



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2023 – 03:24 PM EDT

PDB ID : 3A77
Title : The crystal structure of phosphorylated IRF-3
Authors : Takahasi, K.; Horiuchi, M.; Noda, N.N.; Inagaki, F.
Deposited on : 2009-09-17
Resolution : 1.80 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 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

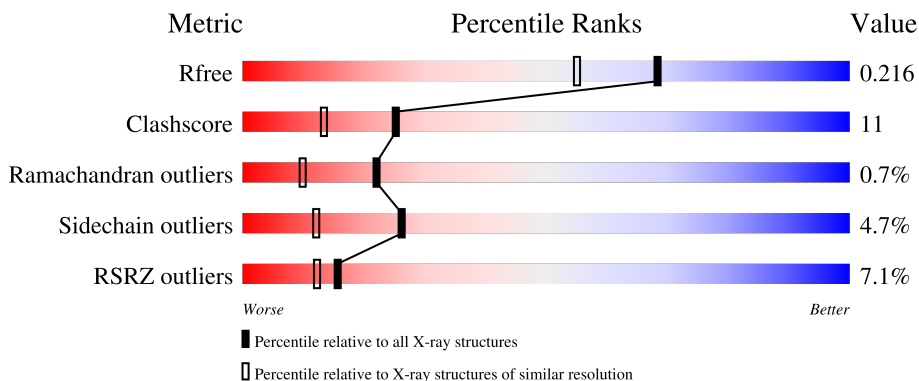
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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	242	 4% 83% 12% . .
1	B	242	 7% 76% 19% . .
1	C	242	 7% 73% 21% . .
1	D	242	 10% 69% 21% 5% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8328 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 Interferon regulatory factor 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	232	1824	1161	312	339	2	10	0	0	0
1	B	234	1836	1168	314	342	2	10	0	0	0
1	C	233	1816	1157	308	339	2	10	0	0	0
1	D	230	1805	1151	309	333	2	10	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	GLY	-	expression tag	UNP Q14653
A	187	ALA	-	expression tag	UNP Q14653
A	188	MET	-	expression tag	UNP Q14653
B	186	GLY	-	expression tag	UNP Q14653
B	187	ALA	-	expression tag	UNP Q14653
B	188	MET	-	expression tag	UNP Q14653
C	186	GLY	-	expression tag	UNP Q14653
C	187	ALA	-	expression tag	UNP Q14653
C	188	MET	-	expression tag	UNP Q14653
D	186	GLY	-	expression tag	UNP Q14653
D	187	ALA	-	expression tag	UNP Q14653
D	188	MET	-	expression tag	UNP Q14653

- Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		

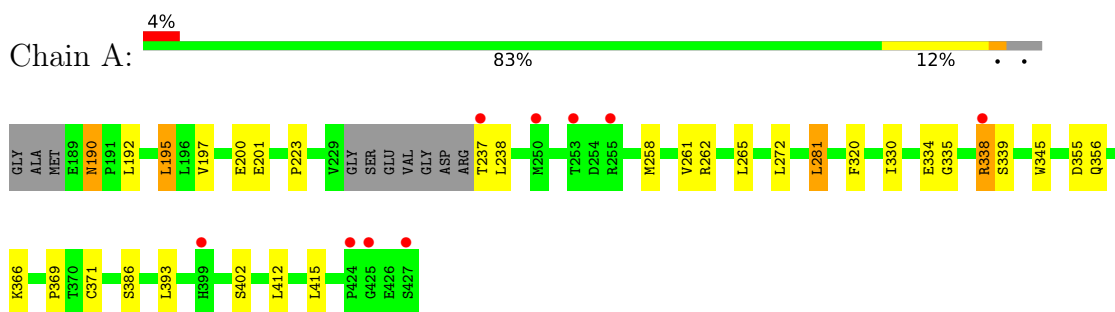
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	266	Total	O	0	0
			266	266		
4	B	275	Total	O	0	0
			275	275		
4	C	254	Total	O	0	0
			254	254		
4	D	212	Total	O	0	0
			212	212		

