Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2016 – 11:26 AM EST

PDB ID	:	4CDR
Title	:	Human O-GlcNAc transferase in complex with a bisubstrate inhibitor, Goblin1
Authors	:	Schimpl, M.; Gundogdu, M.; van Aalten, D.M.F.
Deposited on	:	2013-11-05
Resolution	:	3.15 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 (i) symbol.

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

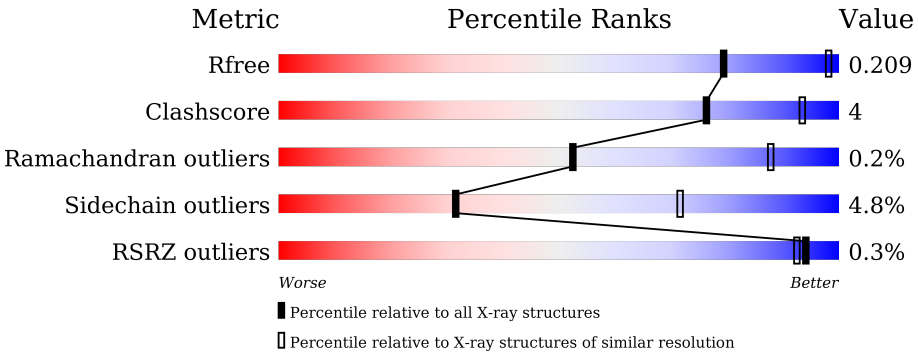
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 3.15 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	723	85% 11%
1	B	723	86% 10%
1	C	723	87% 9%
1	D	723	84% 11%
2	E	9	44% 33% 11% 11%
2	F	9	33% 44% 11% 11%

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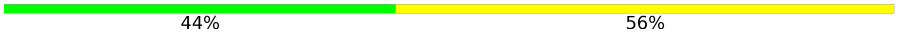
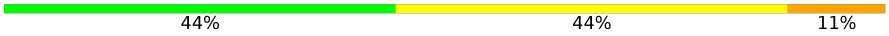
Mol	Chain	Length	Quality of chain
2	G	9	
2	H	9	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22523 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 UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYL GLUCOSAMINYLTRANSFERASE 110 KDA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	698	Total	C	N	O	S	0	0	0
			5514	3499	964	1013	38			
1	B	698	Total	C	N	O	S	0	0	0
			5514	3499	964	1013	38			
1	C	698	Total	C	N	O	S	0	0	0
			5514	3499	964	1013	38			
1	D	698	Total	C	N	O	S	0	0	0
			5514	3499	964	1013	38			

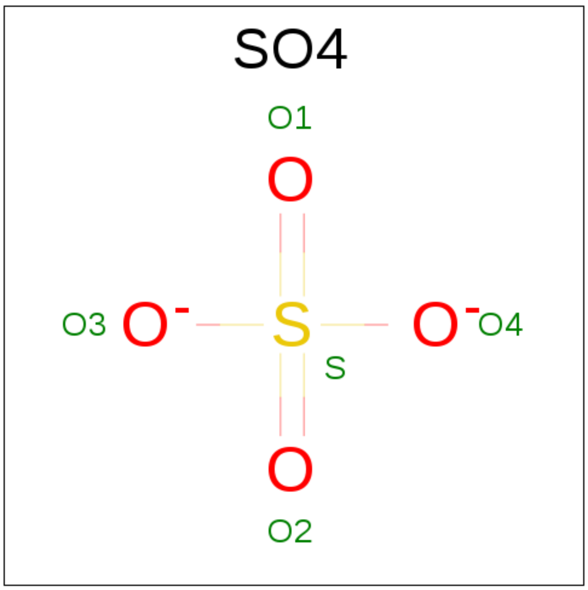
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	GLY	-	EXPRESSION TAG	UNP O15294
A	310	PRO	-	EXPRESSION TAG	UNP O15294
A	311	GLY	-	EXPRESSION TAG	UNP O15294
A	312	SER	-	EXPRESSION TAG	UNP O15294
B	309	GLY	-	EXPRESSION TAG	UNP O15294
B	310	PRO	-	EXPRESSION TAG	UNP O15294
B	311	GLY	-	EXPRESSION TAG	UNP O15294
B	312	SER	-	EXPRESSION TAG	UNP O15294
C	309	GLY	-	EXPRESSION TAG	UNP O15294
C	310	PRO	-	EXPRESSION TAG	UNP O15294
C	311	GLY	-	EXPRESSION TAG	UNP O15294
C	312	SER	-	EXPRESSION TAG	UNP O15294
D	309	GLY	-	EXPRESSION TAG	UNP O15294
D	310	PRO	-	EXPRESSION TAG	UNP O15294
D	311	GLY	-	EXPRESSION TAG	UNP O15294
D	312	SER	-	EXPRESSION TAG	UNP O15294

