



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:56 PM GMT

PDB ID : 3VI7
Title : Human hematopoietic prostaglandin D synthase inhibitor complex structures
Authors : Kado, Y.; Inoue, T.
Deposited on : 2011-09-21
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

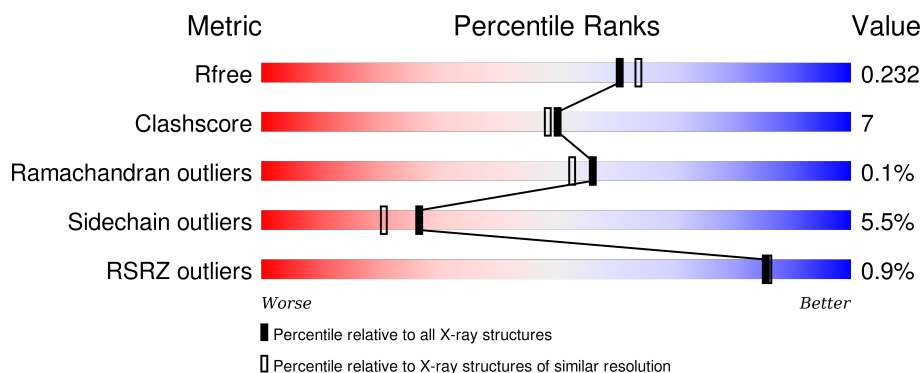
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 $\leq 5\%$. 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>81%</div> <div>15%</div> <div>••</div> </div>
1	B	198	<div> <div>89%</div> <div>9%</div> <div>••</div> </div>
1	C	198	<div> <div>2%</div> <div>84%</div> <div>13%</div> <div>••</div> </div>
1	D	198	<div> <div>2%</div> <div>84%</div> <div>15%</div> <div>•</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GSH	A	200	-	-	-	X
3	CBD	A	201	-	-	-	X
3	CBD	B	401	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7479 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.

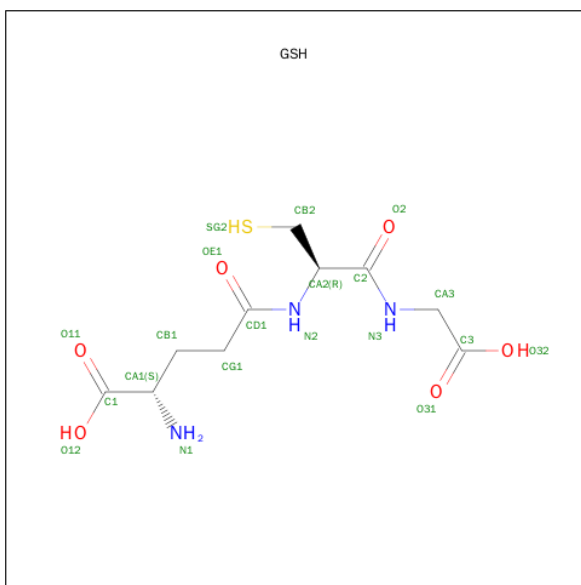
- Molecule 1 is a protein called Hematopoietic prostaglandin D synthase.

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:

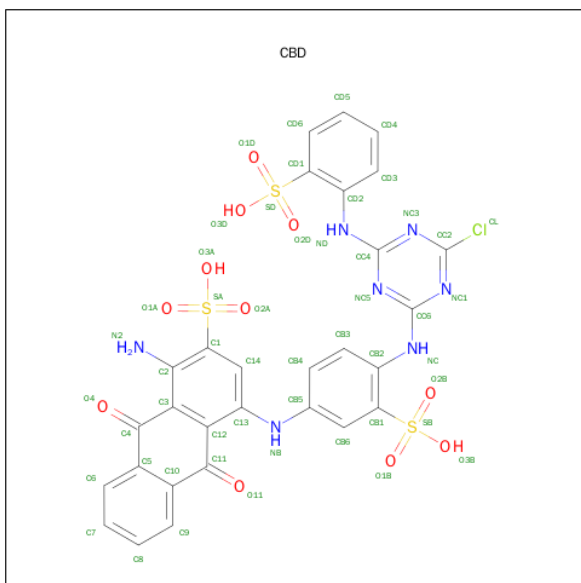
Chain	Residue	Modelled	Actual	Comment	Reference
A	144	MET	ASN	ENGINEERED MUTATION	UNP O60760
B	344	MET	ASN	ENGINEERED MUTATION	UNP O60760
C	544	MET	ASN	ENGINEERED MUTATION	UNP O60760
D	744	MET	ASN	ENGINEERED MUTATION	UNP O60760

- Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: C₁₀H₁₇N₃O₆S).



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

- Molecule 3 is CIBACRON BLUE (three-letter code: CBD) (formula: $\text{C}_{29}\text{H}_{20}\text{ClN}_7\text{O}_{11}\text{S}_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			51	29	1	7	11	3		
3	B	1	Total	C	Cl	N	O	S	0	0
			51	29	1	7	11	3		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

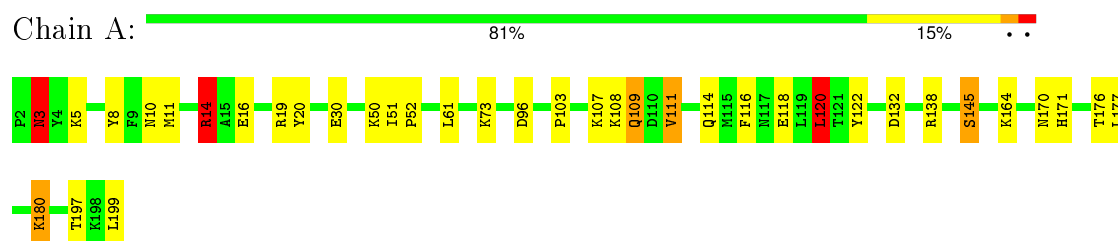
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	219	Total	O	0	0
			219	219		
5	B	216	Total	O	0	0
			216	216		
5	C	145	Total	O	0	0
			145	145		
5	D	163	Total	O	0	0
			163	163		

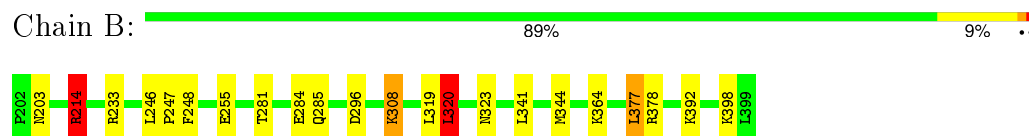
3 Residue-property plots [i](#)

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.

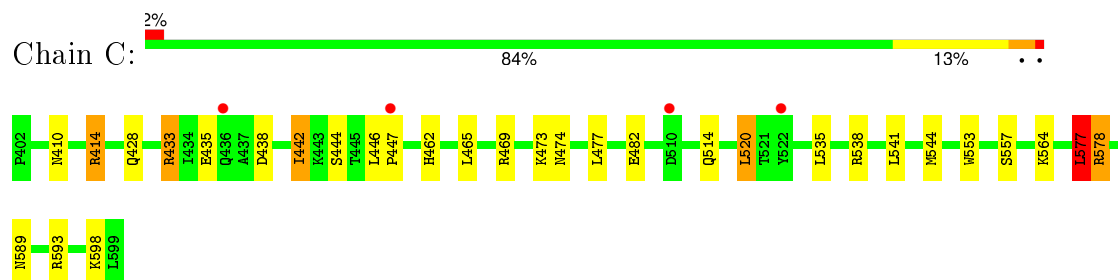
- Molecule 1: Hematopoietic prostaglandin D synthase



