Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:28 PM GMT

PDB ID	:	1KHE
Title	:	PEPCK complex with nonhydrolyzable GTP analog, MAD data
Authors	:	Dunten, P.; Belunis, C.; Crowther, R.; Hollfelder, K.; Kammlott, U.; Levin, W.; Michel, H.; Ramsey, G.B.; Swain, A.; Weber, D.; Wertheimer, S.J.
Deposited on	:	2001-11-29
Resolution	:	2.40 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 ①) were used in the production of this report:

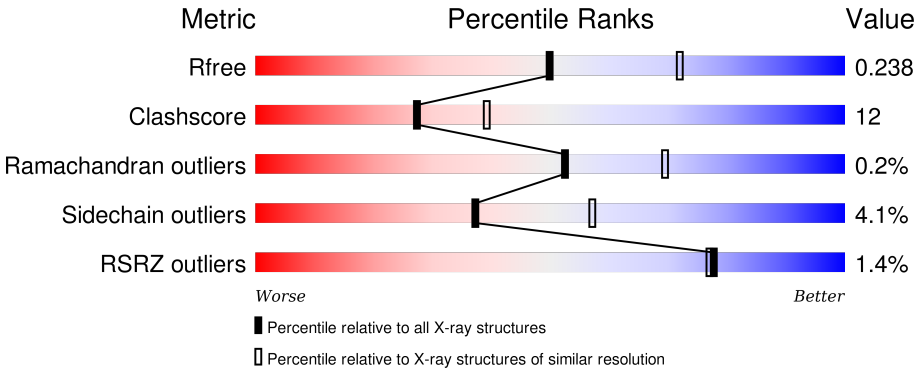
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	625	% 66% 27%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4904 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 Phosphoenolpyruvate Carboxykinase, cytosolic (GTP).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	603	Total	C	N	O	S	Se	0	1	0
			4725	3015	807	867	14	22			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP P35558
A	-1	GLU	-	CLONING ARTIFACT	UNP P35558
A	0	LEU	-	CLONING ARTIFACT	UNP P35558
A	1	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	60	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	117	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	134	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	139	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	146	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	170	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	173	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	176	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	250	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	265	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	267	VAL	ILE	VARIANT	UNP P35558
A	295	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	296	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	315	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	460	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	476	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	482	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	500	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	540	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	574	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	575	MSE	MET	MODIFIED RESIDUE	UNP P35558
A	586	ASP	GLU	VARIANT	UNP P35558
A	597	VAL	GLU	VARIANT	UNP P35558

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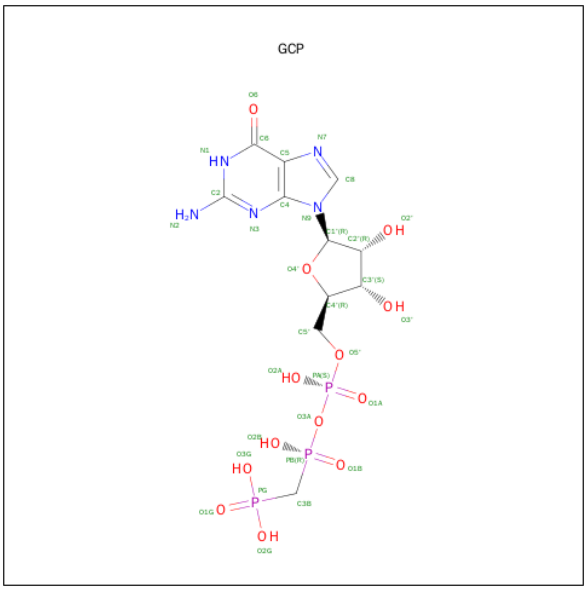
Chain	Residue	Modelled	Actual	Comment	Reference
A	622	MSE	MET	MODIFIED RESIDUE	UNP P35558

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 11	N 5	O 13	P 3	0	0

- Molecule 4 is water.