- Molecule 2 is a protein called GOBLIN1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	E	9	Total C N O 53 34 8 11	0	0	1
2	F	9	Total C N O 53 34 8 11	0	0	1
2	G	9	Total C N O 53 34 8 11	0	0	1
2	H	9	Total C N O 53 34 8 11	0	0	1

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0

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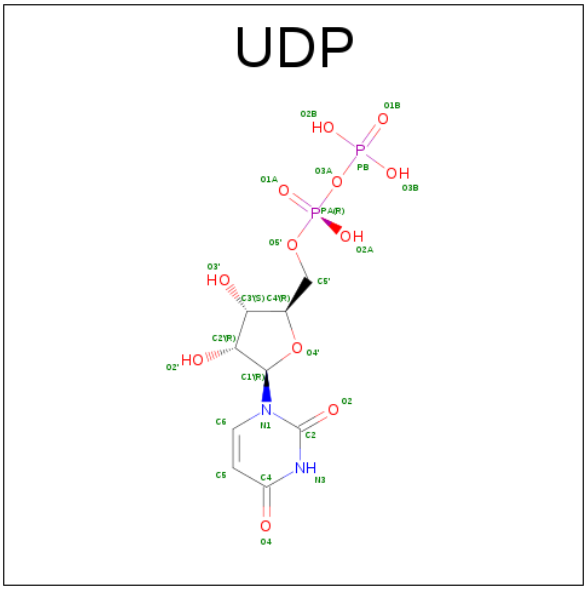
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



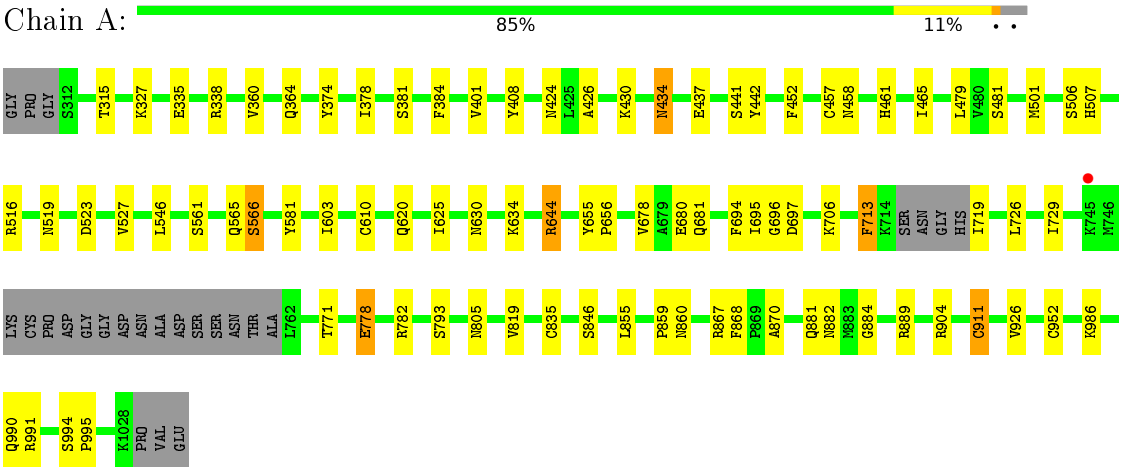
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C N O P 25 9 2 12 2	0	0
4	F	1	Total C N O P 25 9 2 12 2	0	0
4	G	1	Total C N O P 25 9 2 12 2	0	0
4	H	1	Total C N O P 25 9 2 12 2	0	0

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.

