



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:12 AM UTC

PDB ID : 4FTS / pdb_00004fts
Title : Crystal structure of the N363T mutant of the Flock House virus capsid
Authors : Speir, J.A.; Chen, Z.; Reddy, V.S.; Johnson, J.E.
Deposited on : 2012-06-28
Resolution : 3.20 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

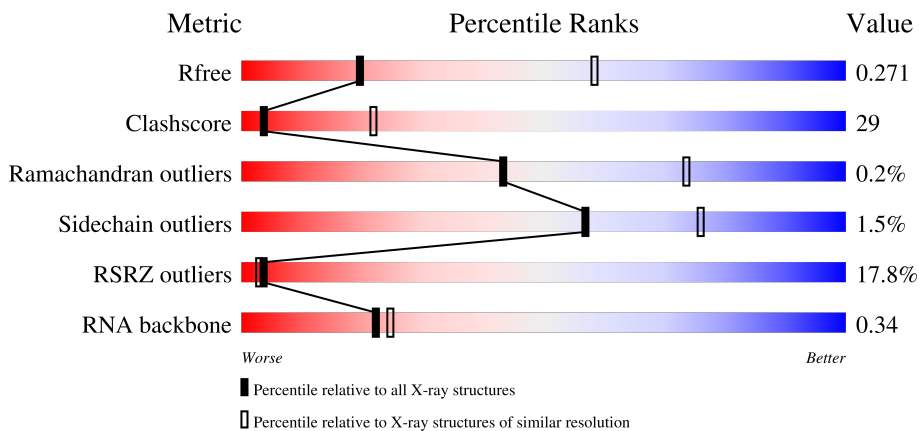
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	407	
1	B	407	
1	C	407	
2	R	15	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8001 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 Capsid protein alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	328	2455	1563	404	477	11	0	0	0
1	B	329	2459	1567	404	476	12	0	0	0
1	C	329	2460	1566	405	478	11	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	363	THR	ASN	engineered mutation	UNP P12870
B	363	THR	ASN	engineered mutation	UNP P12870
C	363	THR	ASN	engineered mutation	UNP P12870

- Molecule 2 is a RNA chain called Random cellular RNAs.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	R	15	302	136	36	115	15	0	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Ca 2	0	0
3	B	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total O S 5 4 1	0	0

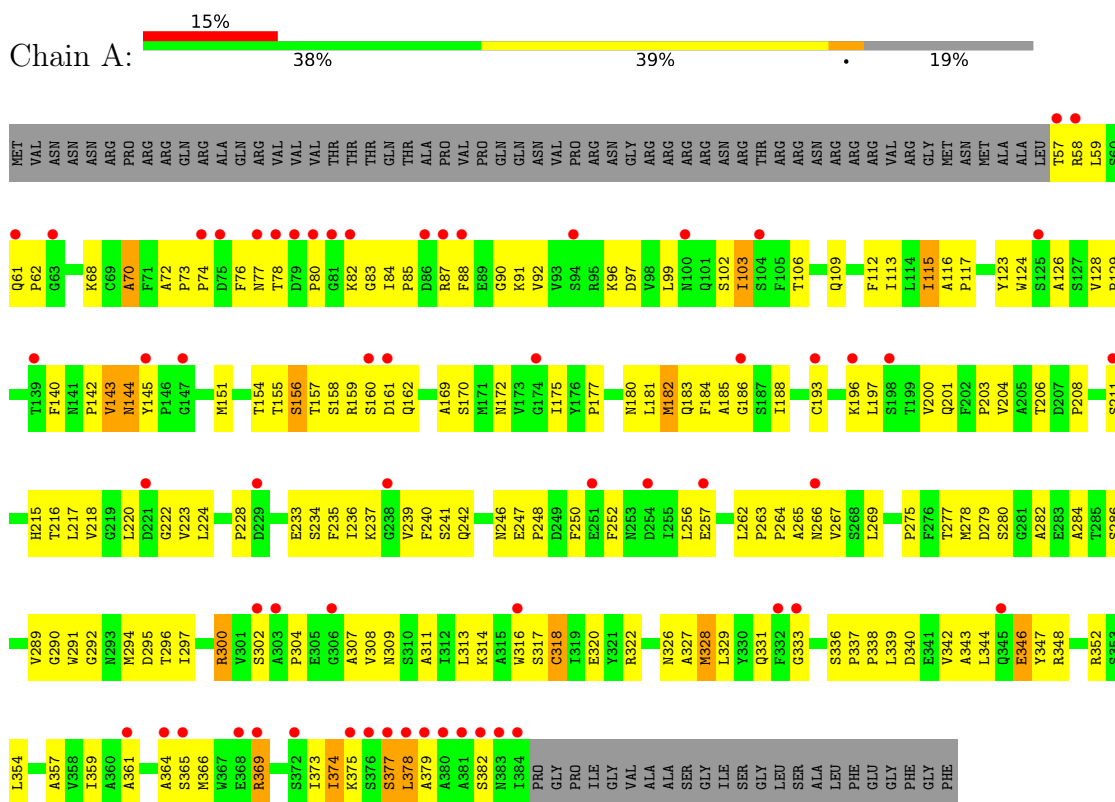
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	74	Total O 74 74	0	0
7	B	101	Total O 101 101	0	0
7	C	92	Total O 92 92	0	0
7	R	3	Total O 3 3	0	0

