Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 10:51 PM EDT

PDB ID	:	2B4H
Title	:	Crystal Structure of the Rhesus Rotavirus VP5 Antigen Domain Dimer
Authors	:	Yoder, J.D.; Dormitzer, P.R.
Deposited on	:	2005-09-24
Resolution	:	1.60 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 (i) 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 (i)) were used in the production of this report:

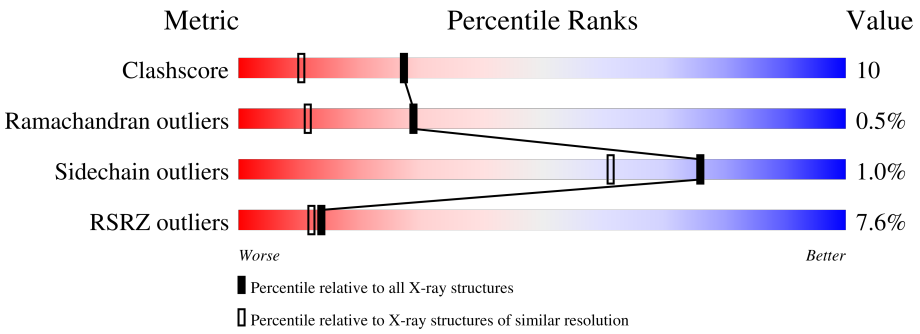
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.60 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))
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 <=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	254	8%, 76%, 13%, •, 11%
1	B	254	6%, 73%, 12%, •, 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3993 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 Outer capsid protein VP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	227	1801	1148	302	345	6	0	0	0
1	B	218	1734	1107	291	330	6	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

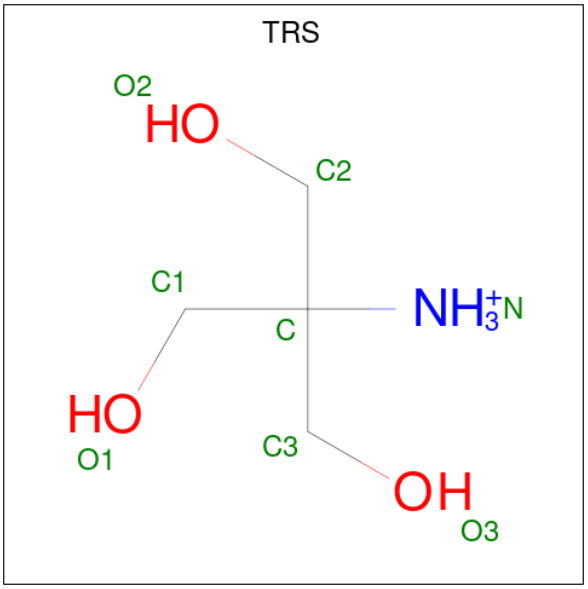
Chain	Residue	Modelled	Actual	Comment	Reference
A	226	MET	-	expression tag	UNP Q91HI9
A	227	GLY	-	expression tag	UNP Q91HI9
A	228	SER	-	expression tag	UNP Q91HI9
A	229	SER	-	expression tag	UNP Q91HI9
A	230	HIS	-	expression tag	UNP Q91HI9
A	231	HIS	-	expression tag	UNP Q91HI9
A	232	HIS	-	expression tag	UNP Q91HI9
A	233	HIS	-	expression tag	UNP Q91HI9
A	234	HIS	-	expression tag	UNP Q91HI9
A	235	HIS	-	expression tag	UNP Q91HI9
A	236	SER	-	expression tag	UNP Q91HI9
A	237	SER	-	expression tag	UNP Q91HI9
A	238	GLY	-	expression tag	UNP Q91HI9
A	239	LEU	-	expression tag	UNP Q91HI9
A	240	VAL	-	expression tag	UNP Q91HI9
A	241	PRO	-	expression tag	UNP Q91HI9
A	242	ARG	-	expression tag	UNP Q91HI9
A	243	GLY	-	expression tag	UNP Q91HI9
A	244	SER	-	expression tag	UNP Q91HI9
A	245	HIS	-	expression tag	UNP Q91HI9
A	246	MET	-	expression tag	UNP Q91HI9
B	226	MET	-	expression tag	UNP Q91HI9
B	227	GLY	-	expression tag	UNP Q91HI9
B	228	SER	-	expression tag	UNP Q91HI9
B	229	SER	-	expression tag	UNP Q91HI9

Continued on next page...