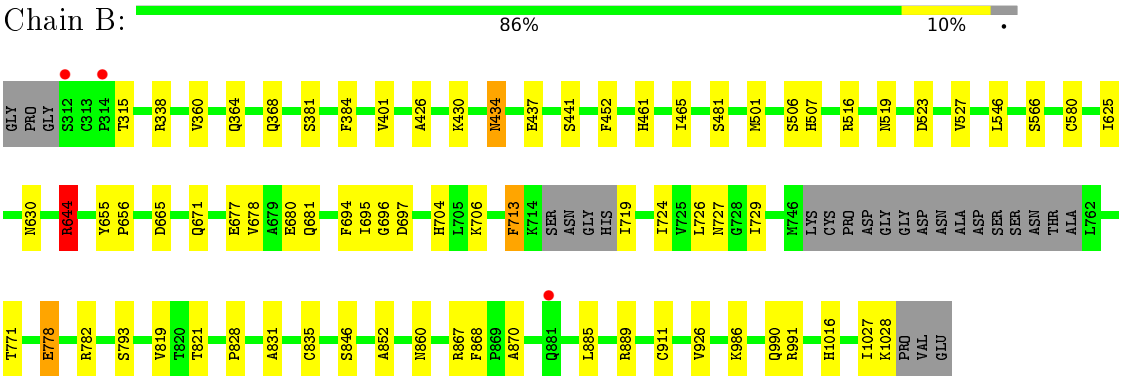
• Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYLTRANSFERASE 110 KDA SUBUNIT

Chain A:



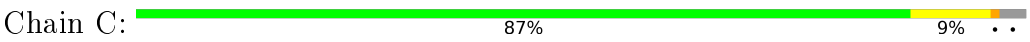
• Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYLTRANSFERASE 110 KDA SUBUNIT

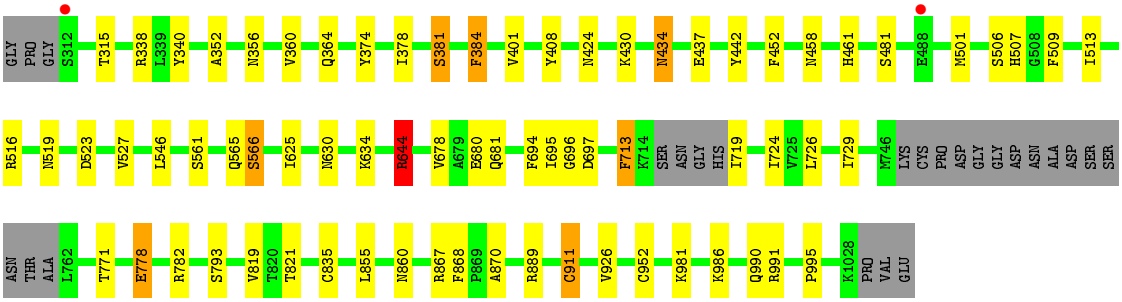
Chain B:



• Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYLTRANSFERASE 110 KDA SUBUNIT

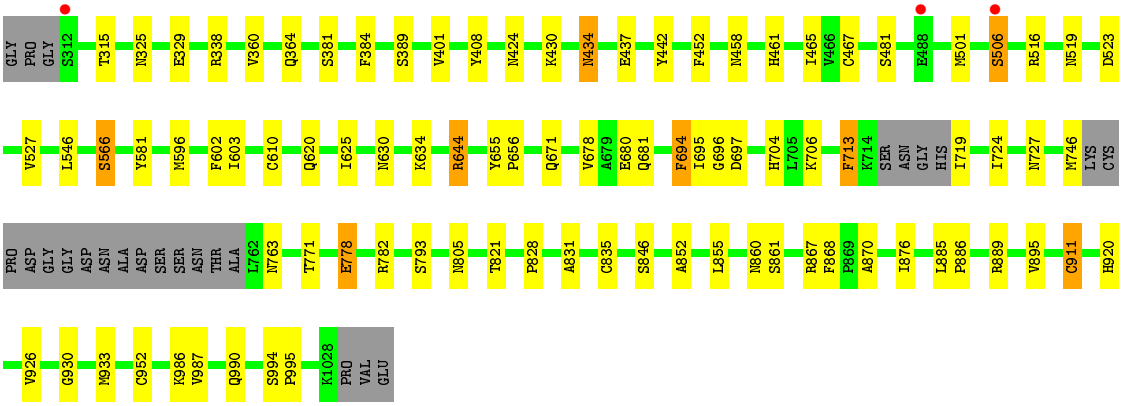
Chain C:





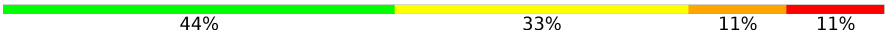
• Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYLTR ANSFERASE 110 KDA SUBUNIT

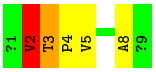
Chain D:



• Molecule 2: GOBLIN1

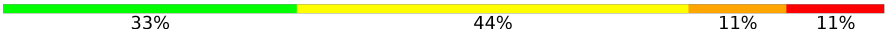
Chain E:

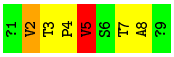




• Molecule 2: GOBLIN1

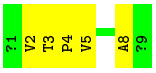
Chain F:





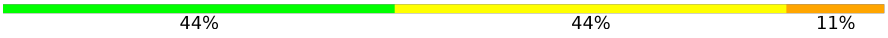
• Molecule 2: GOBLIN1

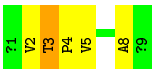
Chain G:



• Molecule 2: GOBLIN1

Chain H:




?1
V2
T3
P4
V5
A8
?9

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	273.73Å 273.73Å 142.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.15 29.87 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-3.15) 99.0 (29.87-3.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.197 , 0.213 0.192 , 0.209	Depositor DCC
R_{free} test set	3141 reflections (3.09%)	DCC
Wilson B-factor (Å^2)	59.0	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 12.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	22523	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: SRZ, UDP, SO4, ACE, NH2

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	0.63	1/5641 (0.0%)	0.66	1/7650 (0.0%)
1	B	0.61	2/5641 (0.0%)	0.65	1/7650 (0.0%)
1	C	0.60	0/5641	0.66	1/7650 (0.0%)
1	D	0.63	1/5641 (0.0%)	0.64	0/7650
2	E	1.82	2/40 (5.0%)	1.74	1/55 (1.8%)
2	F	1.73	2/40 (5.0%)	1.76	1/55 (1.8%)
2	G	1.95	2/40 (5.0%)	1.61	1/55 (1.8%)
2	H	1.89	2/40 (5.0%)	1.59	1/55 (1.8%)
All	All	0.64	12/22724 (0.1%)	0.67	7/30820 (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	1
1	C	0	1
1	D	0	1
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	8	ALA	C-O	7.47	1.37	1.23
2	E	8	ALA	C-O	7.38	1.37	1.23
2	H	8	ALA	C-O	6.87	1.36	1.23
2	F	8	ALA	C-O	6.71	1.36	1.23
2	H	4	PRO	CA-C	-6.40	1.40	1.52
2	G	4	PRO	CA-C	-6.38	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4	PRO	CA-C	-5.99	1.40	1.52
1	B	580	CYS	CB-SG	-5.61	1.72	1.81
1	A	610	CYS	CB-SG	5.52	1.91	1.82
1	B	368	GLN	CB-CG	5.29	1.66	1.52
2	F	4	PRO	CA-C	-5.27	1.42	1.52
1	D	610	CYS	CB-SG	5.06	1.90	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	5	VAL	N-CA-CB	-7.28	95.50	111.50
2	E	5	VAL	N-CA-CB	-6.17	97.93	111.50
1	C	644	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	904	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	H	5	VAL	N-CA-CB	-5.45	99.52	111.50
1	B	644	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	G	5	VAL	N-CA-CB	-5.08	100.32	111.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	506	SER	Peptide
1	B	506	SER	Peptide
1	C	506	SER	Peptide
1	D	506	SER	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	5514	0	5489	47	0
1	B	5514	0	5489	37	0
1	C	5514	0	5489	37	0
1	D	5514	0	5489	49	0
2	E	53	0	55	3	0
2	F	53	0	55	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	53	0	55	0	0
2	H	53	0	55	1	0
3	A	40	0	0	0	0
3	B	35	0	0	0	0
3	C	30	0	0	1	0
3	D	35	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	H	5	0	0	0	0
4	E	25	0	11	0	0
4	F	25	0	11	0	0
4	G	25	0	11	0	0
4	H	25	0	11	0	0
All	All	22523	0	22220	171	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 4.