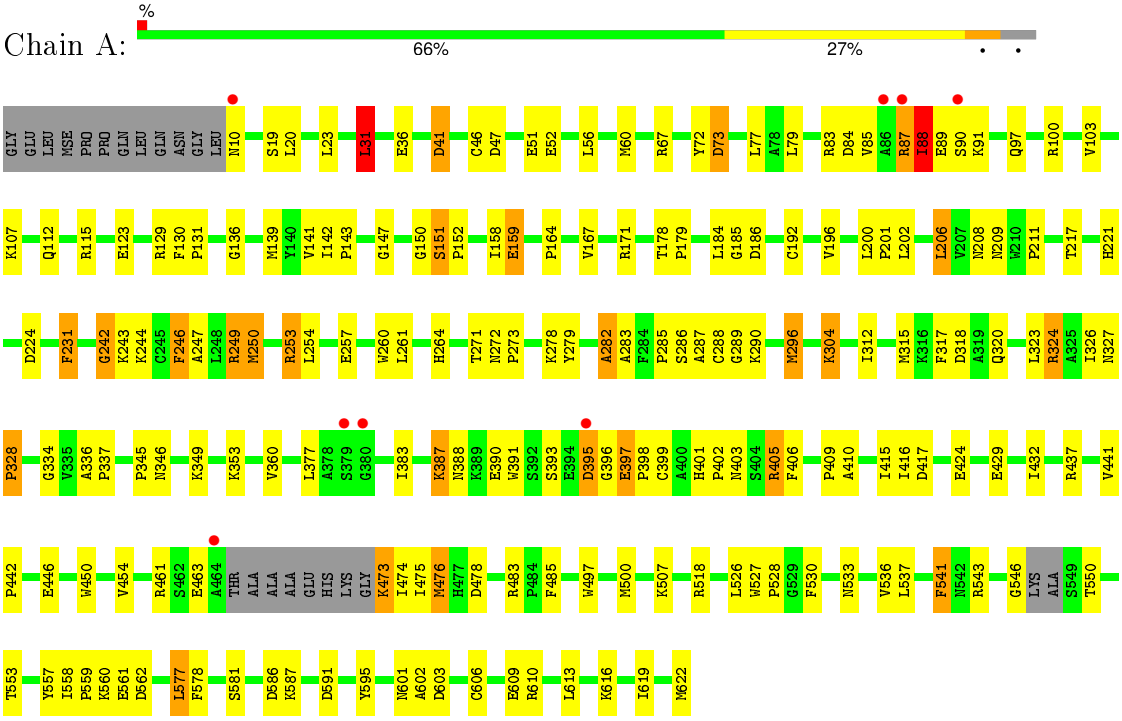
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	145	Total O 145 145	0	0

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: Phosphoenolpyruvate Carboxykinase, cytosolic (GTP)

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	45.39Å 60.54Å 61.83Å 88.36° 70.39° 72.37°	Depositor
Resolution (Å)	20.00 – 2.40 19.89 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.9 (20.00-2.40) 95.3 (19.89-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.02	Depositor
$< I/\sigma(I) >$ [1]	15.12 (at 2.41Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.170 , 0.246 0.169 , 0.238	Depositor DCC
R_{free} test set	1125 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	14.0	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 29.5	EDS
Estimated twinning fraction	0.009 for -h,-l,-k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 22522 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4904	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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