Continued from previous page...

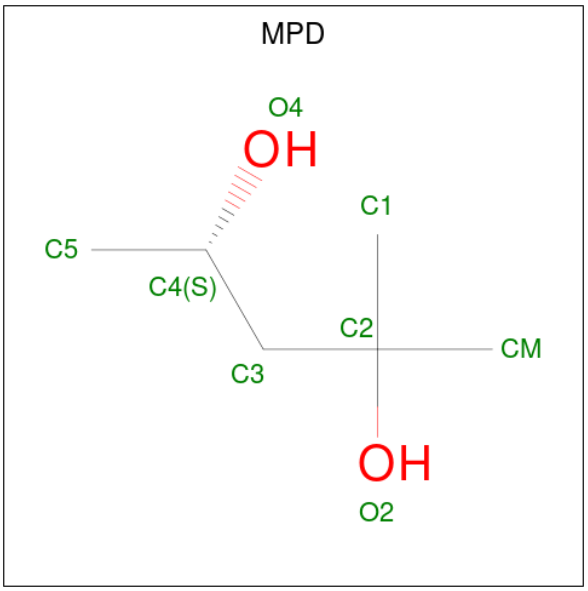
Chain	Residue	Modelled	Actual	Comment	Reference
B	230	HIS	-	expression tag	UNP Q91HI9
B	231	HIS	-	expression tag	UNP Q91HI9
B	232	HIS	-	expression tag	UNP Q91HI9
B	233	HIS	-	expression tag	UNP Q91HI9
B	234	HIS	-	expression tag	UNP Q91HI9
B	235	HIS	-	expression tag	UNP Q91HI9
B	236	SER	-	expression tag	UNP Q91HI9
B	237	SER	-	expression tag	UNP Q91HI9
B	238	GLY	-	expression tag	UNP Q91HI9
B	239	LEU	-	expression tag	UNP Q91HI9
B	240	VAL	-	expression tag	UNP Q91HI9
B	241	PRO	-	expression tag	UNP Q91HI9
B	242	ARG	-	expression tag	UNP Q91HI9
B	243	GLY	-	expression tag	UNP Q91HI9
B	244	SER	-	expression tag	UNP Q91HI9
B	245	HIS	-	expression tag	UNP Q91HI9
B	246	MET	-	expression tag	UNP Q91HI9

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	8	4	1	3	0	0

- 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
			Total	C	O		
3	A	1	8	6	2	0	0
			Total	C	O		
3	A	1	8	6	2	0	0
			Total	C	O		
3	B	1	8	6	2	0	0
			Total	C	O		
3	B	1	8	6	2	0	0

- Molecule 4 is water.

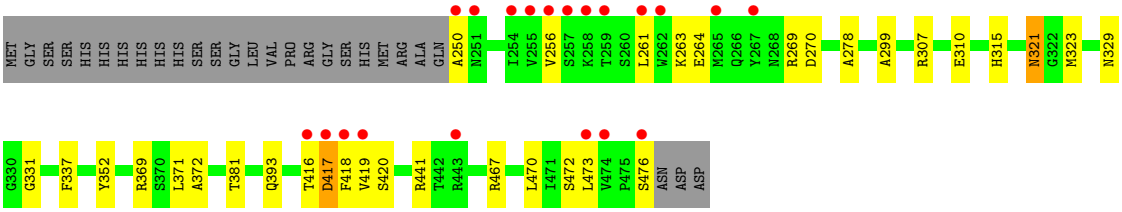
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	222	222	222	0	0
			Total	O		
4	B	196	196	196	0	0

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.

