



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 18, 2024 – 03:20 PM EST

PDB ID : 4FPB
Title : Crystal Structure of Recombinant Human Hexokinase Type I with 1,5-Anhydroglucitol 6-Phosphate
Authors : Shen, L.; Honzatko, R.B.
Deposited on : 2012-06-21
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) 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 : 2.36
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) : 2.36

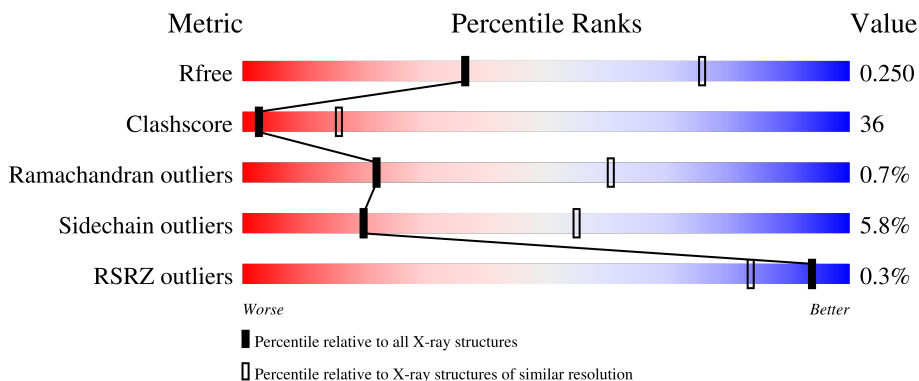
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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 $\leq 5\%$. 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	917	
1	B	917	

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
5	CIT	A	1007	-	-	-	X

2 Entry composition [i](#)

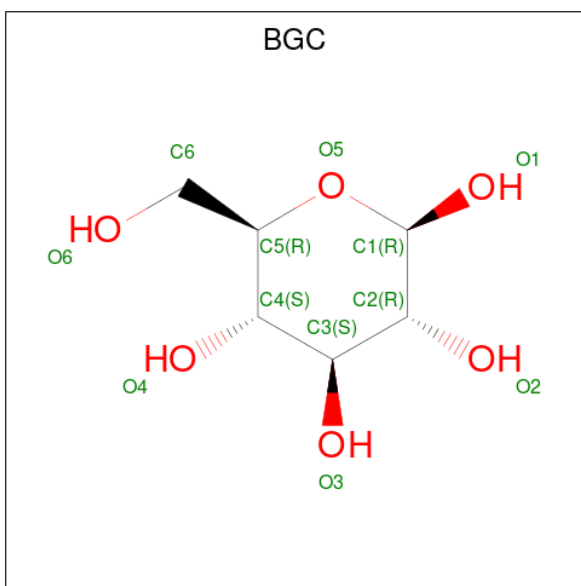
There are 6 unique types of molecules in this entry. The entry contains 14395 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hexokinase-1.

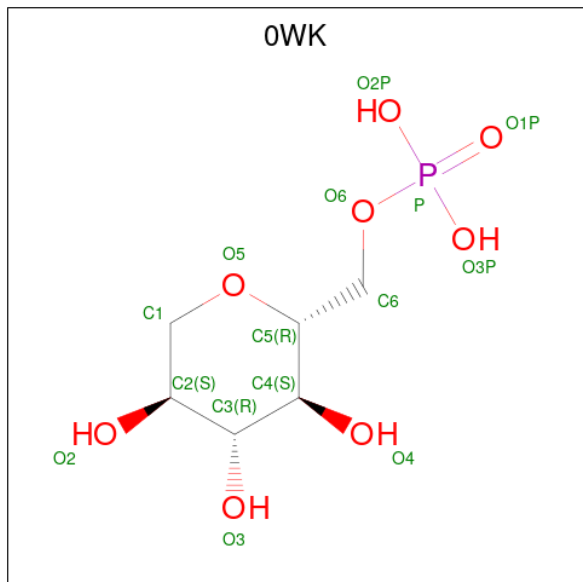
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	899	Total 7032	C 4407	N 1240	O 1332	S 53	0	0	0
1	B	899	Total 7032	C 4407	N 1240	O 1332	S 53	0	0	0