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	1.52	29/4829 (0.6%)	1.39	41/6504 (0.6%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	454	VAL	CB-CG2	9.90	1.73	1.52
1	A	139	MSE	SE-CE	-9.37	1.40	1.95
1	A	296	MSE	SE-CE	-9.07	1.42	1.95
1	A	578	PHE	CE1-CZ	7.33	1.51	1.37
1	A	282	ALA	CA-CB	7.29	1.67	1.52
1	A	72	TYR	CD2-CE2	6.39	1.49	1.39
1	A	196	VAL	CB-CG2	6.15	1.65	1.52
1	A	253	ARG	CZ-NH1	6.15	1.41	1.33
1	A	159	GLU	CD-OE1	6.13	1.32	1.25
1	A	304	LYS	CD-CE	6.09	1.66	1.51
1	A	530	PHE	CB-CG	6.04	1.61	1.51
1	A	83	ARG	CZ-NH1	6.01	1.40	1.33
1	A	247	ALA	CA-CB	6.00	1.65	1.52
1	A	405	ARG	CZ-NH1	5.87	1.40	1.33
1	A	360	VAL	CA-CB	-5.83	1.42	1.54
1	A	211	PRO	CG-CD	5.79	1.69	1.50
1	A	231	PHE	CD2-CE2	-5.75	1.27	1.39
1	A	536	VAL	CB-CG1	5.72	1.64	1.52
1	A	410	ALA	CA-CB	5.69	1.64	1.52
1	A	602	ALA	CA-CB	5.67	1.64	1.52
1	A	250	MSE	SE-CE	5.62	2.28	1.95
1	A	327	ASN	C-O	-5.45	1.13	1.23
1	A	397	GLU	CD-OE2	5.29	1.31	1.25
1	A	206	LEU	N-CA	-5.28	1.35	1.46
1	A	159	GLU	CD-OE2	5.19	1.31	1.25
1	A	429	GLU	CD-OE2	-5.15	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	GLY	C-O	-5.13	1.15	1.23
1	A	595	TYR	CD1-CE1	5.05	1.47	1.39
1	A	283	ALA	CA-CB	5.02	1.62	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	405	ARG	NE-CZ-NH2	-14.97	112.81	120.30
1	A	253	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	A	84	ASP	CB-CG-OD2	11.48	128.63	118.30
1	A	405	ARG	NE-CZ-NH1	11.07	125.83	120.30
1	A	73	ASP	CB-CG-OD1	8.86	126.28	118.30
1	A	603	ASP	CB-CG-OD2	8.58	126.02	118.30
1	A	318	ASP	CB-CG-OD1	8.35	125.81	118.30
1	A	83	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	A	171	ARG	NE-CZ-NH1	-7.97	116.31	120.30
1	A	324	ARG	NE-CZ-NH1	-7.67	116.46	120.30
1	A	224	ASP	CB-CG-OD2	7.22	124.80	118.30
1	A	417	ASP	CB-CG-OD2	7.10	124.69	118.30
1	A	461	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	A	85	VAL	CB-CA-C	-6.80	98.49	111.40
1	A	587	LYS	CD-CE-NZ	6.77	127.27	111.70
1	A	186	ASP	CB-CG-OD1	6.73	124.36	118.30
1	A	395	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	543	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	586	ASP	CB-CG-OD2	6.26	123.94	118.30
1	A	249	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	A	83	ARG	NH1-CZ-NH2	5.87	125.86	119.40
1	A	476	MSE	CA-CB-CG	-5.75	103.53	113.30
1	A	543	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	546	GLY	CA-C-O	-5.72	110.30	120.60
1	A	437	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	409	PRO	N-CD-CG	-5.65	94.72	103.20
1	A	609	GLU	OE1-CD-OE2	-5.63	116.55	123.30
1	A	41	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	289	GLY	N-CA-C	5.56	127.00	113.10
1	A	454	VAL	CG1-CB-CG2	5.51	119.71	110.90
1	A	478	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	591	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	279	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	A	349	LYS	CD-CE-NZ	-5.34	99.42	111.70
1	A	577	LEU	CB-CG-CD1	-5.26	102.05	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	LEU	CB-CG-CD2	5.21	119.87	111.00
1	A	47	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	87	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	88	ILE	CB-CA-C	-5.08	101.44	111.60
1	A	31	LEU	CA-CB-CG	5.08	126.98	115.30
1	A	446	GLU	OE1-CD-OE2	-5.02	117.27	123.30

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	4725	0	4667	111	0
2	A	2	0	0	0	0
3	A	32	0	14	2	0
4	A	145	0	0	2	0
All	All	4904	0	4681	112	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 12.