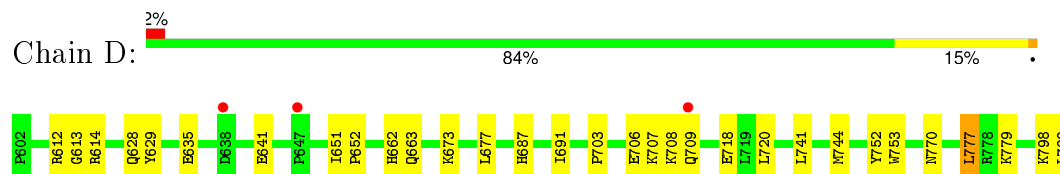
- Molecule 1: Hematopoietic prostaglandin D synthase



- Molecule 1: Hematopoietic prostaglandin D synthase



- Molecule 1: Hematopoietic prostaglandin D synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.04Å 47.36Å 184.94Å 90.00° 97.41° 90.00°	Depositor
Resolution (Å)	45.85 – 2.00 45.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (45.85-2.00) 97.6 (45.85-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.82 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.174 , 0.233 0.174 , 0.232	Depositor DCC
R_{free} test set	2840 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.0	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 56092 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7479	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 31.35 % 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 1.1231e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GSH, CA, CBD

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	1.20	7/1681 (0.4%)	0.98	7/2283 (0.3%)
1	B	1.16	0/1681	0.98	6/2283 (0.3%)
1	C	1.01	0/1681	1.01	9/2283 (0.4%)
1	D	1.12	1/1681 (0.1%)	0.91	1/2283 (0.0%)
All	All	1.12	8/6724 (0.1%)	0.97	23/9132 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	TYR	CD1-CE1	7.18	1.50	1.39
1	A	122	TYR	CD2-CE2	6.68	1.49	1.39
1	A	8	TYR	CD1-CE1	6.65	1.49	1.39
1	D	629	TYR	CD1-CE1	6.34	1.48	1.39
1	A	30	GLU	CB-CG	6.16	1.63	1.52
1	A	16	GLU	CD-OE1	5.88	1.32	1.25
1	A	3	ASN	CB-CG	5.30	1.63	1.51
1	A	20	TYR	CD1-CE1	5.18	1.47	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	414	ARG	NE-CZ-NH1	10.71	125.65	120.30
1	B	214	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	C	414	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	C	538	ARG	NE-CZ-NH1	-6.89	116.86	120.30
1	C	578	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	B	233	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	14	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	C	578	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	19	ARG	NE-CZ-NH1	-5.90	117.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	B	378	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	C	469	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	180	LYS	CD-CE-NZ	5.72	124.86	111.70
1	A	120	LEU	CB-CG-CD1	5.54	120.41	111.00
1	A	11	MET	CA-CB-CG	5.46	122.59	113.30
1	A	14	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	433	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	233	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	C	465	LEU	CB-CG-CD1	-5.28	102.02	111.00
1	D	779	LYS	CD-CE-NZ	-5.28	99.56	111.70
1	A	11	MET	CG-SD-CE	5.22	108.55	100.20
1	B	320	LEU	CA-CB-CG	5.13	127.10	115.30
1	C	577	LEU	CB-CG-CD2	5.03	119.54	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1638	0	1622	28	0
1	B	1638	0	1622	12	0
1	C	1638	0	1622	13	0
1	D	1638	0	1622	25	0
2	A	20	0	15	4	0
2	B	20	0	15	3	0
2	C	20	0	15	0	0
2	D	20	0	15	1	0
3	A	51	0	20	10	0
3	B	51	0	20	10	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	219	0	0	10	0
5	B	216	0	0	5	1
5	C	145	0	0	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	163	0	0	4	0
All	All	7479	0	6588	93	1

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 7.