All (171) 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:889:ARG:HG3	1:A:889:ARG:HH11	1.47	0.79
1:B:889:ARG:HG3	1:B:889:ARG:HH11	1.49	0.78
1:D:889:ARG:HH11	1:D:889:ARG:HG3	1.52	0.74
1:C:889:ARG:HG3	1:C:889:ARG:HH11	1.55	0.72
1:C:360:VAL:O	1:C:364:GLN:HG3	1.95	0.66
1:D:835:CYS:SG	1:D:911:CYS:HB2	2.36	0.66
1:A:644:ARG:HG2	1:A:644:ARG:HH11	1.61	0.65
1:D:644:ARG:HH11	1:D:644:ARG:CG	2.11	0.64
1:B:644:ARG:HH11	1:B:644:ARG:HG2	1.63	0.64
1:A:719:ILE:HG22	1:A:719:ILE:O	1.97	0.63
1:C:719:ILE:HG22	1:C:719:ILE:O	1.97	0.63
1:D:644:ARG:HH11	1:D:644:ARG:HG2	1.63	0.62
1:A:644:ARG:CG	1:A:644:ARG:HH11	2.12	0.62
1:B:644:ARG:HH11	1:B:644:ARG:CG	2.14	0.60
1:D:719:ILE:HG22	1:D:719:ILE:O	2.01	0.60
1:A:884:GLY:O	1:B:1027:ILE:HD12	2.02	0.59
1:B:360:VAL:O	1:B:364:GLN:HG3	2.02	0.59
1:A:360:VAL:O	1:A:364:GLN:HG3	2.02	0.58
1:A:889:ARG:HG3	1:A:889:ARG:NH1	2.14	0.58
1:B:719:ILE:O	1:B:719:ILE:HG22	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:889:ARG:HG3	1:B:889:ARG:NH1	2.18	0.58
1:C:678:VAL:O	1:C:681:GLN:HG3	2.04	0.58
1:A:507:HIS:O	1:A:507:HIS:ND1	2.37	0.58
1:D:360:VAL:O	1:D:364:GLN:HG3	2.06	0.56
1:D:430:LYS:NZ	1:D:461:HIS:HD2	2.04	0.55
1:B:726:LEU:HD22	1:B:819:VAL:HG22	1.88	0.55
1:C:430:LYS:NZ	1:C:461:HIS:HD2	2.05	0.54
1:D:867:ARG:HB3	1:D:870:ALA:HA	1.89	0.54
1:B:867:ARG:HB3	1:B:870:ALA:HA	1.89	0.54
1:A:364:GLN:HB3	1:A:527:VAL:HG11	1.89	0.54
1:C:778:GLU:OE2	1:C:782:ARG:HD3	2.08	0.54
1:C:644:ARG:CG	1:C:644:ARG:HH11	2.20	0.53
1:A:516:ARG:NH1	1:A:519:ASN:HD22	2.07	0.53
1:A:835:CYS:SG	1:A:911:CYS:HB2	2.49	0.53
1:C:724:ILE:HG23	1:C:821:THR:HG22	1.91	0.53
1:C:566:SER:HB2	1:C:697:ASP:OD1	2.09	0.52
1:C:364:GLN:HB3	1:C:527:VAL:HG11	1.91	0.52
1:C:889:ARG:HG3	1:C:889:ARG:NH1	2.23	0.52
1:A:507:HIS:HE2	1:A:681:GLN:CD	2.12	0.52
1:C:434:ASN:HB2	1:C:437:GLU:CG	2.39	0.52
1:D:516:ARG:NH1	1:D:519:ASN:HD22	2.07	0.52
1:D:566:SER:HB2	1:D:697:ASP:OD1	2.10	0.52
1:B:516:ARG:NH1	1:B:519:ASN:HD22	2.08	0.52
1:C:726:LEU:HD22	1:C:819:VAL:HG22	1.91	0.52
1:B:835:CYS:SG	1:B:911:CYS:HB2	2.50	0.52
1:B:644:ARG:CG	1:B:644:ARG:NH1	2.73	0.51