- Molecule 2 is beta-D-glucopyranose (three-letter code: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 12	C 6	O 6	0	0
2	A	1	Total 12	C 6	O 6	0	0
2	B	1	Total 12	C 6	O 6	0	0
2	B	1	Total 12	C 6	O 6	0	0

- Molecule 3 is 1,5-anhydro-6-O-phosphono-D-glucitol (three-letter code: 0WK) (formula: $C_6H_{13}O_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			15	6	8	1		
3	A	1	Total	C	O	P	0	0
			15	6	8	1		
3	B	1	Total	C	O	P	0	0
			15	6	8	1		
3	B	1	Total	C	O	P	0	0
			15	6	8	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		
4	B	2	Total	Na	0	0
			2	2		

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 6 7	0	0
5	B	1	Total C O 13 6 7	0	0

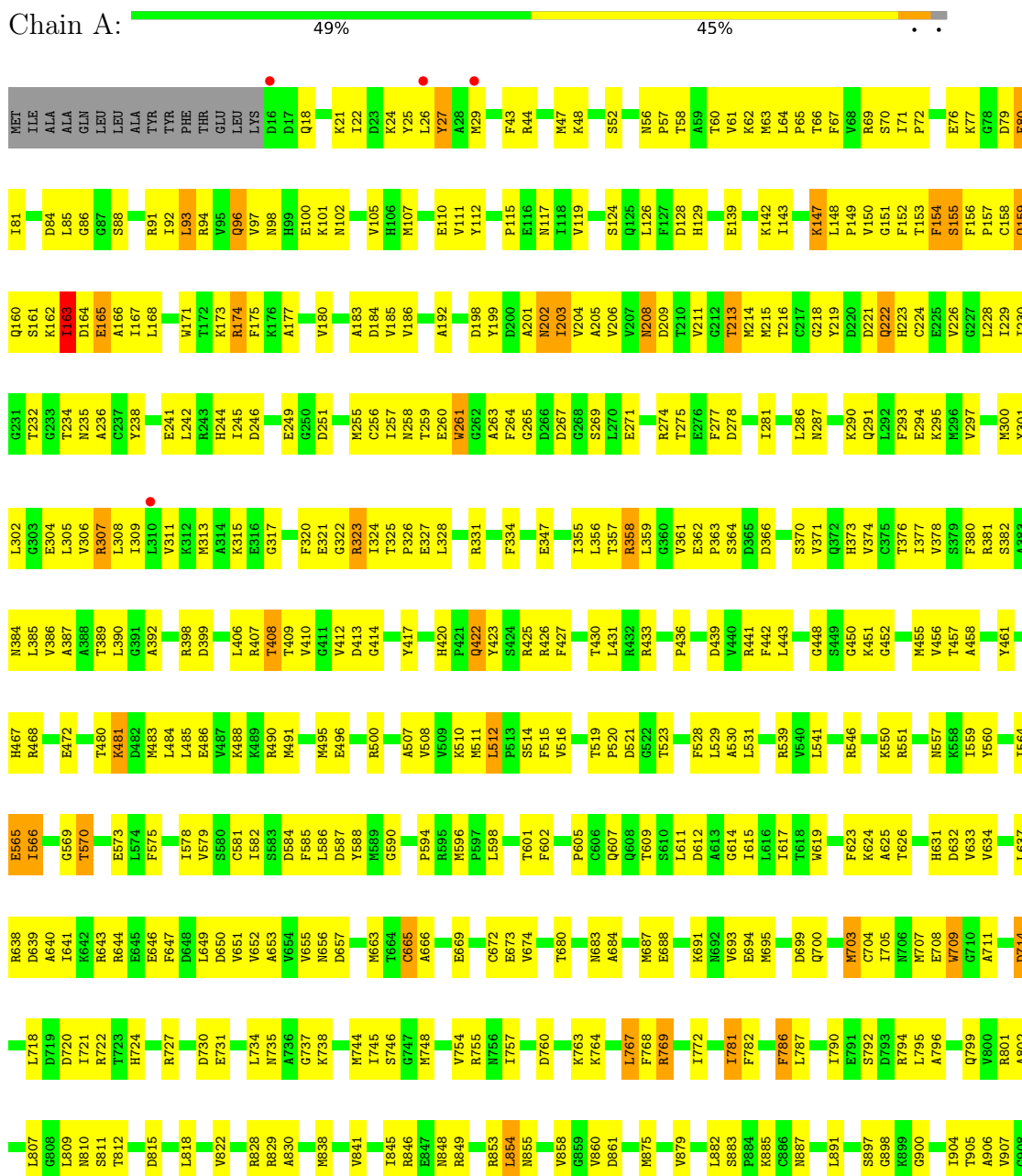
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	94	Total O 94 94	0	0
6	B	99	Total O 99 99	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: Hexokinase-1