All (93) 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:D:612:ARG:H	1:D:799:LEU:HD21	1.03	1.11
1:A:199:LEU:HD13	3:A:201:CBD:HB4	1.43	1.00
2:B:400:GSH:HB22	3:B:401:CBD:O1B	1.61	0.98
3:A:201:CBD:H14	3:A:201:CBD:CB6	1.99	0.92
1:D:613:GLY:H	1:D:799:LEU:HD11	1.36	0.91
1:D:612:ARG:N	1:D:799:LEU:HD21	1.89	0.88
1:A:14:ARG:NH2	1:A:96:ASP:OD1	2.08	0.85
1:B:214:ARG:NH1	2:B:400:GSH:O11	2.09	0.85
1:A:132:ASP:OD1	1:A:171:HIS:HD2	1.60	0.84
1:D:770:ASN:ND2	5:D:840:HOH:O	2.11	0.82
1:D:613:GLY:H	1:D:799:LEU:CD1	1.92	0.82
3:A:201:CBD:C14	3:A:201:CBD:HB6	2.11	0.80
1:A:138:ARG:NH1	5:A:285:HOH:O	2.17	0.77
1:D:613:GLY:N	1:D:799:LEU:HD11	2.00	0.77
1:A:176:THR:HG22	1:A:180:LYS:HE2	1.67	0.76
1:D:706:GLU:OE1	1:D:708:LYS:HG3	1.87	0.75
3:A:201:CBD:H14	3:A:201:CBD:HB6	1.67	0.74
1:D:612:ARG:HB2	1:D:799:LEU:HG	1.68	0.74
3:A:201:CBD:CL	5:A:288:HOH:O	2.42	0.73
1:C:410:ASN:HD22	1:C:433:ARG:HH11	1.34	0.73
1:B:320:LEU:HG	1:B:364:LYS:HB2	1.71	0.72
3:A:201:CBD:CB6	3:A:201:CBD:C14	2.58	0.72
1:A:50:LYS:HD3	2:A:200:GSH:HG12	1.72	0.71
5:A:413:HOH:O	1:D:662:HIS:HD2	1.74	0.70
1:D:651:ILE:HB	1:D:652:PRO:HA	1.71	0.70
1:B:319:LEU:HA	1:B:323:ASN:HD22	1.56	0.70
3:B:401:CBD:HD5	5:B:679:HOH:O	1.90	0.70
1:A:120:LEU:HG	1:A:164:LYS:HB2	1.75	0.69
1:A:14:ARG:HD2	2:A:200:GSH:HB12	1.78	0.65
1:A:108:LYS:HB2	1:A:111:VAL:HG13	1.78	0.65
1:B:255:GLU:OE1	5:B:418:HOH:O	2.16	0.63
1:A:14:ARG:NH1	2:A:200:GSH:O11	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:541:LEU:HG	1:C:577:LEU:HD11	1.81	0.61
1:B:284:GLU:OE2	5:B:774:HOH:O	2.16	0.61
1:A:177:LEU:HA	1:A:180:LYS:HE3	1.81	0.61
5:B:691:HOH:O	1:C:462:HIS:HE1	1.85	0.60
3:B:401:CBD:CB6	3:B:401:CBD:H14	2.32	0.59
3:B:401:CBD:H9	5:B:37:HOH:O	2.02	0.59
1:C:589:ASN:HB3	5:C:616:HOH:O	2.02	0.58
3:A:201:CBD:H9	5:A:653:HOH:O	2.03	0.58
1:A:114:GLN:NE2	1:A:118:GLU:OE1	2.27	0.57
1:A:14:ARG:CD	2:A:200:GSH:HB12	2.35	0.57
1:A:14:ARG:HH22	1:A:96:ASP:CG	2.07	0.56
1:D:612:ARG:NH2	1:D:799:LEU:HB2	2.20	0.56
1:C:410:ASN:ND2	1:C:433:ARG:HH11	2.02	0.56
3:A:201:CBD:O11	3:A:201:CBD:NB	2.36	0.55
1:D:753:TRP:CD1	1:D:777:LEU:HD13	2.43	0.54
1:C:482:GLU:HG2	5:C:788:HOH:O	2.09	0.53
3:B:401:CBD:O11	3:B:401:CBD:NB	2.29	0.52
1:D:741:LEU:HG	1:D:777:LEU:HD11	1.92	0.52
1:D:799:LEU:CD2	1:D:799:LEU:N	2.73	0.51
