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wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:50 PM GMT

PDB ID	:	1HH4
Title	:	RAC1-RHOGDI COMPLEX INVOLVED IN NADPH OXIDASE ACTIVATION
Authors	:	Grizot, S.; Faure, J.; Fieschi, F.; Vignais, P.V.; Dagher, M.-C.; Pebay-Peyroula, E.
Deposited on	:	2000-12-20
Resolution	:	2.70 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

http://wwpdb.org/validation/2016/XrayValidationReportHelp

with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.70 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.
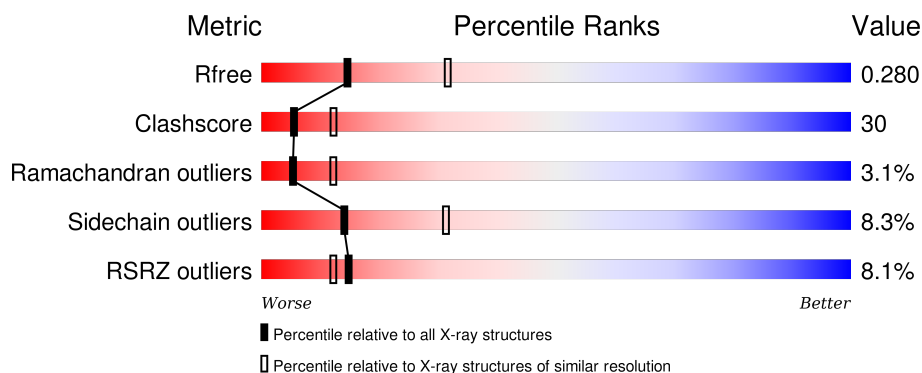
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 <=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	192	6% / 54% / 41%
1	B	192	8% / 43% / 50% / 5%
2	D	204	9% / 48% / 39% / 9%
2	E	204	7% / 44% / 39% / 5% / 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	B	1191	-	-	-	X
5	GER	D	1502	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5908 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 RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total 1448	C 928	N 243	O 268	S 9	0	0	0
1	B	189	Total 1446	C 924	N 243	O 270	S 9	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	SER	PHE	CLONING ARTIFACT	UNP P15154
A	1	PRO	MET	CLONING ARTIFACT	UNP P15154
B	78	SER	PHE	CLONING ARTIFACT	UNP P15154
B	1	PRO	MET	CLONING ARTIFACT	UNP P15154