Y909
R910
L911
R912
T913
E914
ALA
SER
SER

● Molecule 1: Hexokinase-1



MET	D16	D17	D18	D19	D20	D21	D22	D23	D24	D25	D26	D27	D28	D29	D30	D31	D32	D33	D34	D35	D36	D37	D38	D39	D40	D41	D42	D43	D44	D45	D46	D47	D48	D49	D50	D51	D52	D53	D54	D55	D56	D57	D58	D59	D60	D61	D62	D63	D64	D65	D66	D67	D68	D69	D70	D71	D72	D73	D74	D75	D76	D77	D78	D79	D80	D81	D82	D83	D84	D85	D86	D87	D88	D89	D90	D91	D92	D93	D94	D95	D96	D97	D98	D99	E00	E01	E02	E03	E04	E05	E06	E07	E08	E09	E10	E11	E12	E13	E14	E15	E16	E17	E18	E19	E20	E21	E22	E23	E24	E25	E26	E27	E28	E29	E30	E31	E32	E33	E34	E35	E36	E37	E38	E39	E40	E41	E42	E43	E44	E45	E46	E47	E48	E49	E50	E51	E52	E53	E54	E55	E56	E57	E58	E59	E60	E61	E62	E63	E64	E65	E66	E67	E68	E69	E70	E71	E72	E73	E74	E75	E76	E77	E78	E79	E80	E81	E82	E83	E84	E85	E86	E87	E88	E89	E90	E91	E92	E93	E94	E95	E96	E97	E98	E99	F00	F01	F02	F03	F04	F05	F06	F07	F08	F09	F10	F11	F12	F13	F14	F15	F16	F17	F18	F19	F20	F21	F22	F23	F24	F25	F26	F27	F28	F29	F30	F31	F32	F33	F34	F35	F36	F37	F38	F39	F40	F41	F42	F43	F44	F45	F46	F47	F48	F49	F50	F51	F52	F53	F54	F55	F56	F57	F58	F59	F60	F61	F62	F63	F64	F65	F66	F67	F68	F69	F70	F71	F72	F73	F74	F75	F76	F77	F78	F79	F80	F81	F82	F83	F84	F85	F86	F87	F88	F89	F90	F91	F92	F93	F94	F95	F96	F97	F98	F99	G00	G01	G02	G03	G04	G05	G06	G07	G08	G09	G10	G11	G12	G13	G14	G15	G16	G17	G18	G19	G20	G21	G22	G23	G24	G25	G26	G27	G28	G29	G30	G31	G32	G33	G34	G35	G36	G37	G38	G39	G40	G41	G42	G43	G44	G45	G46	G47	G48	G49	G50	G51	G52	G53	G54	G55	G56	G57	G58	G59	G60	G61	G62	G63	G64	G65	G66	G67	G68	G69	G70	G71	G72	G73	G74	G75	G76	G77	G78	G79	G80	G81	G82	G83	G84	G85	G86	G87	G88	G89	G90	G91	G92	G93	G94	G95	G96	G97	G98	G99	H00	H01	H02	H03	H04	H05	H06	H07	H08	H09	H10	H11	H12	H13	H14	H15	H16	H17	H18	H19	H20	H21	H22	H23	H24	H25	H26	H27	H28	H29	H30	H31	H32	H33	H34	H35	H36	H37	H38	H39	H40	H41	H42	H43	H44	H45	H46	H47	H48	H49	H50	H51	H52	H53	H54	H55	H56	H57	H58	H59	H60	H61	H62	H63	H64	H65	H66	H67	H68	H69	H70	H71	H72	H73	H74	H75	H76	H77	H78	H79	H80	H81	H82	H83	H84	H85	H86	H87	H88	H89	H90	H91	H92	H93	H94	H95	H96	H97	H98	H99	I00	I01	I02	I03	I04	I05	I06	I07	I08	I09	I10	I11	I12	I13	I14	I15	I16	I17	I18	I19	I20	I21	I22	I23	I24	I25	I26	I27	I28	I29	I30	I31	I32	I33	I34	I35	I36	I37	I38	I39	I40	I41	I42	I43	I44	I45	I46	I47	I48	I49	I50	I51	I52	I53	I54	I55	I56	I57	I58	I59	I60	I61	I62	I63	I64	I65	I66	I67	I68	I69	I70	I71	I72	I73	I74	