1:C:410:ASN:HD22	1:C:433:ARG:HD3	1.76	0.51
1:C:553:TRP:CD1	1:C:577:LEU:HD13	2.46	0.51
2:B:400:GSH:CB2	3:B:401:CBD:O1B	2.47	0.50
1:B:281:THR:O	1:B:285:GLN:HG3	2.12	0.50
1:A:199:LEU:CD1	3:A:201:CBD:HB4	2.28	0.50
1:A:5:LYS:HE3	5:A:651:HOH:O	2.10	0.50
1:C:473:LYS:O	1:C:474:ASN:HB2	2.12	0.50
1:B:214:ARG:NH2	1:B:296:ASP:OD1	2.44	0.50
1:D:691:ILE:HG12	5:D:827:HOH:O	2.12	0.50
1:D:628:GLN:NE2	5:D:348:HOH:O	2.44	0.50
1:C:557:SER:OG	1:C:578:ARG:HD2	2.13	0.49
1:A:103:PRO:HD2	1:A:116:PHE:CE1	2.49	0.48
1:D:612:ARG:H	1:D:799:LEU:CD2	1.97	0.48
1:D:703:PRO:HB2	1:D:706:GLU:HB2	1.95	0.48
1:D:799:LEU:HD22	1:D:799:LEU:N	2.28	0.48
1:D:614:ARG:HE	2:D:800:GSH:C1	2.27	0.48
1:A:50:LYS:HE2	5:D:573:HOH:O	2.13	0.47
1:B:247:PRO:HB2	1:B:248:PHE:CD1	2.49	0.47
1:A:170:ASN:ND2	5:A:840:HOH:O	2.39	0.47
1:D:662:HIS:O	1:D:663:GLN:HB2	2.14	0.46
3:B:401:CBD:C14	3:B:401:CBD:CB6	2.89	0.46
5:A:413:HOH:O	1:D:662:HIS:CD2	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASN:O	1:A:197:THR:HG21	2.16	0.46
1:B:341:LEU:HG	1:B:377:LEU:HD11	1.99	0.45
3:B:401:CBD:HB6	3:B:401:CBD:C14	2.47	0.45
1:A:109:GLN:NE2	1:A:109:GLN:HA	2.32	0.44
1:C:435:GLU:HB3	5:C:626:HOH:O	2.17	0.44
1:A:132:ASP:OD1	1:A:171:HIS:CD2	2.53	0.44
1:A:199:LEU:HD13	3:A:201:CBD:CB4	2.31	0.44
3:B:401:CBD:HB6	3:B:401:CBD:H14	1.99	0.44
1:B:398:LYS:HD3	3:B:401:CBD:HD6	2.00	0.43
1:A:145:SER:HB3	5:A:460:HOH:O	2.17	0.43
1:A:3:ASN:ND2	5:A:287:HOH:O	2.53	0.42
1:B:308:LYS:HE2	1:B:308:LYS:HB2	1.63	0.42
1:D:798:LYS:O	1:D:799:LEU:HB2	2.19	0.41
1:C:438:ASP:O	1:C:442:ILE:HG13	2.21	0.41
1:B:392:LYS:HE3	1:B:392:LYS:HB3	1.82	0.41
1:A:171:HIS:HE1	5:A:202:HOH:O	2.03	0.40
1:D:651:ILE:CB	1:D:652:PRO:HA	2.47	0.40
1:A:61:LEU:HD23	1:D:687:HIS:CE1	2.57	0.40
1:A:51:ILE:HB	1:A:52:PRO:HA	2.04	0.40
1:C:520:LEU:HG	1:C:564:LYS:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:846:HOH:O	5:C:801:HOH:O[1_565]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	192 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	196/198 (99%)	192 (98%)	4 (2%)	0	100	100
1	C	196/198 (99%)	191 (97%)	4 (2%)	1 (0%)	34	26
1	D	196/198 (99%)	190 (97%)	6 (3%)	0	100	100
All	All	784/792 (99%)	765 (98%)	18 (2%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	444	SER