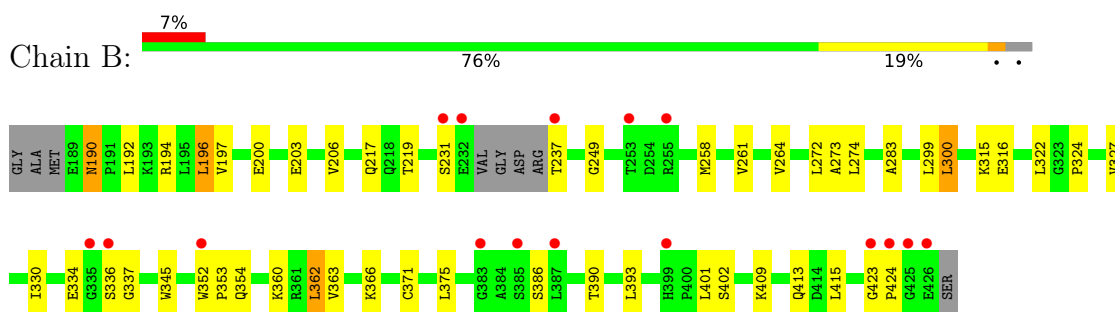
3 Residue-property plots [i](#)

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.

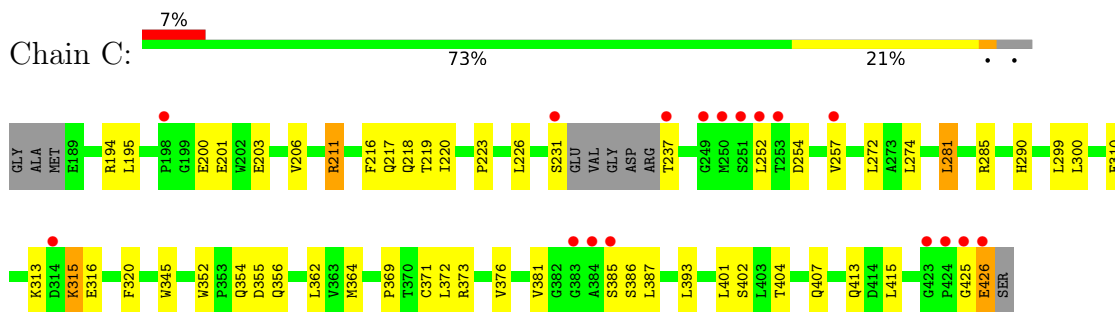
- Molecule 1: Interferon regulatory factor 3



- Molecule 1: Interferon regulatory factor 3

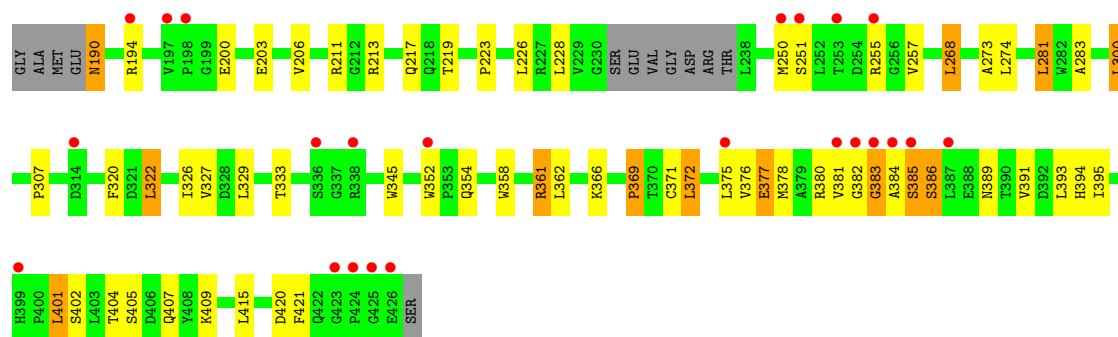


- Molecule 1: Interferon regulatory factor 3



- Molecule 1: Interferon regulatory factor 3





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	163.47Å 102.46Å 68.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 19.94 – 1.80	Depositor EDS
% Data completeness (in resolution range)	87.7 (20.00-1.80) 97.5 (19.94-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.69 (at 1.80Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.194 , 0.221 0.189 , 0.216	Depositor DCC
R_{free} test set	10726 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8328	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.28% 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: SEP, MPD, ACY

