



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 03:13 am GMT

PDB ID : 2CVD  
Title : Crystal structure analysis of human hematopoietic prostaglandin D synthase complexed with HQL-79  
Authors : Aritake, K.; Kado, Y.; Inoue, T.; Miyano, M.; Urade, Y.  
Deposited on : 2005-06-02  
Resolution : 1.45 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

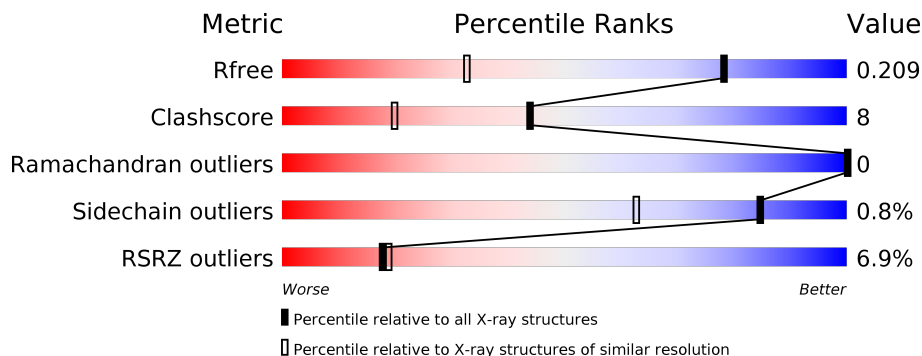
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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))
$R_{free}$	100719	1510 (1.48-1.44)
Clashscore	112137	1573 (1.48-1.44)
Ramachandran outliers	110173	1555 (1.48-1.44)
Sidechain outliers	110143	1555 (1.48-1.44)
RSRZ outliers	101464	1516 (1.48-1.44)

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  $\geq 3$ , 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	198	<div> <div>10%</div> <div>84%</div> <div>16%</div> </div>
1	B	198	<div> <div>10%</div> <div>86%</div> <div>14%</div> </div>
1	C	198	<div> <div>5%</div> <div>85%</div> <div>15%</div> </div>
1	D	198	<div> <div>4%</div> <div>87%</div> <div>13%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GSH	B	2002	-	-	-	X
4	HQL	A	2201	-	-	-	X
4	HQL	B	2401	-	-	-	X
4	HQL	C	2601	-	-	-	X
4	HQL	D	2801	-	-	-	X
5	GOL	A	3006	-	-	-	X
5	GOL	B	3005	-	-	-	X
5	GOL	B	3007	-	-	-	X
5	GOL	C	3001	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8172 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 Glutathione-requiring prostaglandin D synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1638	1058	273	298	9			
1	B	198	Total	C	N	O	S	0	0	0
			1638	1058	273	298	9			
1	C	198	Total	C	N	O	S	0	0	0
			1638	1058	273	298	9			
1	D	198	Total	C	N	O	S	0	0	0
			1638	1058	273	298	9			

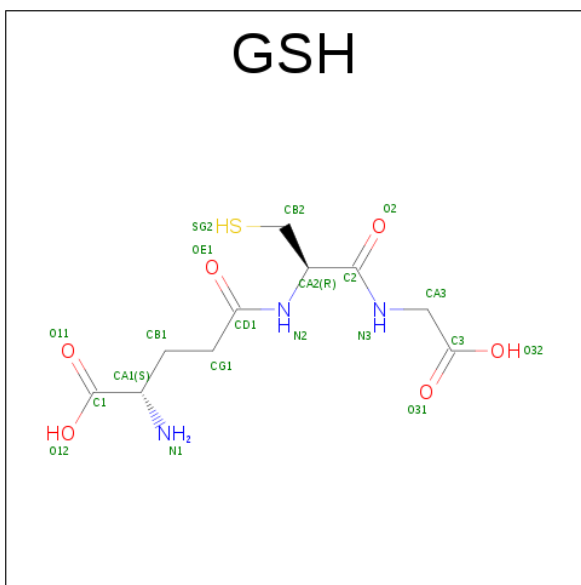
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	MET	ASN	CONFLICT	UNP O60760
B	144	MET	ASN	CONFLICT	UNP O60760
C	144	MET	ASN	CONFLICT	UNP O60760
D	144	MET	ASN	CONFLICT	UNP O60760