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%)	170 (96%)	8 (4%)	34	29
1	B	178/178 (100%)	171 (96%)	7 (4%)	39	35
1	C	178/178 (100%)	165 (93%)	13 (7%)	17	11
1	D	178/178 (100%)	167 (94%)	11 (6%)	23	16
All	All	712/712 (100%)	673 (94%)	39 (6%)	27	21

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	14	ARG
1	A	73	LYS
1	A	107	LYS
1	A	109	GLN
1	A	111	VAL
1	A	120	LEU
1	A	145	SER
1	B	203	ASN
1	B	214	ARG

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Mol	Chain	Res	Type
1	B	246	LEU
1	B	308	LYS
1	B	320	LEU
1	B	344	MET
1	B	377	LEU
1	C	414	ARG
1	C	428	GLN
1	C	442	ILE
1	C	446	LEU
1	C	447	PRO
1	C	477	LEU
1	C	514	GLN
1	C	520	LEU
1	C	535	LEU
1	C	544	MET
1	C	577	LEU
1	C	593	ARG
1	C	598	LYS
1	D	635	GLU
1	D	641	GLU
1	D	673	LYS
1	D	677	LEU
1	D	707	LYS
1	D	709	GLN
1	D	718	GLU
1	D	720	LEU
1	D	744	MET
1	D	752	TYR
1	D	777	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	62	HIS
1	A	109	GLN
1	A	123	ASN
1	A	170	ASN
1	A	171	HIS
1	B	262	HIS
1	B	314	GLN
1	B	323	ASN

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Mol	Chain	Res	Type
1	C	410	ASN
1	C	432	HIS
1	C	462	HIS
1	C	480	ASN
1	C	509	GLN
1	C	514	GLN
1	C	517	ASN
1	C	570	ASN
1	D	603	ASN
1	D	628	GLN
1	D	662	HIS
1	D	680	ASN
1	D	709	GLN
1	D	770	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
2	GSH	A	200	-	13,19,19	3.42	2 (15%)	15,24,24	1.45	1 (6%)
3	CBD	A	201	-	55,56,56	2.97	12 (21%)	76,87,87	2.37	16 (21%)
2	GSH	B	400	-	13,19,19	3.36	2 (15%)	15,24,24	1.83	4 (26%)
3	CBD	B	401	-	55,56,56	2.85	12 (21%)	76,87,87	2.53	24 (31%)
2	GSH	C	600	-	13,19,19	3.36	2 (15%)	15,24,24	0.99	1 (6%)
2	GSH	D	800	-	13,19,19	3.45	2 (15%)	15,24,24	1.86	3 (20%)