I75	I76	I77	I78	I79	I80	I81	I82	I83	I84	I85	I86	I87	I88	I89	I90	I91	I92	I93	I94	I95	I96	I97	I98	I99	J00	J01	J02	J03	J04	J05	J06	J07	J08	J09	J10	J11	J12	J13	J14	J15	J16	J17	J18	J19	J20	J21	J22	J23	J24	J25	J26	J27	J28	J29	J30	J31	J32	J33	J34	J35	J36	J37	J38	J39	J40	J41	J42	J43	J44	J45	J46	J47	J48	J49	J50	J51	J52	J53	J54	J55	J56	J57	J58	J59	J60	J61	J62	J63	J64	J65	J66	J67	J68	J69	J70	J71	J72	J73	J74	J75	J76	J77	J78	J79	J80	J81	J82	J83	J84	J85	J86	J87	J88	J89	J90	J91	J92	J93	J94	J95	J96	J97	J98	J99	K00	K01	K02	K03	K04	K05	K06	K07	K08	K09	K10	K11	K12	K13	K14	K15	K16	K17	K18	K19	K20	K21	K22	K23	K24	K25	K26	K27	K28	K29	K30	K31	K32	K33	K34	K35	K36	K37	K38	K39	K40	K41	K42	K43	K44	K45	K46	K47	K48	K49	K50	K51	K52	K53	K54	K55	K56	K57	K58	K59	K60	K61	K62	K63	K64	K65	K66	K67	K68	K69	K70	K71	K72	K73	K74	K75	K76	K77	K78	K79	K80	K81	K82	K83	K84	K85	K86	K87	K88	K89	K90	K91	K92	K93	K94	K95	K96	K97	K98	K99	L00	L01	L02	L03	L04	L05	L06	L07	L08	L09	L10	L11	L12	L13	L14	L15	L16	L17	L18	L19	L20	L21	L22	L23	L24	L25	L26	L27	L28	L29	L30	L31	L32	L33	L34	L35	L36	L37	L38	L39	L40	L41	L42	L43	L44	L45	L46	L47	L48	L49	L50	L51	L52	L53	L54	L55	L56	L57	L58	L59	L60	L61	L62	L63	L64	L65	L66	L67	L68	L69	L70	L71	L72	L73	L74	L75	L76	L77	L78	L79	L80	L81	L82	L83	L84	L85	L86	L87	L88	L89	L90	L91	L92	L93	L94	L95	L96	L97	L98	L99	M00	M01	M02	M03	M04	M05	M06	M07	M08	M09	M10	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20	M21	M22	M23	M24	M25	M26	M27	M28	M29	M30	M31	M32	M33	M34	M35	M36	M37	M38	M39	M40	M41	M42	M43	M44	M45	M46	M47	M48	M49	M50	M51	M52	M53	M54	M55	M56	M57	M58	M59	M60	M61	M62	M63	M64	M65	M66	M67	M68	M69	M70	M71	M72	M73	M74	M75	M76	M77	M78	M79	M80	M81	M82	M83	M84	M85	M86	M87	M88	M89	M90	M91	M92	M93	M94	M95	M96	M97	M98	M99	N00	N01	N02	N03	N04	N05	N06	N07	N08	N09	N10	N11	N12	N13	N14	N15	N16	N17	N18	N19	N20	N21	N22	N23	N24	N25	N26	N27	N28	N29	N30	N31	N32	N33	N34	N35	N36	N37	N38	N39	N40	N41	N42	N43	N44	N45	N46	N47	N48	N49	N50	N51	N52	N53	N54	N55	N56	N57	N58	N59	N60	N61	N62	N63	N64	N65	N66	N67	N68	N69	N70	N71	N72	N73	N74	N75	N76	N77	N78	N79	N80	N81	N82	N83	N84	N85	N86	N87	N88	N89	N90	N91	N92	N93	N94	N95	N96	N97	N98	N99	O00	O01	O02	O03	O04	O05	O06	O07	O08	O09	O10	O11	O12	O13	O14	O15	O16	O17	O18	O19	O20	O21	O22	O23	O24	O25	O26	O27	O28	O29	O30	O31	O32	O33	O34	O35	O36	O37	O38	O39	O40	O41	O42	O43	O44	O45	O46	O47	O48	O49	