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	0.30	0/1855	0.59	1/2524 (0.0%)
1	B	0.31	0/1867	0.60	1/2541 (0.0%)
1	C	0.30	0/1846	0.58	0/2514
1	D	0.30	0/1836	0.60	1/2499 (0.0%)
All	All	0.30	0/7404	0.59	3/10078 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	PRO	N-CA-C	-5.20	98.57	112.10
1	D	369	PRO	N-CA-C	-5.18	98.62	112.10
1	B	300	LEU	CA-CB-CG	5.09	127.01	115.30

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	1824	0	1756	20	0
1	B	1836	0	1765	37	0
1	C	1816	0	1743	48	0
1	D	1805	0	1739	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	3	0	0
2	C	4	0	3	0	0
3	A	8	0	14	0	0
3	B	8	0	14	1	0
3	C	8	0	14	1	0
3	D	8	0	14	0	0
4	A	266	0	0	2	0
4	B	275	0	0	5	0
4	C	254	0	0	5	0
4	D	212	0	0	1	0
All	All	8328	0	7065	154	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 11.

The worst 5 of 154 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:264:VAL:HG21	1:B:363:VAL:HG21	1.52	0.91
1:D:405:SER:O	1:D:409:LYS:HD3	1.72	0.90
3:B:3001:MPD:O4	3:B:3001:MPD:H13	1.84	0.77
1:B:352:TRP:HE1	1:B:354:GLN:HE21	1.33	0.76
3:C:3003:MPD:O4	3:C:3003:MPD:H13	1.84	0.74

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	226/242 (93%)	222 (98%)	4 (2%)	0	100 100
1	B	228/242 (94%)	222 (97%)	4 (2%)	2 (1%)	17 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	227/242 (94%)	222 (98%)	5 (2%)	0	100	100
1	D	224/242 (93%)	214 (96%)	6 (3%)	4 (2%)	8	2
All	All	905/968 (94%)	880 (97%)	19 (2%)	6 (1%)	22	10

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	384	ALA
1	B	337	GLY
1	D	383	GLY
1	D	385	SER
1	D	251	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	194/201 (96%)	188 (97%)	6 (3%)	40	25
1	B	195/201 (97%)	187 (96%)	8 (4%)	30	16
1	C	192/201 (96%)	185 (96%)	7 (4%)	35	20
1	D	191/201 (95%)	176 (92%)	15 (8%)	12	4
All	All	772/804 (96%)	736 (95%)	36 (5%)	26	12

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	327	VAL
1	D	415	LEU
1	D	361	ARG
1	D	375	LEU
1	B	375	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	422	GLN
1	D	284	GLN
1	D	214	GLN
1	D	288	HIS
1	B	190	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](#)

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SEP	B	402	1	8,9,10	1.07	0	8,12,14	1.63	2 (25%)
1	SEP	A	402	1	8,9,10	1.01	0	8,12,14	1.41	1 (12%)
1	SEP	C	402	1	8,9,10	1.05	0	8,12,14	1.88	2 (25%)
1	SEP	B	386	1	8,9,10	1.01	0	8,12,14	1.84	2 (25%)
1	SEP	A	386	1	8,9,10	0.92	0	8,12,14	1.23	1 (12%)
1	SEP	C	386	1	8,9,10	1.05	0	8,12,14	1.80	2 (25%)
1	SEP	D	402	1	8,9,10	1.08	0	8,12,14	1.65	2 (25%)
1	SEP	D	386	1	8,9,10	1.23	0	8,12,14	2.19	2 (25%)

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
1	SEP	B	402	1	-	3/5/8/10	-
1	SEP	A	402	1	-	0/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	C	402	1	-	0/5/8/10	-
1	SEP	B	386	1	-	0/5/8/10	-
1	SEP	A	386	1	-	0/5/8/10	-
1	SEP	C	386	1	-	1/5/8/10	-
1	SEP	D	402	1	-	3/5/8/10	-
1	SEP	D	386	1	-	1/5/8/10	-