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
2	GSH	A	200	-	-	0/18/24/24	0/0/0/0
3	CBD	A	201	-	-	1/30/46/46	0/6/6/6
2	GSH	B	400	-	-	0/18/24/24	0/0/0/0
3	CBD	B	401	-	-	2/30/46/46	0/6/6/6
2	GSH	C	600	-	-	0/18/24/24	0/0/0/0
2	GSH	D	800	-	-	0/18/24/24	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	CBD	CB1-SB	-10.99	1.61	1.78
3	B	401	CBD	CD1-SD	-10.42	1.62	1.78
3	A	201	CBD	C1-SA	-10.02	1.63	1.78
3	A	201	CBD	CD1-SD	-9.81	1.63	1.78
3	B	401	CBD	C1-SA	-9.61	1.63	1.78
3	B	401	CBD	CB1-SB	-9.46	1.63	1.78
3	A	201	CBD	C10-C11	-3.81	1.40	1.48
3	A	201	CBD	C5-C4	-3.73	1.40	1.48
3	A	201	CBD	CB5-NB	-3.26	1.33	1.40
3	B	401	CBD	CB5-NB	-3.10	1.34	1.40
3	B	401	CBD	C5-C4	-2.92	1.42	1.48
3	A	201	CBD	C12-C11	-2.92	1.40	1.47
3	A	201	CBD	C3-C4	-2.71	1.40	1.47
3	B	401	CBD	C12-C11	-2.54	1.41	1.47
3	B	401	CBD	C3-C4	-2.13	1.42	1.47
3	B	401	CBD	C10-C11	-2.04	1.44	1.48
3	A	201	CBD	CC2-CL	2.02	1.79	1.74
3	A	201	CBD	CC2-NC1	2.40	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	CBD	O4-C4	2.40	1.27	1.22
3	B	401	CBD	CC2-NC3	2.88	1.36	1.32
3	A	201	CBD	CC2-NC3	3.24	1.36	1.32
3	B	401	CBD	CC2-NC1	3.44	1.36	1.32
3	A	201	CBD	O11-C11	7.61	1.36	1.22
2	A	200	GSH	O2-C2	7.82	1.38	1.23
3	B	401	CBD	O11-C11	7.90	1.37	1.22
2	C	600	GSH	O2-C2	8.33	1.39	1.23
2	D	800	GSH	O2-C2	8.42	1.39	1.23
2	B	400	GSH	O2-C2	8.43	1.39	1.23
2	B	400	GSH	OE1-CD1	8.49	1.41	1.23
2	C	600	GSH	OE1-CD1	8.58	1.41	1.23
2	D	800	GSH	OE1-CD1	8.83	1.41	1.23
2	A	200	GSH	OE1-CD1	9.37	1.42	1.23

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	CBD	NC3-CC2-NC1	-6.60	120.47	129.68
3	B	401	CBD	NC3-CC2-NC1	-6.46	120.67	129.68
2	D	800	GSH	CA2-CB2-SG2	-4.83	108.22	114.16
2	A	200	GSH	CA2-CB2-SG2	-4.77	108.30	114.16
3	A	201	CBD	NC5-CC4-NC3	-4.75	118.91	126.22
3	B	401	CBD	NC5-CC4-NC3	-4.05	120.00	126.22
3	B	401	CBD	NC5-CC6-NC1	-3.81	120.36	126.22
2	B	400	GSH	OE1-CD1-CG1	-3.45	116.03	121.98
3	B	401	CBD	CD6-CD1-CD2	-3.28	117.44	120.21
3	A	201	CBD	NC5-CC6-NC1	-3.21	121.29	126.22
3	B	401	CBD	CD2-ND-CC4	-3.13	120.97	129.22
3	B	401	CBD	O11-C11-C12	-3.04	116.12	121.49
2	B	400	GSH	CB2-CA2-C2	-2.94	103.04	109.66
3	A	201	CBD	CD6-CD1-CD2	-2.84	117.81	120.21
3	A	201	CBD	CD2-ND-CC4	-2.82	121.79	129.22
3	B	401	CBD	C12-C13-NB	-2.59	117.84	120.47
2	C	600	GSH	CB1-CG1-CD1	-2.52	107.28	113.27
3	B	401	CBD	CB2-NC-CC6	-2.40	122.89	129.22
3	A	201	CBD	C7-C8-C9	-2.35	116.75	120.19
3	B	401	CBD	CB6-CB1-CB2	-2.22	118.11	120.67
3	A	201	CBD	CB5-NB-C13	-2.16	120.54	126.60
2	D	800	GSH	C3-CA3-N3	-2.13	106.25	111.74
3	B	401	CBD	C5-C4-C3	2.02	121.44	117.99
3	B	401	CBD	CB3-CB2-CB1	2.04	120.97	117.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	CBD	CB3-CB2-CB1	2.10	121.07	117.84
3	B	401	CBD	CD3-CD2-CD1	2.18	121.20	117.84
3	B	401	CBD	C9-C10-C11	2.24	123.00	119.28
3	B	401	CBD	CL-CC2-NC3	2.34	117.90	115.08
3	B	401	CBD	O2D-SD-CD1	2.37	108.90	106.17
3	A	201	CBD	O1B-SB-CB1	2.47	109.01	106.17
3	B	401	CBD	O1B-SB-CB1	2.62	109.19	106.17
3	B	401	CBD	O2B-SB-CB1	2.68	109.26	106.17
3	B	401	CBD	O2A-SA-C1	2.89	109.50	106.17
2	B	400	GSH	CA3-N3-C2	2.91	126.35	122.34
2	B	400	GSH	CG1-CD1-N2	2.92	120.59	115.83
3	A	201	CBD	O1D-SD-CD1	2.98	109.60	106.17
3	A	201	CBD	CL-CC2-NC1	3.00	118.71	115.08
2	D	800	GSH	CA3-N3-C2	3.19	126.73	122.34
3	A	201	CBD	O2D-SD-CD1	3.47	110.17	106.17
3	A	201	CBD	CC6-NC5-CC4	4.05	119.94	113.99
3	B	401	CBD	CC6-NC5-CC4	4.06	119.95	113.99
3	B	401	CBD	O1D-SD-CD1	4.45	111.30	106.17
3	A	201	CBD	CL-CC2-NC3	4.75	120.82	115.08
3	B	401	CBD	O1A-SA-C1	5.21	112.18	106.17
3	B	401	CBD	CL-CC2-NC1	5.26	121.43	115.08
3	A	201	CBD	CC6-NC1-CC2	8.36	118.92	112.49
3	B	401	CBD	CC6-NC1-CC2	8.66	119.15	112.49
3	B	401	CBD	CC4-NC3-CC2	9.60	119.88	112.49
3	A	201	CBD	CC4-NC3-CC2	10.36	120.46	112.49