O50	O51	O52	O53	O54	O55	O56	O57	O58	O59	O60	O61	O62	O63	O64	O65	O66	O67	O68	O69	O70	O71	O72	O73	O74	O75	O76	O77	O78	O79	O80	O81	O82	O83	O84	O85	O86	O87	O88	O89	O90	O91	O92	O93	O94	O95	O96	O97	O98	O99	P00	P01	P02	P03	P04	P05	P06	P07	P08	P09	P10	P11	P12	P13	P14	P15	P16	P17	P18	P19	P20	P21	P22	P23	P24	P25	P26	P27	P28	P29	P30	P31	P32	P33	P34	P35	P36	P37	P38	P39	P40	P41	P42	P43	P44	P45	P46	P47	P48	P49	P50	P51	P52	P53	P54	P55	P56	P57	P58	P59	P60	P61	P62	P63	P64	P65	P66	P67	P68	P69	P70	P71	P72	P73	P74	P75	P76	P77	P78	P79	P80	P81	P82	P83	P84	P85	P86	P87	P88	P89	P90	P91	P92	P93	P94	P95	P96	P97	P98	P99	Q00	Q01	Q02	Q03	Q04	Q05	Q06	Q07	Q08	Q09	Q10	Q11	Q12	Q13	Q14	Q15	Q16	Q17	Q18	Q19	Q20	Q21	Q22	Q23	Q24	Q25	Q26	Q27	Q28	Q29	Q30	Q31	Q32	Q33	Q34	Q35	Q36	Q37	Q38	Q39	Q40	Q41	Q42	Q43	Q44	Q45	Q46	Q47	Q48	Q49	Q50	Q51	Q52	Q53	Q54	Q55	Q56	Q57	Q58	Q59	Q60	Q61	Q62	Q63	Q64	Q65	Q66	Q67	Q68	Q69	Q70	Q71	Q72	Q73	Q74	Q75	Q76	Q77	Q78	Q79	Q80	Q81	Q82	Q83	Q84	Q85	Q86	Q87	Q88	Q89	Q90	Q91	Q92	Q93	Q94	Q95	Q96	Q97	Q98	Q99	R00	R01	R02	R03	R04	R05	R06	R07	R08	R09	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19	R20	R21	R22	R23	R24	R25	R26	R27	R28	R29	R30	R31	R32	R33	R34	R35	R36	R37	R38	R39	R40	R41	R42	R43	R44	R45	R46	R47	R48	R49	R50	R51	R52	R53	R54	R55	R56	R57	R58	R59	R60	R61	R62	R63	R64	R65	R66	R67	R68	R69	R70	R71	R72	R73	R74	R75	R76	R77	R78	R79	R80	R81	R82	R83	R84	R85	R86	R87	R88	R89	R90	R91	R92	R93	R94	R95	R96	R97	R98	R99	S00	S01	S02	S03	S04	S05	S06	S07	S08	S09	S10	S11	S12	S13	S14	S15	S16	S17	S18	S19	S20	S21	S22	S23	S24	S25	S26	S27	S28	S29	S30	S31	S32	S33	S34	S35	S36	S37	S38	S39	S40	S41	S42	S43	S44	S45	S46	S47	S48	S49	S50	S51	S52	S53	S54	S55	S56	S57	S58	S59	S60	S61	S62	S63	S64	S65	S66	S67	S68	S69	S70	S71	S72	S73	S74	S75	S76	S77	S78	S79	S80	S81	S82	S83	S84	S85	S86	S87	S88	S89	S90	S91	S92	S93	S94	S95	S96	S97	S98	S99	T00	T01	T02	T03	T04	T05	T06	T07	T08	T09	T10	T11	T12	T13	T14	T15	T16	T17	T18	T19	T20	T21	T22	T23	T24	T25	T26	T27	T28	T29	T30	T31	T32	T33	T34	T35	T36	T37	T38	T39	T40	T41	T42	T43	T44	T45	T46	T47	T48	T49	T50	T51	T52	T53	T54	T55	T56	T57	T58	T59	T60	T61	T62	T63	T64	T65	T66	T67	T68	T69	T70	T71	T72	T73	T74	T75	T76	T77	T78	T79	T80	T81	T82	T83	T84	T85	T86	T87	T88	T89	T90	T91	T92	T93	T94	T95	T96	T97	T98	T99	U00	U01	U02	U03	U04	U05	U06	U07	U08	U
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	---