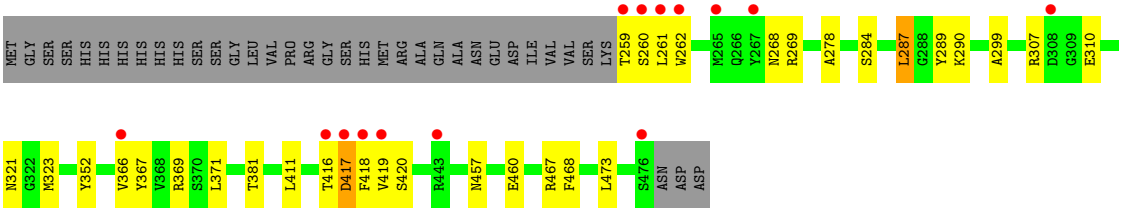
- Molecule 1: Outer capsid protein VP4

Chain A:



- Molecule 1: Outer capsid protein VP4

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	163.36Å 54.80Å 65.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.50 – 1.60 45.51 – 1.50	Depositor EDS
% Data completeness (in resolution range)	93.6 (45.50-1.60) 83.6 (45.51-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 1.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.203 , 0.225 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	16.6	Xtriage
Anisotropy	0.939	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3993	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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 26.95 % 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 2.3998e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

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

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	0.59	0/1846	0.77	0/2508
1	B	0.62	0/1779	0.80	0/2417
All	All	0.61	0/3625	0.78	0/4925

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1801	0	1735	40	0
1	B	1734	0	1667	40	0
2	A	8	0	11	0	0
3	A	16	0	28	5	0
3	B	16	0	28	0	0
4	A	222	0	0	2	0
4	B	196	0	0	8	0
All	All	3993	0	3469	71	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 10.