- Molecule 2 is a protein called RHO GDP-DISSOCIATION INHIBITOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	186	Total 1445	C 912	N 245	O 285	S 3	0	0	0
2	E	180	Total 1441	C 915	N 243	O 279	S 4	0	0	0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GERAN-8-YL GERAN (three-letter code: GER) (formula: $C_{20}H_{34}$).
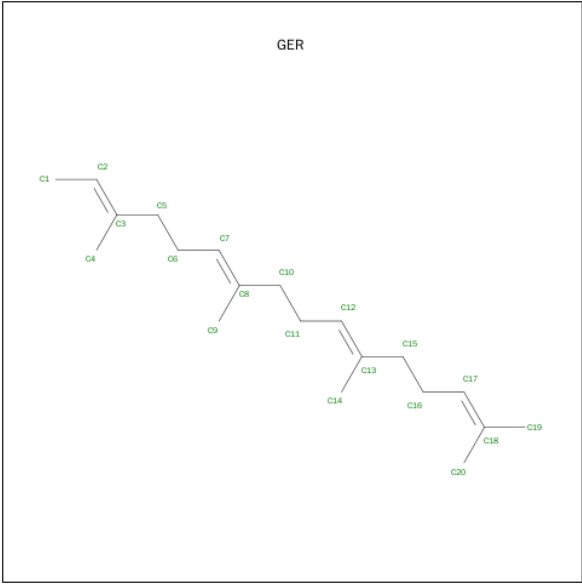
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total 20	C 20	0	0
5	E	1	Total 20	C 20	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total 12	O 12	0	0
6	B	6	Total 6	O 6	0	0
6	D	7	Total 7	O 7	0	0
6	E	5	Total 5	O 5	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
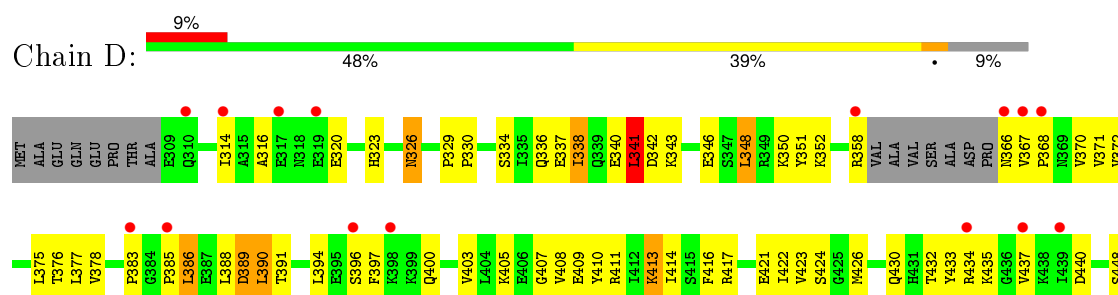
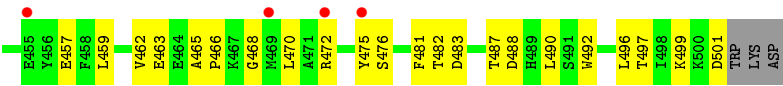- Molecule 1: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE 1
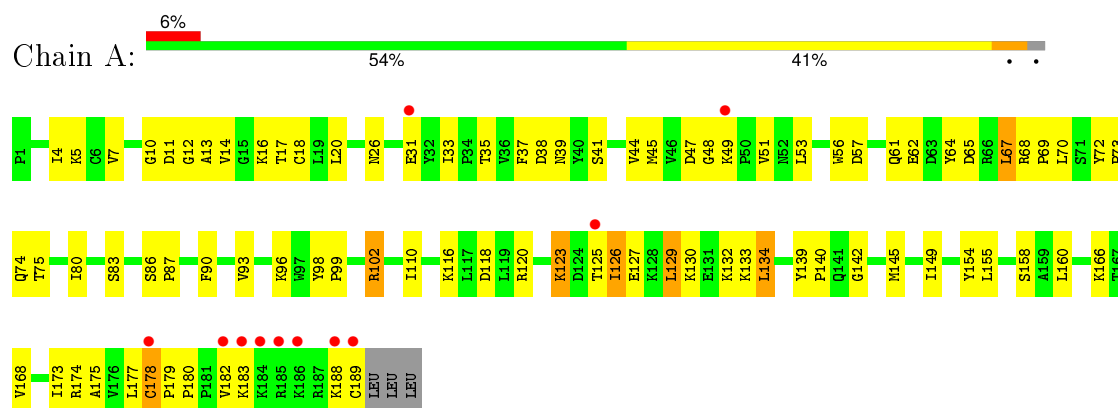
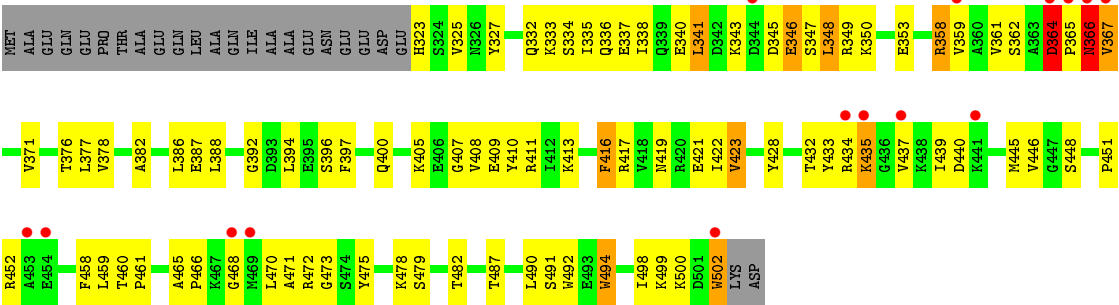- Molecule 1: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE 1
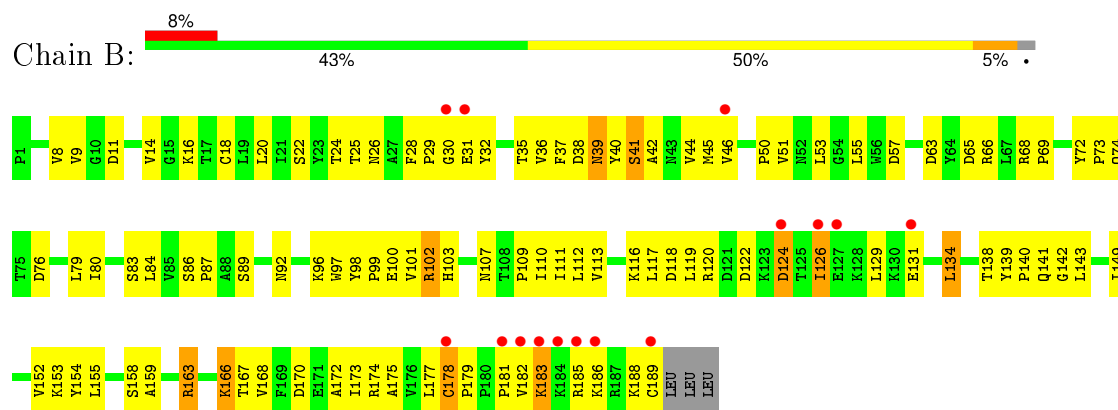
- Molecule 2: RHO GDP-DISSOCIATION INHIBITOR 1