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	CBD	NC1-CC6-NC-CB2
3	B	401	CBD	NC5-CC6-NC-CB2
3	A	201	CBD	NC5-CC6-NC-CB2

There are no ring outliers.

5 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	200	GSH	4	0
3	A	201	CBD	10	0
2	B	400	GSH	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	CBD	10	0
2	D	800	GSH	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	198/198 (100%)	-0.62	0 100 100	9, 16, 31, 42	0
1	B	198/198 (100%)	-0.60	0 100 100	7, 15, 31, 39	0
1	C	198/198 (100%)	-0.35	4 (2%) 68 69	9, 23, 49, 61	0
1	D	198/198 (100%)	-0.36	3 (1%) 76 77	9, 22, 49, 55	0
All	All	792/792 (100%)	-0.48	7 (0%) 85 86	7, 19, 41, 61	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	522	TYR	4.3
1	C	510	ASP	2.6
1	D	709	GLN	2.4
1	C	436	GLN	2.2
1	D	647	PRO	2.2
1	D	638	ASP	2.1
1	C	447	PRO	2.1

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

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

6.3 Carbohydrates ⓘ

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 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(Å ²)	Q<0.9
2	GSH	A	200	20/20	0.93	0.17	6.74	14,39,58,60	0
3	CBD	B	401	51/51	0.72	0.25	6.41	34,76,104,104	0
3	CBD	A	201	51/51	0.68	0.29	3.99	58,86,117,118	0
2	GSH	B	400	20/20	0.93	0.13	1.74	10,33,40,41	0
2	GSH	D	800	20/20	0.91	0.15	1.26	17,36,50,51	0
2	GSH	C	600	20/20	0.94	0.11	0.43	14,28,41,41	0
4	CA	C	902	1/1	0.97	0.06	-0.53	43,43,43,43	0
4	CA	D	901	1/1	0.97	0.06	-2.35	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.