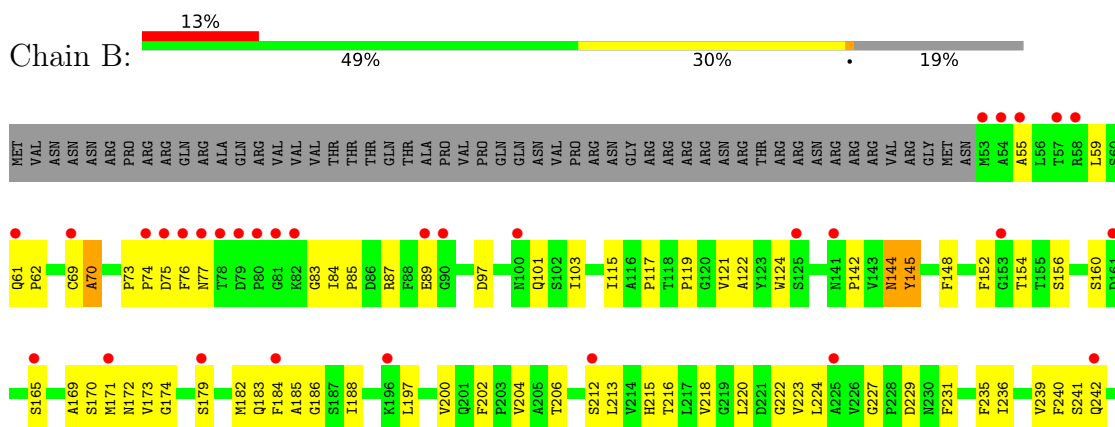
3 Residue-property plots [i](#)

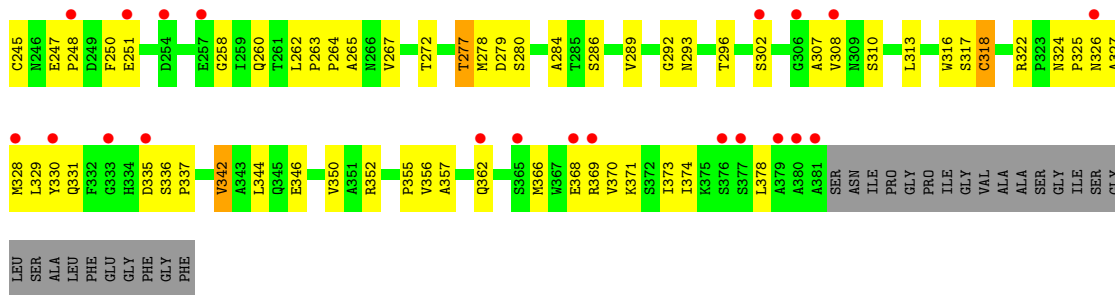
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