• Molecule 2: RHO GDP-DISSOCIATION INHIBITOR 1

Chain E:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	154.70Å 88.70Å 62.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.70 29.62 – 2.67	Depositor EDS
% Data completeness (in resolution range)	85.1 (19.80-2.70) 83.7 (29.62-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.68Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.256 , 0.280 0.256 , 0.280	Depositor DCC
R_{free} test set	1063 reflections (5.14%)	DCC
Wilson B-factor (Å^2)	47.9	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 67.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Outliers	1 of 21152 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5908	wwPDB-VP
Average B, all atoms (Å^2)	58.0	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 35.42 % 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 5.8543e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GDP, GER, MG

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	0.50	0/1480	0.71	0/2015
1	B	0.48	0/1478	0.77	0/2015
2	D	0.49	0/1472	0.75	1/1990 (0.1%)
2	E	0.44	0/1472	0.75	1/1989 (0.1%)
All	All	0.48	0/5902	0.74	2/8009 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	358	ARG	NE-CZ-NH2	7.42	124.01	120.30
2	D	316	ALA	N-CA-CB	7.23	120.22	110.10

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	1448	0	1473	70	0
1	B	1446	0	1455	124	0
2	D	1445	0	1385	69	0
2	E	1441	0	1426	96	0
3	A	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	D	20	0	34	5	0
5	E	20	0	34	6	0
6	A	12	0	0	1	0
6	B	6	0	0	1	0
6	D	7	0	0	0	0
6	E	5	0	0	2	0
All	All	5908	0	5831	346	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 30.

The worst 5 of 346 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:177:LEU:O	1:B:178:CYS:SG	1.99	1.19
1:A:64:TYR:CE1	2:D:341:LEU:HD12	1.89	1.07
2:E:472:ARG:NH1	2:E:500:LYS:HD2	1.73	1.04
1:B:65:ASP:HA	1:B:68:ARG:HH12	1.25	1.02
1:B:155:LEU:HD23	1:B:168:VAL:HA	1.42	0.98