All (112) 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:250:MSE:CE	1:A:250:MSE:SE	2.28	1.31
1:A:497:TRP:HA	1:A:500[A]:MSE:HE2	1.50	0.94
1:A:90:SER:O	1:A:115:ARG:NH1	2.02	0.93
1:A:395:ASP:OD1	1:A:396:GLY:N	2.05	0.88
1:A:497:TRP:CA	1:A:500[A]:MSE:HE2	2.03	0.87
1:A:497:TRP:CE3	1:A:500[A]:MSE:HE1	2.12	0.84
1:A:90:SER:C	1:A:115:ARG:HH11	1.83	0.81
1:A:398:PRO:HD2	4:A:716:HOH:O	1.80	0.80
1:A:497:TRP:O	1:A:500[A]:MSE:HE2	1.84	0.78
1:A:497:TRP:O	1:A:500[A]:MSE:CE	2.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:MSE:HA	1:A:324:ARG:O	1.87	0.75
1:A:619:ILE:O	1:A:622:MSE:HG2	1.87	0.73
1:A:473:LYS:O	1:A:474:ILE:HD13	1.88	0.73
1:A:90:SER:C	1:A:115:ARG:NH1	2.43	0.71
1:A:346:ASN:ND2	1:A:415:ILE:HD13	2.05	0.71
1:A:613:LEU:HD12	1:A:616:LYS:HD2	1.73	0.70
1:A:142:ILE:HD11	1:A:167:VAL:HG22	1.75	0.68
1:A:242:GLY:HA2	1:A:246:PHE:HB3	1.80	0.63
1:A:497:TRP:C	1:A:500[A]:MSE:HE2	2.20	0.62
1:A:41:ASP:OD2	1:A:136:GLY:HA2	2.01	0.61
1:A:450:TRP:HZ2	1:A:500[A]:MSE:CE	2.15	0.60
1:A:264:HIS:CD2	1:A:290:LYS:HE3	2.35	0.60
1:A:377:LEU:HD11	1:A:383:ILE:HD11	1.83	0.60
1:A:317:PHE:CE1	1:A:500[B]:MSE:HE3	2.37	0.59
1:A:90:SER:CA	1:A:115:ARG:HH11	2.17	0.57
1:A:497:TRP:O	1:A:500[A]:MSE:HE3	2.04	0.56
1:A:178:THR:N	1:A:179:PRO:CD	2.68	0.56
1:A:67:ARG:HH21	1:A:79:LEU:HD12	1.71	0.56
1:A:336:ALA:HB3	1:A:337:PRO:HD3	1.88	0.56
1:A:31:LEU:C	1:A:31:LEU:HD12	2.26	0.56
1:A:250:MSE:CE	1:A:250:MSE:HB2	2.37	0.55
1:A:424:GLU:H	1:A:424:GLU:CD	2.09	0.55
1:A:272:ASN:HB2	1:A:273:PRO:CD	2.36	0.55
1:A:178:THR:HB	1:A:179:PRO:HD3	1.89	0.55
1:A:19:SER:O	1:A:20:LEU:C	2.44	0.54
1:A:282:ALA:HB2	1:A:432:ILE:HB	1.88	0.54
1:A:67:ARG:HH22	1:A:388:ASN:ND2	2.05	0.54
1:A:89:GLU:O	1:A:90:SER:C	2.46	0.53
1:A:23:LEU:CD1	1:A:31:LEU:HD23	2.39	0.53
1:A:260:TRP:HB2	1:A:315:MSE:O	2.09	0.53
1:A:202:LEU:HD11	1:A:206:LEU:HD22	1.91	0.53
1:A:296:MSE:HE1	1:A:533:ASN:HB2	1.92	0.52
1:A:31:LEU:HD22	1:A:141:VAL:HG21	1.91	0.51
1:A:450:TRP:HZ2	1:A:500[A]:MSE:HE3	1.76	0.51
1:A:88:ILE:HD13	1:A:91:LYS:HD3	1.91	0.51
1:A:320:GLN:O	1:A:507:LYS:NZ	2.43	0.51
1:A:474:ILE:HG22	1:A:476:MSE:HG3	1.92	0.51
1:A:463:GLU:HA	1:A:475:ILE:HA	1.91	0.51
1:A:450:TRP:CZ2	1:A:500[A]:MSE:HE3	2.46	0.50
1:A:326:ILE:HG13	1:A:326:ILE:O	2.10	0.50
1:A:261:LEU:HD11	1:A:500[A]:MSE:SE	2.62	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LYS:HG3	1:A:541:PHE:CE1	2.47	0.49
1:A:73:ASP:HB3	1:A:353:LYS:HG2	1.95	0.48
1:A:200:LEU:HA	1:A:201:PRO:C	2.33	0.48
1:A:334:GLY:HA3	1:A:406:PHE:CZ	2.49	0.48
1:A:353:LYS:HE2	1:A:353:LYS:HB2	1.68	0.48
1:A:441:VAL:HA	1:A:442:PRO:HD3	1.57	0.48