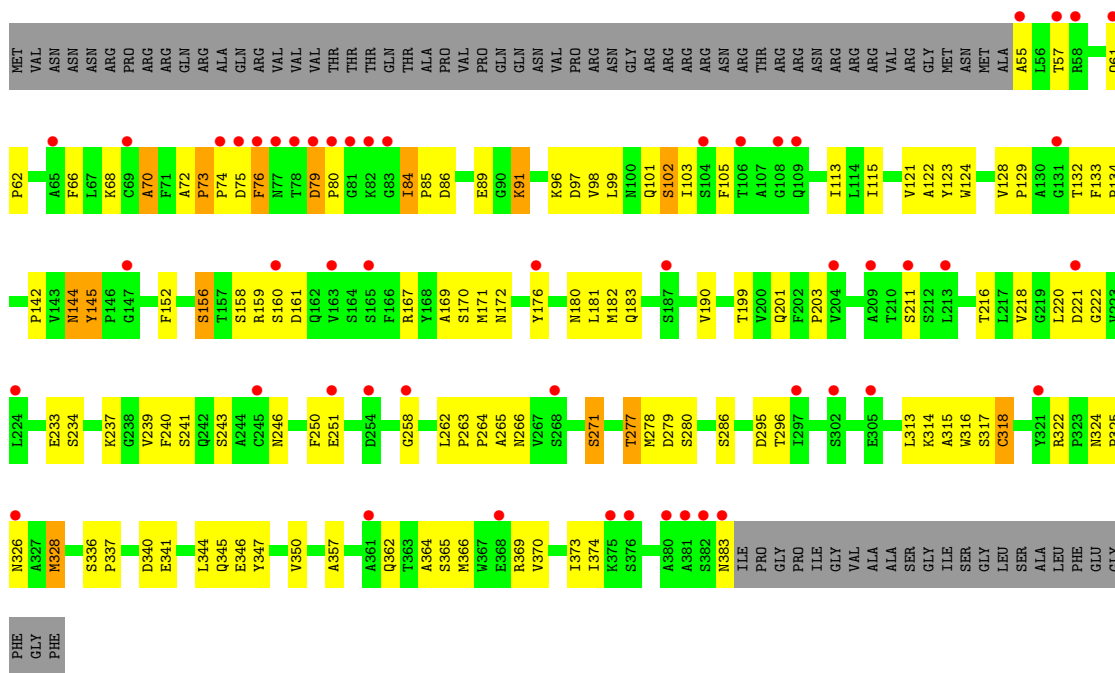


- Molecule 1: Capsid protein alpha

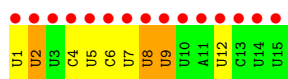




● Molecule 1: Capsid protein alpha



● Molecule 2: Random cellular RNAs



4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	326.04Å 326.04Å 770.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.20 40.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.8 (40.00-3.20) 91.7 (40.00-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.19Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.259 , (Not available) 0.266 , 0.271	Depositor DCC
R_{free} test set	9099 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtrriage
Anisotropy	0.004	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	0.000 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k +1/3*l 0.000 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/ 3*k+1/3*l 0.000 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+ 1/3*l,-4/3*h+4/3*k+1/3*l 0.000 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3* k-1/3*l 0.000 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k- 1/3*l,4/3*h-4/3*k-1/3*l 0.000 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3 *k-1/3*l 0.000 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.35	EDS
Total number of atoms	8001	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.20% 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: SO4, CA, EPE, CL

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	0.63	0/2519	1.11	19/3445 (0.6%)
1	B	0.62	0/2523	1.06	7/3450 (0.2%)
1	C	0.64	0/2524	1.08	12/3452 (0.3%)
2	R	0.30	0/332	0.57	0/511
All	All	0.62	0/7898	1.06	38/10858 (0.3%)

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.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	271	SER	N-CA-C	-8.33	102.28	111.36
1	A	80	PRO	N-CA-C	-8.25	102.06	113.53
1	B	83	GLY	N-CA-C	8.05	119.69	111.56
1	A	378	LEU	N-CA-C	-7.78	103.89	113.15
1	C	73	PRO	N-CA-C	-7.22	101.89	110.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	79	ASP	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2455	0	2399	175	0
1	B	2459	0	2407	147	0
1	C	2460	0	2404	139	0
2	R	302	0	155	10	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	15	0	18	0	0
4	B	15	0	18	1	0
4	C	15	0	18	0	0
5	B	1	0	0	0	0
6	C	5	0	0	0	0
7	A	74	0	0	0	0
7	B	101	0	0	1	0
7	C	92	0	0	1	0
7	R	3	0	0	0	0
All	All	8001	0	7419	440	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 29.