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.72Å 121.21Å 120.79Å 90.00° 93.12° 90.00°	Depositor
Resolution (Å)	46.24 – 3.00 46.24 – 3.00	Depositor EDS
% Data completeness (in resolution range)	82.7 (46.24-3.00) 82.7 (46.24-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.229 , 0.256 0.225 , 0.250	Depositor DCC
R_{free} test set	1955 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtrriage
Anisotropy	0.100	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 19.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14395	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 0WK, BGC, NA, CIT

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	0.36	1/7138 (0.0%)	0.49	1/9606 (0.0%)
1	B	0.35	2/7138 (0.0%)	0.51	2/9606 (0.0%)
All	All	0.35	3/14276 (0.0%)	0.50	3/19212 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	ARG	CZ-NH2	14.91	1.52	1.33
1	B	595	ARG	CZ-NH2	12.36	1.49	1.33
1	B	595	ARG	CZ-NH1	9.11	1.44	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	595	ARG	NE-CZ-NH1	-11.74	114.43	120.30
1	A	323	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	B	595	ARG	NE-CZ-NH2	5.73	123.16	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	PHE	Peptide
1	B	595	ARG	Sidechain
1	B	668	GLU	Peptide

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	7032	0	7090	521	0
1	B	7032	0	7090	508	0
2	A	24	0	24	4	0
2	B	24	0	24	4	0
3	A	30	0	22	2	0
3	B	30	0	22	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	13	0	5	1	0
5	B	13	0	5	4	0
6	A	94	0	0	10	0
6	B	99	0	0	25	0
All	All	14395	0	14282	1025	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 36.

The worst 5 of 1025 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:319:LEU:HB3	1:B:320:PHE:CE1	1.36	1.56
1:A:320:PHE:CZ	1:A:361:VAL:HG21	1.64	1.31
1:A:570:THR:CG2	1:A:573:GLU:HG3	1.58	1.31
1:A:520:PRO:HD3	1:A:663:MET:CE	1.65	1.25
1:B:319:LEU:CB	1:B:320:PHE:CE1	2.25	1.20

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	897/917 (98%)	794 (88%)	97 (11%)	6 (1%)	22	60
1	B	897/917 (98%)	777 (87%)	114 (13%)	6 (1%)	22	60
All	All	1794/1834 (98%)	1571 (88%)	211 (12%)	12 (1%)	22	60

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	ILE
1	A	251	ASP
1	A	694	GLU
1	A	307	ARG
1	B	276	GLU

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	774/788 (98%)	726 (94%)	48 (6%)	18	52
1	B	774/788 (98%)	732 (95%)	42 (5%)	22	57
All	All	1548/1576 (98%)	1458 (94%)	90 (6%)	20	55