1:A:334:GLY:O	1:A:405:ARG:HA	2.13	0.47
1:A:254:LEU:O	1:A:257:GLU:HB2	2.14	0.47
1:A:345:PRO:HD2	4:A:761:HOH:O	2.15	0.47
1:A:221:HIS:CE1	1:A:249:ARG:HD2	2.50	0.47
1:A:129:ARG:HB3	1:A:231:PHE:CZ	2.50	0.47
1:A:558:ILE:HB	1:A:559:PRO:CD	2.45	0.47
1:A:90:SER:O	1:A:115:ARG:HD3	2.15	0.46
1:A:56:LEU:HA	1:A:56:LEU:HD23	1.52	0.46
1:A:221:HIS:NE2	1:A:249:ARG:HD2	2.30	0.46
1:A:606:CYS:O	1:A:610:ARG:HG3	2.16	0.46
1:A:527:TRP:CD2	1:A:528:PRO:HD2	2.51	0.45
1:A:550:THR:HB	1:A:557:TYR:HB3	1.98	0.45
1:A:130:PHE:N	1:A:131:PRO:CD	2.79	0.45
1:A:282:ALA:CB	1:A:432:ILE:HB	2.46	0.45
1:A:553:THR:HG21	1:A:558:ILE:HD13	1.99	0.45
1:A:159:GLU:HA	1:A:192:CYS:HB2	1.98	0.45
1:A:271:THR:HB	1:A:304:LYS:HB3	2.00	0.44
1:A:518:ARG:HG2	1:A:526:LEU:HD12	2.00	0.44
1:A:112:GLN:HB3	1:A:483:ARG:HH21	1.82	0.44
1:A:244:LYS:HD2	1:A:485:PHE:CE2	2.53	0.44
1:A:286:SER:O	1:A:287:ALA:HB3	2.18	0.44
1:A:387:LYS:O	1:A:388:ASN:CB	2.65	0.44
1:A:20:LEU:HD23	1:A:20:LEU:HA	1.76	0.43
1:A:107:LYS:NZ	1:A:601:ASN:OD1	2.45	0.43
1:A:51:GLU:H	1:A:51:GLU:CD	2.20	0.43
1:A:390:GLU:HG3	1:A:391:TRP:N	2.32	0.43
1:A:67:ARG:HH22	1:A:388:ASN:HD21	1.66	0.43
1:A:88:ILE:HD12	1:A:88:ILE:H	1.84	0.42
1:A:147:GLY:HA2	1:A:328:PRO:HA	2.01	0.42
1:A:184:LEU:O	1:A:185:GLY:C	2.56	0.42
1:A:323:LEU:HD12	1:A:323:LEU:HA	1.77	0.42
3:A:703:GCP:H3B2	3:A:703:GCP:O2A	2.18	0.42
1:A:143:PRO:HA	1:A:158:ILE:HD13	2.01	0.42
1:A:473:LYS:C	1:A:474:ILE:HD13	2.39	0.42
1:A:208:ASN:O	1:A:209:ASN:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:MSE:SE	1:A:164:PRO:HB2	2.70	0.42
1:A:272:ASN:CB	1:A:273:PRO:CD	2.96	0.42
1:A:217:THR:HA	1:A:231:PHE:O	2.19	0.42
1:A:391:TRP:CD2	1:A:399:CYS:HB3	2.54	0.42
1:A:150:GLY:O	1:A:151:SER:C	2.58	0.42
1:A:129:ARG:HG3	1:A:129:ARG:HH11	1.85	0.42
1:A:151:SER:HA	1:A:152:PRO:HD3	1.77	0.42
1:A:130:PHE:N	1:A:131:PRO:HD3	2.35	0.41
1:A:401:HIS:CE1	1:A:402:PRO:HD2	2.55	0.41
1:A:474:ILE:HD13	1:A:474:ILE:HA	1.72	0.41
1:A:285:PRO:O	1:A:288:CYS:HB2	2.20	0.41
1:A:397:GLU:HB2	1:A:398:PRO:HD2	2.03	0.41
1:A:243:LYS:HG3	1:A:243:LYS:O	2.20	0.41
1:A:46:CYS:HA	1:A:52:GLU:OE2	2.20	0.41
1:A:561:GLU:O	1:A:562:ASP:HB2	2.21	0.41
1:A:290:LYS:HB2	3:A:703:GCP:O1B	2.20	0.40
1:A:158:ILE:HG23	1:A:158:ILE:HD12	1.82	0.40
1:A:442:PRO:HA	1:A:577:LEU:O	2.21	0.40
1:A:416:ILE:HA	1:A:416:ILE:HD12	1.99	0.40
1:A:500[A]:MSE:HE3	1:A:500[A]:MSE:HB2	1.97	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	598/625 (96%)	571 (96%)	26 (4%)	1 (0%)	52 69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	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	509/501 (102%)	488 (96%)	21 (4%)	37 57