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	386	SEP	OG-CB-CA	4.11	112.14	108.14
1	C	402	SEP	P-OG-CB	-3.97	107.36	118.30
1	B	386	SEP	P-OG-CB	-3.97	107.36	118.30
1	D	386	SEP	P-OG-CB	-3.91	107.52	118.30
1	C	386	SEP	P-OG-CB	-3.71	108.09	118.30

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	402	SEP	CB-OG-P-O2P
1	B	402	SEP	CB-OG-P-O3P
1	C	386	SEP	N-CA-CB-OG
1	D	402	SEP	CB-OG-P-O2P
1	D	402	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	386	SEP	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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
3	MPD	C	3003	-	7,7,7	1.16	1 (14%)	9,10,10	4.10	5 (55%)
3	MPD	D	3004	-	7,7,7	0.48	0	9,10,10	0.38	0
2	ACY	C	2003	-	3,3,3	0.59	0	3,3,3	0.83	0
3	MPD	A	3002	-	7,7,7	0.49	0	9,10,10	0.41	0
2	ACY	A	2001	-	3,3,3	0.58	0	3,3,3	0.80	0
3	MPD	B	3001	-	7,7,7	1.13	1 (14%)	9,10,10	4.09	5 (55%)

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	MPD	A	3002	-	-	0/5/5/5	-
3	MPD	D	3004	-	-	0/5/5/5	-
3	MPD	C	3003	-	-	0/5/5/5	-
3	MPD	B	3001	-	-	0/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3003	MPD	C3-C2	2.50	1.60	1.53
3	B	3001	MPD	C3-C2	2.43	1.60	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3003	MPD	O2-C2-C3	-7.34	82.22	109.80
3	B	3001	MPD	O2-C2-C3	-7.31	82.35	109.80
3	B	3001	MPD	CM-C2-C3	-5.84	82.75	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3003	MPD	CM-C2-C3	-5.79	82.98	109.96
3	C	3003	MPD	O2-C2-C1	5.49	125.68	108.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3003	MPD	1	0
3	B	3001	MPD	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	230/242 (95%)	0.06	9 (3%) 39 33	10, 16, 36, 47	0
1	B	232/242 (95%)	0.17	16 (6%) 16 13	9, 16, 42, 63	0
1	C	231/242 (95%)	0.23	17 (7%) 14 11	11, 20, 43, 57	0
1	D	228/242 (94%)	0.45	23 (10%) 7 5	11, 20, 46, 64	0
All	All	921/968 (95%)	0.23	65 (7%) 16 12	9, 18, 43, 64	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	384	ALA	9.4
1	D	425	GLY	8.1
1	D	423	GLY	6.9
1	C	231	SER	6.1
1	B	424	PRO	5.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	C	386	10/11	0.47	0.30	51,56,63,64	0
1	SEP	D	402	10/11	0.67	0.22	33,39,50,50	0
1	SEP	D	386	10/11	0.71	0.23	58,62,63,64	0
1	SEP	B	402	10/11	0.74	0.21	32,39,49,49	0
1	SEP	C	402	10/11	0.76	0.17	26,32,45,45	0
1	SEP	B	386	10/11	0.79	0.22	54,56,61,62	0
1	SEP	A	402	10/11	0.90	0.12	16,20,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	SEP	A	386	10/11	0.98	0.07	11,13,15,15	0

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
3	MPD	C	3003	8/8	0.59	0.34	59,61,61,61	0
3	MPD	A	3002	8/8	0.63	0.33	53,55,55,55	0
3	MPD	B	3001	8/8	0.70	0.31	59,59,60,61	0
2	ACY	A	2001	4/4	0.72	0.22	35,38,38,40	0
3	MPD	D	3004	8/8	0.74	0.22	58,59,59,59	0
2	ACY	C	2003	4/4	0.84	0.15	29,33,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.