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

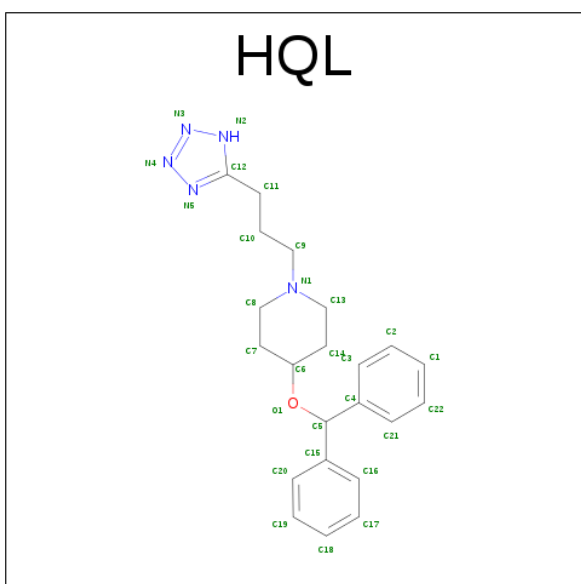
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GLUTATHIONE (three-letter code: GSH) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>3</sub>O<sub>6</sub>S).



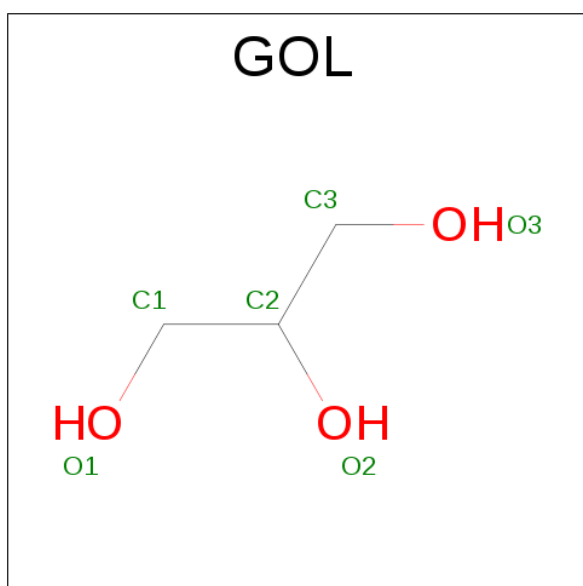
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 20	C 10	N 3	O 6	S 1	0	0
3	B	1	Total 20	C 10	N 3	O 6	S 1	0	0
3	C	1	Total 20	C 10	N 3	O 6	S 1	0	0
3	D	1	Total 20	C 10	N 3	O 6	S 1	0	0

- Molecule 4 is 4-(BENZHYDRYLOXY)-1-[3-(1H-TETRAAZOL-5-YL)PROPYL]PIPERIDINE (three-letter code: HQL) (formula: C<sub>22</sub>H<sub>27</sub>N<sub>5</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			28	22	5	1		
4	B	1	Total	C	N	O	0	0
			28	22	5	1		
4	C	1	Total	C	N	O	0	0
			28	22	5	1		
4	D	1	Total	C	N	O	0	0
			28	22	5	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



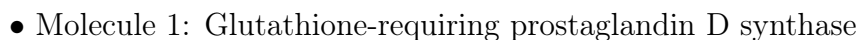
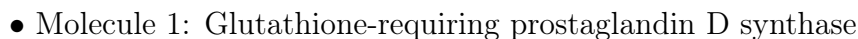
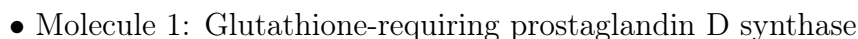
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	344	Total 344	O 344	0	0
6	B	282	Total 282	O 282	0	0
6	C	390	Total 390	O 390	0	0
6	D	368	Total 368	O 368	0	0

i

- Molecule 1: Glutathione-requiring prostaglandin D synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.94Å 49.09Å 93.14Å 85.83° 88.71° 89.98°	Depositor
Resolution (Å)	34.98 – 1.45 34.98 – 1.45	Depositor EDS
% Data completeness (in resolution range)	87.0 (34.98-1.45) 85.7 (34.98-1.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 1.45Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.192 , 0.209 0.192 , 0.209	Depositor DCC
$R_{free}$ test set	6414 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	6.5	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.109 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8172	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, MG, HQL, GSH