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	249	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	432	ARG
1	B	281	ILE
1	B	347	GLU
1	B	562	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	351	ASN
1	B	506	ASN
1	B	384	ASN
1	B	466	GLN
1	B	607	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	BGC	A	1001	-	12,12,12	0.38	0	17,17,17	0.99	1 (5%)
2	BGC	B	1003	-	12,12,12	0.46	0	17,17,17	1.34	2 (11%)
3	0WK	B	1002	-	15,15,15	0.45	0	22,22,22	0.78	0
5	CIT	B	1007	-	12,12,12	1.00	0	17,17,17	1.46	1 (5%)
2	BGC	A	1003	-	12,12,12	0.31	0	17,17,17	1.40	2 (11%)
5	CIT	A	1007	-	12,12,12	1.00	0	17,17,17	1.64	1 (5%)
3	0WK	A	1004	-	15,15,15	0.48	0	22,22,22	0.79	0
3	0WK	B	1004	-	15,15,15	0.43	0	22,22,22	0.85	0
3	0WK	A	1002	-	15,15,15	0.46	0	22,22,22	0.94	0
2	BGC	B	1001	-	12,12,12	0.34	0	17,17,17	0.94	1 (5%)

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	BGC	A	1001	-	-	0/2/22/22	0/1/1/1
2	BGC	B	1003	-	-	0/2/22/22	0/1/1/1
3	0WK	B	1002	-	-	2/6/23/23	0/1/1/1
5	CIT	B	1007	-	-	9/16/16/16	-
2	BGC	A	1003	-	-	2/2/22/22	0/1/1/1
5	CIT	A	1007	-	-	9/16/16/16	-
3	0WK	A	1004	-	-	4/6/23/23	0/1/1/1
3	0WK	B	1004	-	-	4/6/23/23	0/1/1/1
3	0WK	A	1002	-	-	2/6/23/23	0/1/1/1
2	BGC	B	1001	-	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1007	CIT	O6-C6-C3	4.61	121.06	113.05
5	B	1007	CIT	O6-C6-C3	3.98	119.97	113.05
2	A	1003	BGC	O5-C1-C2	-3.69	103.70	110.28
2	B	1003	BGC	O5-C1-C2	-3.54	103.96	110.28
2	A	1001	BGC	C6-C5-C4	-3.06	105.83	113.00

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	0WK	C6-O6-P-O2P
3	A	1004	0WK	C6-O6-P-O2P
3	A	1004	0WK	C6-O6-P-O3P
3	B	1004	0WK	C6-O6-P-O3P
5	A	1007	CIT	C2-C3-C4-C5

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	BGC	1	0
2	B	1003	BGC	1	0
5	B	1007	CIT	4	0
2	A	1003	BGC	3	0
5	A	1007	CIT	1	0
3	B	1004	0WK	1	0
3	A	1002	0WK	2	0
2	B	1001	BGC	3	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	899/917 (98%)	-0.30	4 (0%) 92 79	45, 76, 106, 143	0
1	B	899/917 (98%)	-0.35	2 (0%) 95 87	44, 76, 106, 143	0
All	All	1798/1834 (98%)	-0.32	6 (0%) 94 84	44, 76, 106, 143	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	16	ASP	3.6
1	A	29	MET	3.6
1	A	310	LEU	3.3
1	A	26	LEU	2.9
1	A	16	ASP	2.8

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(\AA^2)	Q<0.9
5	CIT	B	1007	13/13	0.68	0.27	124,126,127,127	0
5	CIT	A	1007	13/13	0.74	0.41	127,127,129,129	0
4	NA	A	1005	1/1	0.89	0.09	74,74,74,74	0
4	NA	B	1005	1/1	0.90	0.12	77,77,77,77	0
2	BGC	B	1001	12/12	0.91	0.31	78,79,79,80	0
4	NA	B	1006	1/1	0.92	0.08	54,54,54,54	0
2	BGC	A	1001	12/12	0.92	0.50	80,81,81,82	0
2	BGC	B	1003	12/12	0.92	0.26	53,55,56,56	0
3	0WK	A	1002	15/15	0.94	0.32	79,80,80,80	0
2	BGC	A	1003	12/12	0.95	0.21	51,54,55,56	0
4	NA	A	1006	1/1	0.95	0.05	55,55,55,55	0
3	0WK	B	1002	15/15	0.95	0.21	77,78,78,78	0
3	0WK	A	1004	15/15	0.96	0.22	59,60,61,61	0
3	0WK	B	1004	15/15	0.96	0.29	60,60,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.