All (71) 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:A:419:VAL:HG12	1:A:420:SER:H	1.39	0.88
1:B:419:VAL:HG12	1:B:420:SER:H	1.37	0.87
1:A:337:PHE:H	3:A:3001:MPD:H12	1.47	0.79
1:A:416:THR:HG22	1:A:417:ASP:H	1.52	0.73
1:A:416:THR:HG22	1:A:417:ASP:N	2.05	0.72
1:A:321:ASN:HB2	1:A:352:TYR:HE1	1.55	0.69
1:A:419:VAL:HG12	1:A:420:SER:N	2.08	0.68
1:B:419:VAL:HG12	1:B:420:SER:N	2.09	0.67
1:B:260:SER:HB2	1:B:262:TRP:HE1	1.60	0.67
1:B:416:THR:O	1:B:418:PHE:N	2.29	0.66
1:A:307:ARG:O	1:A:310:GLU:HG2	1.97	0.64
1:A:263:LYS:HD3	1:A:264:GLU:H	1.63	0.62
1:B:381:THR:CG2	4:B:4152:HOH:O	2.48	0.62
1:A:261:LEU:HD23	1:B:261:LEU:HD23	1.81	0.61
1:A:441:ARG:O	3:A:3001:MPD:H51	2.01	0.60
1:A:261:LEU:HB3	1:A:476:SER:HB3	1.85	0.58
1:B:284:SER:HB2	1:B:290:LYS:HB2	1.85	0.57
1:A:315:HIS:ND1	3:A:2001:MPD:H4	2.19	0.57
1:A:416:THR:O	1:A:418:PHE:N	2.38	0.56
1:A:416:THR:CG2	1:A:417:ASP:H	2.17	0.56
1:B:307:ARG:O	1:B:310:GLU:HG2	2.06	0.56
1:A:419:VAL:CG1	1:A:420:SER:H	2.16	0.56
1:A:250:ALA:O	1:B:269:ARG:HA	2.07	0.55
1:A:337:PHE:H	3:A:3001:MPD:C1	2.19	0.54
1:A:250:ALA:O	1:B:269:ARG:CA	2.56	0.54
1:A:269:ARG:HH11	1:A:269:ARG:HG3	1.73	0.54
1:B:366:VAL:HG13	1:B:367:TYR:N	2.24	0.53
1:B:287:LEU:HD22	1:B:289:TYR:CE1	2.44	0.53
1:B:287:LEU:HD23	1:B:287:LEU:O	2.08	0.53
1:A:250:ALA:HB3	1:B:268:ASN:HB3	1.91	0.53
1:B:416:THR:HG22	1:B:417:ASP:N	2.24	0.51
1:A:416:THR:CG2	1:A:417:ASP:N	2.72	0.51
1:A:263:LYS:CD	1:A:264:GLU:H	2.23	0.51
1:A:261:LEU:HD22	1:B:259:THR:CG2	2.41	0.50
1:B:460:GLU:HG2	4:B:4079:HOH:O	2.11	0.49
1:A:467:ARG:HD2	4:A:5087:HOH:O	2.11	0.49
1:A:278:ALA:HB2	1:A:299:ALA:HB2	1.95	0.49
1:B:369:ARG:HG2	1:B:369:ARG:HH11	1.77	0.49
1:A:381:THR:HG21	4:A:5067:HOH:O	2.12	0.49
1:B:371:LEU:HD22	1:B:468:PHE:CZ	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LEU:HD23	4:B:4085:HOH:O	2.13	0.48
1:B:381:THR:HG22	4:B:4152:HOH:O	2.12	0.48
1:B:260:SER:CB	1:B:262:TRP:HE1	2.25	0.48
1:B:366:VAL:HG13	1:B:367:TYR:H	1.77	0.48
1:A:337:PHE:N	3:A:3001:MPD:H12	2.25	0.48
1:B:381:THR:HG23	4:B:4152:HOH:O	2.12	0.47
1:B:287:LEU:HD21	4:B:4052:HOH:O	2.14	0.47
1:B:366:VAL:CG1	4:B:4111:HOH:O	2.63	0.46
1:B:381:THR:O	1:B:457:ASN:HB2	2.15	0.46
1:B:366:VAL:HG12	4:B:4111:HOH:O	2.14	0.46
1:B:287:LEU:HD22	1:B:289:TYR:HE1	1.79	0.46
1:A:470:LEU:HD21	1:A:472:SER:HB3	1.97	0.46
1:B:369:ARG:HG2	1:B:369:ARG:NH1	2.29	0.46
1:A:250:ALA:N	1:B:467:ARG:HG2	2.31	0.45
1:B:419:VAL:CG1	1:B:420:SER:H	2.17	0.45
1:A:369:ARG:HB2	1:B:367:TYR:OH	2.17	0.45
1:A:419:VAL:CG1	1:A:420:SER:N	2.78	0.45
1:A:329:ASN:ND2	1:A:331:GLY:H	2.15	0.45
1:A:256:VAL:O	1:A:256:VAL:HG12	2.17	0.45
1:A:270:ASP:OD1	1:A:467:ARG:HG2	2.16	0.45
1:A:261:LEU:HD22	1:B:259:THR:HG21	1.98	0.44
1:A:371:LEU:HD23	1:A:372:ALA:N	2.32	0.44
1:A:269:ARG:HG3	1:A:269:ARG:NH1	2.32	0.43
1:A:393:GLN:HB3	1:A:441:ARG:CZ	2.48	0.43
1:B:278:ALA:HB2	1:B:299:ALA:HB2	2.00	0.43
1:B:321:ASN:HB2	1:B:352:TYR:HE1	1.84	0.43
1:A:371:LEU:HD23	1:A:371:LEU:C	2.39	0.42
1:B:416:THR:CG2	1:B:417:ASP:N	2.83	0.42
1:B:371:LEU:HD11	1:B:411:LEU:HB2	2.03	0.41
1:A:473:LEU:HD23	1:B:473:LEU:CD2	2.51	0.41
1:B:262:TRP:HB3	1:B:473:LEU:HG	2.03	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	225/254 (89%)	217 (96%)	7 (3%)	1 (0%)	34	15
1	B	216/254 (85%)	210 (97%)	5 (2%)	1 (0%)	29	11
All	All	441/508 (87%)	427 (97%)	12 (3%)	2 (0%)	29	11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	417	ASP
1	B	417	ASP