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	0/1681	0.54	0/2283
1	B	0.29	0/1681	0.54	0/2283
1	C	0.31	0/1681	0.57	0/2283
1	D	0.32	0/1681	0.57	0/2283
All	All	0.31	0/6724	0.55	0/9132

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	1638	0	1622	32	0
1	B	1638	0	1622	22	0
1	C	1638	0	1622	31	0
1	D	1638	0	1622	25	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	20	0	15	0	0
3	B	20	0	15	0	0
3	C	20	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	20	0	15	0	0
4	A	28	0	27	2	0
4	B	28	0	27	1	0
4	C	28	0	27	2	0
4	D	28	0	27	1	0
5	A	6	0	8	1	0
5	B	12	0	16	2	0
5	C	24	0	32	0	0
6	A	344	0	0	8	0
6	B	282	0	0	6	0
6	C	390	0	0	5	0
6	D	368	0	0	4	0
All	All	8172	0	6712	102	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 8.

The worst 5 of 102 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:85:GLN:HE21	1:D:73:LYS:NZ	1.78	0.80
1:A:85:GLN:NE2	1:D:73:LYS:HZ3	1.79	0.79
1:A:143:GLY:H	5:A:3006:GOL:H12	1.48	0.78
1:B:115:MET:HG3	6:B:4247:HOH:O	1.83	0.78
1:C:112:LYS:HA	1:C:115:MET:HE2	1.67	0.75

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	196/198 (99%)	191 (97%)	5 (3%)	0	100	100
1	B	196/198 (99%)	190 (97%)	6 (3%)	0	100	100
1	C	196/198 (99%)	191 (97%)	5 (3%)	0	100	100
1	D	196/198 (99%)	192 (98%)	4 (2%)	0	100	100
All	All	784/792 (99%)	764 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	178/178 (100%)	177 (99%)	1 (1%)	89	70
1	B	178/178 (100%)	177 (99%)	1 (1%)	89	70
1	C	178/178 (100%)	177 (99%)	1 (1%)	89	70
1	D	178/178 (100%)	175 (98%)	3 (2%)	66	29
All	All	712/712 (100%)	706 (99%)	6 (1%)	85	63

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	144	MET
1	D	144	MET
1	D	3	ASN
1	B	144	MET
1	D	36	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	28	GLN
1	C	114	GLN
1	D	171	HIS

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Mol	Chain	Res	Type
1	C	80	ASN
1	C	170	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	GSH	A	2001	-	11,19,19	1.02	1 (9%)	14,24,24	1.09	2 (14%)
4	HQL	A	2201	-	31,31,31	4.85	23 (74%)	36,40,40	2.38	8 (22%)
5	GOL	A	3006	-	5,5,5	0.97	0	5,5,5	0.32	0
3	GSH	B	2002	-	11,19,19	1.08	1 (9%)	14,24,24	1.11	2 (14%)
4	HQL	B	2401	-	31,31,31	4.79	19 (61%)	36,40,40	2.36	9 (25%)
5	GOL	B	3005	-	5,5,5	0.84	0	5,5,5	0.52	0
5	GOL	B	3007	-	5,5,5	0.97	0	5,5,5	0.39	0
3	GSH	C	2003	-	11,19,19	1.05	1 (9%)	14,24,24	1.09	2 (14%)
4	HQL	C	2601	-	31,31,31	4.44	18 (58%)	36,40,40	2.51	12 (33%)
5	GOL	C	3001	-	5,5,5	0.92	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	C	3002	-	5,5,5	1.02	0	5,5,5	0.40	0
5	GOL	C	3003	-	5,5,5	1.04	0	5,5,5	0.33	0
5	GOL	C	3004	-	5,5,5	0.98	0	5,5,5	0.42	0
3	GSH	D	2004	-	11,19,19	1.03	1 (9%)	14,24,24	1.15	2 (14%)
4	HQL	D	2801	-	31,31,31	4.64	20 (64%)	36,40,40	2.78	11 (30%)