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	31	LEU
1	A	36	GLU
1	A	87	ARG
1	A	88	ILE
1	A	97	GLN
1	A	100	ARG
1	A	103	VAL
1	A	123	GLU
1	A	246	PHE
1	A	253	ARG
1	A	312	ILE
1	A	328	PRO
1	A	387	LYS
1	A	393	SER
1	A	403	ASN
1	A	473	LYS
1	A	537	LEU
1	A	541	PHE
1	A	560	LYS
1	A	581	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	GCP	A	703	2	26,34,34	2.09	8 (30%)	34,54,54	2.81	13 (38%)

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	GCP	A	703	2	-	0/15/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	GCP	C4-N3	-4.60	1.28	1.35
3	A	703	GCP	PB-O2B	-3.53	1.47	1.56
3	A	703	GCP	PG-O2G	-2.96	1.47	1.54
3	A	703	GCP	C5-C4	-2.24	1.35	1.40
3	A	703	GCP	O3'-C3'	2.26	1.48	1.43
3	A	703	GCP	PB-O3A	2.42	1.61	1.58
3	A	703	GCP	O4'-C1'	3.62	1.45	1.41
3	A	703	GCP	C6-N1	5.41	1.43	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	703	GCP	C5-C6-N1	-7.84	112.86	123.59
3	A	703	GCP	O2G-PG-O1G	-4.96	99.72	112.40
3	A	703	GCP	C4'-O4'-C1'	-4.71	104.54	109.72
3	A	703	GCP	N3-C2-N1	-3.74	121.75	127.44
3	A	703	GCP	O3G-PG-O1G	-3.64	103.09	112.40
3	A	703	GCP	C5'-C4'-C3'	-2.42	105.61	115.21
3	A	703	GCP	PA-O3A-PB	-2.16	126.67	132.73
3	A	703	GCP	O2B-PB-C3B	2.32	116.97	106.88
3	A	703	GCP	O2G-PG-C3B	2.39	112.20	106.40
3	A	703	GCP	O2A-PA-O1A	2.56	126.43	112.53
3	A	703	GCP	O1B-PB-C3B	4.22	119.64	109.02
3	A	703	GCP	C6-N1-C2	4.62	122.36	115.94
3	A	703	GCP	O1G-PG-C3B	6.25	125.39	111.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	GCP	2	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, 95^{th} 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	582/625 (93%)	-0.42	8 (1%)	78	77	3, 10, 28, 48	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	ASN	3.9
1	A	86	ALA	3.8
1	A	90	SER	3.0
1	A	395	ASP	2.9
1	A	380	GLY	2.5
1	A	87	ARG	2.2
1	A	464	ALA	2.2
1	A	379	SER	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

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^{th} 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
3	GCP	A	703	32/32	0.97	0.11	0.25	2,8,21,23	0
2	MN	A	701	1/1	0.99	0.05	-3.54	6,6,6,6	0
2	MN	A	702	1/1	1.00	0.02	-	6,6,6,6	0

6.5 Other polymers (i)

There are no such residues in this entry.