98%)	211 (81%)	39 (15%)	11 (4%)	3	10
1	E	261/267 (98%)	208 (80%)	41 (16%)	12 (5%)	2	8
1	F	261/267 (98%)	205 (78%)	42 (16%)	14 (5%)	2	6
All	All	1566/1602 (98%)	1219 (78%)	256 (16%)	91 (6%)	2	5

5 of 91 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
1	A	47	LYS
1	A	56	HIS
1	A	64	PRO
1	A	128	TYR

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	227/231 (98%)	213 (94%)	14 (6%)	20	50
1	B	226/231 (98%)	203 (90%)	23 (10%)	8	24
1	C	227/231 (98%)	213 (94%)	14 (6%)	20	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	227/231 (98%)	210 (92%)	17 (8%)	15	39
1	E	227/231 (98%)	209 (92%)	18 (8%)	13	37
1	F	227/231 (98%)	207 (91%)	20 (9%)	11	31
All	All	1361/1386 (98%)	1255 (92%)	106 (8%)	14	37

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	235	ASN
1	D	114	SER
1	F	156	VAL
1	C	259	ILE
1	D	55	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	196	ASN
1	D	240	ASN
1	F	258	HIS
1	C	240	ASN
1	D	179	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	ESA	A	500	2	5,5,5	3.03	1 (20%)	7,7,7	2.34	2 (28%)
3	ESA	B	500	2	5,5,5	3.07	1 (20%)	7,7,7	2.34	3 (42%)
3	ESA	C	500	2	5,5,5	2.89	1 (20%)	7,7,7	2.30	3 (42%)
3	ESA	D	500	2	5,5,5	2.82	1 (20%)	7,7,7	2.33	3 (42%)
3	ESA	E	500	2	5,5,5	2.97	1 (20%)	7,7,7	2.32	3 (42%)
3	ESA	F	500	2	5,5,5	3.01	1 (20%)	7,7,7	2.47	2 (28%)

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	ESA	A	500	2	-	0/3/3/3	0/0/0/0
3	ESA	B	500	2	-	0/3/3/3	0/0/0/0
3	ESA	C	500	2	-	0/3/3/3	0/0/0/0
3	ESA	D	500	2	-	0/3/3/3	0/0/0/0
3	ESA	E	500	2	-	0/3/3/3	0/0/0/0
3	ESA	F	500	2	-	0/3/3/3	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	ESA	C1-C2	-6.67	1.26	1.50
3	A	500	ESA	C1-C2	-6.64	1.26	1.50
3	F	500	ESA	C1-C2	-6.61	1.26	1.50
3	E	500	ESA	C1-C2	-6.44	1.27	1.50
3	C	500	ESA	C1-C2	-6.29	1.28	1.50

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	500	ESA	O1-S-C2	-3.47	102.73	106.92
3	A	500	ESA	O1-S-C2	-2.94	103.37	106.92
3	B	500	ESA	O1-S-C2	-2.81	103.53	106.92
3	B	500	ESA	O3-S-C2	-2.78	103.57	106.92
3	E	500	ESA	O3-S-C2	-2.68	103.69	106.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	500	ESA	1	0
3	C	500	ESA	3	0
3	E	500	ESA	1	0
3	F	500	ESA	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	263/267 (98%)	-0.44	1 (0%) 92 90	12, 37, 60, 67	0
1	B	263/267 (98%)	-0.34	6 (2%) 60 51	6, 36, 65, 77	0
1	C	263/267 (98%)	-0.37	1 (0%) 92 90	11, 37, 60, 69	0
1	D	263/267 (98%)	-0.47	3 (1%) 80 75	5, 36, 58, 68	0
1	E	263/267 (98%)	-0.46	3 (1%) 80 75	4, 35, 58, 65	0
1	F	263/267 (98%)	-0.48	2 (0%) 86 81	9, 33, 54, 60	0
All	All	1578/1602 (98%)	-0.43	16 (1%) 82 77	4, 36, 60, 77	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	222	ASP	3.4
1	B	77	LEU	2.7
1	D	222	ASP	2.6
1	B	63	MET	2.5
1	E	220	ASN	2.4

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 carbohydrates 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	MG	A	501	1/1	0.83	0.16	4,4,4,4	0
2	MG	F	501	1/1	0.95	0.25	18,18,18,18	0
3	ESA	C	500	6/6	0.96	0.21	39,43,44,44	0
2	MG	C	501	1/1	0.96	0.15	1,1,1,1	0
2	MG	E	501	1/1	0.97	0.23	3,3,3,3	0
3	ESA	A	500	6/6	0.98	0.17	30,32,33,34	0
3	ESA	D	500	6/6	0.98	0.14	27,29,29,29	0
3	ESA	E	500	6/6	0.98	0.16	24,25,26,27	0
2	MG	B	501	1/1	0.98	0.23	8,8,8,8	0
3	ESA	F	500	6/6	0.98	0.19	35,37,38,39	0
3	ESA	B	500	6/6	0.98	0.19	33,35,35,36	0
2	MG	D	501	1/1	0.99	0.25	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.