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	GSH	A	2001	-	-	0/18/24/24	0/0/0/0
4	HQL	A	2201	-	-	0/18/28/28	0/4/4/4
5	GOL	A	3006	-	-	0/4/4/4	0/0/0/0
3	GSH	B	2002	-	-	0/18/24/24	0/0/0/0
4	HQL	B	2401	-	-	0/18/28/28	0/4/4/4
5	GOL	B	3005	-	-	0/4/4/4	0/0/0/0
5	GOL	B	3007	-	-	0/4/4/4	0/0/0/0
3	GSH	C	2003	-	-	0/18/24/24	0/0/0/0
4	HQL	C	2601	-	-	0/18/28/28	0/4/4/4
5	GOL	C	3001	-	-	0/4/4/4	0/0/0/0
5	GOL	C	3002	-	-	0/4/4/4	0/0/0/0
5	GOL	C	3003	-	-	0/4/4/4	0/0/0/0
5	GOL	C	3004	-	-	0/4/4/4	0/0/0/0
3	GSH	D	2004	-	-	0/18/24/24	0/0/0/0
4	HQL	D	2801	-	-	0/18/28/28	0/4/4/4

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2201	HQL	C11-C12	-5.55	1.45	1.50
4	A	2201	HQL	C12-N2	-5.29	1.29	1.33
4	A	2201	HQL	N2-N3	-3.33	1.29	1.34
4	A	2201	HQL	N5-N4	-2.78	1.30	1.34
4	C	2601	HQL	N2-N3	-2.63	1.30	1.34

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2801	HQL	C9-N1-C8	-7.64	91.68	111.26
4	C	2601	HQL	C9-N1-C8	-7.17	92.86	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2401	HQL	C9-N1-C8	-7.10	93.05	111.26
4	A	2201	HQL	C9-N1-C8	-6.19	95.38	111.26
4	A	2201	HQL	C7-C8-N1	-5.07	102.86	110.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2201	HQL	2	0
5	A	3006	GOL	1	0
4	B	2401	HQL	1	0
5	B	3005	GOL	2	0
4	C	2601	HQL	2	0
4	D	2801	HQL	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	198/198 (100%)	0.46	20 (10%) 8 8	3, 13, 27, 30	0
1	B	198/198 (100%)	0.47	19 (9%) 9 10	3, 13, 27, 33	0
1	C	198/198 (100%)	0.15	9 (4%) 34 35	1, 8, 18, 30	0
1	D	198/198 (100%)	0.11	7 (3%) 44 46	2, 8, 18, 30	0
All	All	792/792 (100%)	0.30	55 (6%) 18 19	1, 10, 26, 33	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	110	ASP	5.4
1	A	110	ASP	5.2
1	B	122	TYR	5.1
1	D	108	LYS	5.0
1	B	110	ASP	5.0

### 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 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, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	HQL	A	2201	28/28	0.57	0.22	8.03	16,18,27,27	0
4	HQL	B	2401	28/28	0.57	0.21	5.64	16,18,26,27	0
4	HQL	C	2601	28/28	0.72	0.20	4.62	11,13,22,23	0
5	GOL	B	3007	6/6	0.50	0.26	4.45	40,40,40,40	0
4	HQL	D	2801	28/28	0.71	0.20	3.38	12,14,23,24	0
5	GOL	C	3001	6/6	0.85	0.12	2.47	24,24,24,24	0
5	GOL	A	3006	6/6	0.59	0.25	2.38	38,38,39,39	0
5	GOL	B	3005	6/6	0.66	0.24	2.36	38,38,39,39	0
3	GSH	B	2002	20/20	0.89	0.13	2.20	8,12,18,18	0
3	GSH	D	2004	20/20	0.94	0.12	1.91	5,9,15,15	0
3	GSH	C	2003	20/20	0.94	0.11	1.67	6,9,13,13	0
3	GSH	A	2001	20/20	0.91	0.13	1.33	8,12,19,19	0
5	GOL	C	3003	6/6	0.90	0.11	0.95	18,19,19,19	0
2	MG	A	4001	1/1	1.00	0.03	-2.99	6,6,6,6	0
2	MG	B	4002	1/1	1.00	0.02	-3.92	6,6,6,6	0
5	GOL	C	3004	6/6	0.80	0.18	-	19,20,20,21	0
5	GOL	C	3002	6/6	0.75	0.21	-	21,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.