The worst 5 of 440 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:74:PRO:HG3	1:B:316:TRP:CZ2	1.45	1.49
1:A:74:PRO:HG3	1:A:316:TRP:CE2	1.54	1.42
1:B:74:PRO:HB3	1:B:316:TRP:NE1	1.48	1.29
1:B:74:PRO:CB	1:B:316:TRP:HE1	1.50	1.23
1:B:218:VAL:HG13	1:C:160:SER:HB2	1.20	1.19

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	326/407 (80%)	306 (94%)	20 (6%)	0	100	100
1	B	327/407 (80%)	299 (91%)	28 (9%)	0	100	100
1	C	327/407 (80%)	300 (92%)	25 (8%)	2 (1%)	21	56
All	All	980/1221 (80%)	905 (92%)	73 (7%)	2 (0%)	43	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	365	SER
1	C	156	SER

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	272/336 (81%)	267 (98%)	5 (2%)	51	74
1	B	271/336 (81%)	267 (98%)	4 (2%)	57	76
1	C	272/336 (81%)	269 (99%)	3 (1%)	65	79
All	All	815/1008 (81%)	803 (98%)	12 (2%)	57	76

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	318	CYS

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Mol	Chain	Res	Type
1	B	342	VAL
1	C	318	CYS
1	C	76	PHE
1	A	328	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	246	ASN
1	C	383	ASN
1	B	331	GLN
1	C	266	ASN
1	B	293	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	14/15 (93%)	6 (42%)	0

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	2	U
2	R	4	C
2	R	5	U
2	R	8	U
2	R	9	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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
4	EPE	A	503	-	15,15,15	1.27	1 (6%)	19,20,20	1.33	2 (10%)
6	SO4	C	502	-	4,4,4	0.46	0	6,6,6	0.12	0
4	EPE	C	503	-	15,15,15	1.41	1 (6%)	19,20,20	1.41	2 (10%)
4	EPE	B	503	-	15,15,15	1.44	1 (6%)	19,20,20	1.53	2 (10%)

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
4	EPE	A	503	-	-	0/9/19/19	0/1/1/1
4	EPE	C	503	-	-	0/9/19/19	0/1/1/1
4	EPE	B	503	-	-	1/9/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	EPE	C10-S	3.55	1.82	1.77
4	B	503	EPE	C10-S	3.39	1.82	1.77
4	A	503	EPE	C10-S	2.23	1.80	1.77

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	EPE	O1S-S-C10	5.07	114.39	106.73
4	C	503	EPE	O1S-S-C10	3.72	112.35	106.73
4	A	503	EPE	O1S-S-C10	3.54	112.07	106.73
4	C	503	EPE	O3S-S-O2S	-3.28	103.18	111.40
4	A	503	EPE	O3S-S-O2S	-3.05	103.78	111.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	EPE	N4-C7-C8-O8

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	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 [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	328/407 (80%)	1.34	60 (18%) 3 3	46, 70, 136, 236	0
1	B	329/407 (80%)	1.27	52 (15%) 5 4	46, 71, 135, 216	0
1	C	329/407 (80%)	1.26	51 (15%) 5 4	45, 70, 115, 196	0
2	R	15/15 (100%)	5.02	15 (100%) 0 0	213, 289, 331, 334	0
All	All	1001/1236 (80%)	1.35	178 (17%) 4 3	45, 71, 146, 334	0

The worst 5 of 178 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	ALA	13.4
1	A	383	ASN	11.1
1	A	381	ALA	10.4
1	C	383	ASN	10.0
1	C	382	SER	10.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	A	502	1/1	0.67	0.34	112,112,112,112	0
5	CL	B	502	1/1	0.86	0.17	95,95,95,95	0
6	SO4	C	502	5/5	0.92	0.22	124,128,150,190	0
3	CA	C	501	1/1	0.93	0.09	61,61,61,61	0
4	EPE	A	503	15/15	0.93	0.21	56,86,162,162	0
4	EPE	B	503	15/15	0.94	0.20	55,98,145,156	0
4	EPE	C	503	15/15	0.95	0.17	51,102,157,161	0
3	CA	B	501	1/1	0.96	0.12	58,58,58,58	0
3	CA	A	501	1/1	0.98	0.08	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.