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	198/221 (90%)	196 (99%)	2 (1%)	76	61
1	B	190/221 (86%)	188 (99%)	2 (1%)	73	57
All	All	388/442 (88%)	384 (99%)	4 (1%)	76	61

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	ASN
1	A	323	MET
1	B	287	LEU
1	B	323	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
1	A	321	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	329	ASN
1	A	414	GLN
1	B	376	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	B	4001	-	7,7,7	0.58	0	9,10,10	0.44	0
3	MPD	A	3001	-	7,7,7	0.42	0	9,10,10	0.68	0
2	TRS	A	5001	-	7,7,7	1.64	2 (28%)	9,9,9	1.96	3 (33%)
3	MPD	A	2001	-	7,7,7	0.55	0	9,10,10	0.49	0
3	MPD	B	1001	-	7,7,7	0.47	0	9,10,10	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	B	4001	-	-	2/5/5/5	-
3	MPD	A	3001	-	-	0/5/5/5	-
2	TRS	A	5001	-	-	3/9/9/9	-
3	MPD	A	2001	-	-	2/5/5/5	-
3	MPD	B	1001	-	-	0/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5001	TRS	C2-C	-3.70	1.41	1.53
2	A	5001	TRS	O1-C1	-2.23	1.34	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	5001	TRS	O3-C3-C	3.69	122.70	111.00
2	A	5001	TRS	C3-C-N	2.60	115.73	107.98
2	A	5001	TRS	C2-C-C1	-2.10	104.31	110.81

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5001	TRS	C1-C-C3-O3
2	A	5001	TRS	C2-C-C3-O3
2	A	5001	TRS	N-C-C3-O3
3	A	2001	MPD	C1-C2-C3-C4
3	B	4001	MPD	CM-C2-C3-C4
3	A	2001	MPD	O2-C2-C3-C4
3	B	4001	MPD	O2-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3001	MPD	4	0
3	A	2001	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	227/254 (89%)	0.39	20 (8%)	10	9	16, 26, 59, 94	0
1	B	218/254 (85%)	0.26	14 (6%)	19	17	14, 27, 55, 96	0
All	All	445/508 (87%)	0.33	34 (7%)	13	12	14, 27, 58, 96	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	PHE	13.2
1	B	418	PHE	10.6
1	A	419	VAL	8.0
1	A	417	ASP	7.8
1	A	250	ALA	7.5
1	B	417	ASP	7.5
1	B	419	VAL	6.6
1	A	256	VAL	5.8
1	A	416	THR	5.2
1	A	261	LEU	5.1
1	A	258	LYS	4.5
1	B	476	SER	4.1
1	B	261	LEU	3.9
1	B	259	THR	3.8
1	A	262	TRP	3.5
1	B	262	TRP	3.4
1	A	255	VAL	3.3
1	A	476	SER	3.2
1	A	254	ILE	3.2
1	B	366	VAL	3.2
1	A	259	THR	3.1
1	A	257	SER	2.9
1	B	416	THR	2.9
1	A	474	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	308	ASP	2.7
1	A	265	MET	2.5
1	B	260	SER	2.5
1	A	251	ASN	2.4
1	A	473	LEU	2.4
1	B	265	MET	2.3
1	B	443	ARG	2.3
1	A	267	TYR	2.3
1	B	267	TYR	2.0
1	A	443	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MPD	B	4001	8/8	0.47	0.30	53,54,55,55	0
2	TRS	A	5001	8/8	0.68	0.21	71,71,71,72	0
3	MPD	A	3001	8/8	0.73	0.28	60,61,61,62	0
3	MPD	A	2001	8/8	0.80	0.26	52,53,53,53	0
3	MPD	B	1001	8/8	0.81	0.16	29,35,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.