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	187/192 (97%)	173 (92%)	11 (6%)	3 (2%)	12 30
1	B	187/192 (97%)	164 (88%)	18 (10%)	5 (3%)	6 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	182/204 (89%)	148 (81%)	27 (15%)	7 (4%)	4 9
2	E	178/204 (87%)	147 (83%)	23 (13%)	8 (4%)	3 6
All	All	734/792 (93%)	632 (86%)	79 (11%)	23 (3%)	5 12

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	CYS
2	E	362	SER
2	E	366	ASN
2	D	314	ILE
2	D	383	PRO

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	160/168 (95%)	144 (90%)	16 (10%)	9 22
1	B	159/168 (95%)	147 (92%)	12 (8%)	17 38
2	D	152/180 (84%)	139 (91%)	13 (9%)	13 29
2	E	159/180 (88%)	148 (93%)	11 (7%)	19 43
All	All	630/696 (90%)	578 (92%)	52 (8%)	14 31

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	163	ARG
2	D	326	ASN
2	E	416	PHE
1	B	166	LYS
1	B	186	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	162	GLN
2	D	326	ASN
2	E	339	GLN
1	B	141	GLN
2	D	430	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 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	$\#|Z| > 2$
3	GDP	A	1190	4	23,30,30	2.94	9 (39%)	30,47,47	3.16	9 (30%)
3	GDP	B	1190	4	23,30,30	3.04	11 (47%)	30,47,47	3.10	10 (33%)
5	GER	D	1502	-	19,19,19	1.57	4 (21%)	22,22,22	3.12	13 (59%)
5	GER	E	1503	-	19,19,19	1.60	4 (21%)	22,22,22	3.10	14 (63%)

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	GDP	A	1190	4	-	0/12/32/32	0/3/3/3
3	GDP	B	1190	4	-	0/12/32/32	0/3/3/3
5	GER	D	1502	-	-	0/20/20/20	0/0/0/0
5	GER	E	1503	-	-	0/20/20/20	0/0/0/0

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1190	GDP	PB-O2B	-4.56	1.38	1.54
3	B	1190	GDP	PB-O2B	-4.25	1.39	1.54
3	A	1190	GDP	O4'-C4'	2.02	1.49	1.45
3	B	1190	GDP	C3'-C4'	2.03	1.58	1.53
3	B	1190	GDP	C6-N1	2.03	1.36	1.33

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1190	GDP	C6-C5-C4	-9.85	109.12	120.90
3	B	1190	GDP	C6-C5-C4	-9.32	109.76	120.90
3	B	1190	GDP	C4-C5-N7	-6.09	103.88	109.48
3	A	1190	GDP	C4-C5-N7	-6.03	103.93	109.48
3	A	1190	GDP	N2-C2-N1	-5.79	107.61	117.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1190	GDP	2	0
5	D	1502	GER	5	0
5	E	1503	GER	6	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	189/192 (98%)	0.02	11 (5%)	26	25	4, 31, 98, 132	0
1	B	189/192 (98%)	0.33	15 (7%)	15	13	11, 46, 113, 132	0
2	D	186/204 (91%)	0.51	19 (10%)	9	6	24, 67, 119, 132	0
2	E	180/204 (88%)	0.50	15 (8%)	14	11	21, 68, 110, 132	0
All	All	744/792 (93%)	0.34	60 (8%)	15	12	4, 52, 115, 132	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	189	CYS	7.1
1	A	189	CYS	6.4
2	E	359	VAL	6.4
1	B	181	PRO	6.2
2	E	367	VAL	6.2

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

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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	LLDF	B-factors(Å²)	Q<0.9
4	MG	B	1191	1/1	0.94	0.59	13.47	48,48,48,48	0
5	GER	D	1502	20/20	0.57	0.49	2.36	78,78,78,78	0
5	GER	E	1503	20/20	0.71	0.33	1.17	78,78,78,78	0
4	MG	A	1191	1/1	0.97	0.17	0.19	48,48,48,48	0
3	GDP	A	1190	28/28	0.98	0.15	-0.29	38,38,38,38	0
3	GDP	B	1190	28/28	0.94	0.14	-0.89	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.