2:E:2:VAL:CG2	2:E:3:THR:HG22	2.40	0.51
1:A:644:ARG:CG	1:A:644:ARG:NH1	2.72	0.51
1:B:1028:LYS:HG3	1:B:1028:LYS:O	2.11	0.51
1:B:778:GLU:OE2	1:B:782:ARG:HD3	2.11	0.51
1:B:678:VAL:O	1:B:681:GLN:HG3	2.12	0.50
1:D:389:SER:OG	1:D:424:ASN:ND2	2.44	0.50
1:A:566:SER:HB2	1:A:697:ASP:OD1	2.12	0.50
1:B:430:LYS:NZ	1:B:461:HIS:HD2	2.09	0.50
1:A:546:LEU:HD21	1:A:625:ILE:HD12	1.93	0.50
1:B:364:GLN:HB3	1:B:527:VAL:HG11	1.94	0.50
1:D:678:VAL:O	1:D:681:GLN:HG3	2.12	0.50
1:D:828:PRO:HG2	1:D:831:ALA:HB3	1.93	0.50
1:A:434:ASN:HB2	1:A:437:GLU:CG	2.42	0.49
1:D:889:ARG:NH1	1:D:889:ARG:HG3	2.24	0.49
1:C:713:PHE:HD1	1:C:713:PHE:H	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:GLN:HB3	1:D:527:VAL:HG11	1.95	0.49
1:A:726:LEU:HD22	1:A:819:VAL:HG22	1.95	0.49
1:B:828:PRO:HG2	1:B:831:ALA:HB3	1.93	0.49
1:D:546:LEU:HD21	1:D:625:ILE:HD12	1.94	0.49
1:A:881:GLN:HB3	1:B:677:GLU:HG3	1.93	0.49
1:D:644:ARG:NH1	1:D:644:ARG:CG	2.71	0.48
1:C:644:ARG:HG2	1:C:644:ARG:HH11	1.78	0.48
1:D:778:GLU:OE2	1:D:782:ARG:HD3	2.13	0.48
1:A:461:HIS:O	1:A:465:ILE:HG13	2.13	0.48
1:A:430:LYS:NZ	1:A:461:HIS:HD2	2.12	0.48
1:C:434:ASN:HB2	1:C:437:GLU:HG2	1.96	0.48
1:C:516:ARG:NH1	1:C:519:ASN:HD22	2.12	0.48
1:D:434:ASN:HB2	1:D:437:GLU:CG	2.44	0.48
1:B:713:PHE:HD1	1:B:713:PHE:H	1.61	0.48
1:C:561:SER:O	1:C:565:GLN:HB3	2.14	0.48
1:C:986:LYS:O	1:C:990:GLN:HG2	2.14	0.47
1:A:713:PHE:HD1	1:A:713:PHE:H	1.61	0.47
1:D:442:TYR:CZ	1:D:458:ASN:HB3	2.49	0.47
1:D:805:ASN:HD22	1:D:805:ASN:H	1.61	0.47
1:D:895:VAL:HG11	2:H:3:THR:HG21	1.96	0.47
1:D:713:PHE:HD1	1:D:713:PHE:H	1.63	0.47
1:C:835:CYS:SG	1:C:911:CYS:HB2	2.54	0.47
1:C:546:LEU:HD21	1:C:625:ILE:HD12	1.95	0.47
1:A:678:VAL:O	1:A:681:GLN:HG3	2.14	0.46
1:A:859:PRO:HG2	1:B:1016:HIS:ND1	2.31	0.46
1:C:507:HIS:O	1:C:507:HIS:ND1	2.48	0.46
1:A:442:TYR:CZ	1:A:458:ASN:HB3	2.49	0.46
1:B:986:LYS:O	1:B:990:GLN:HG2	2.16	0.46
1:A:855:LEU:O	1:A:889:ARG:NH2	2.48	0.46
1:C:719:ILE:CG2	1:C:719:ILE:O	2.62	0.46
1:A:695:ILE:HG13	1:A:696:GLY:N	2.31	0.46
1:A:867:ARG:HB3	1:A:870:ALA:HA	1.98	0.46
1:D:434:ASN:HB2	1:D:437:GLU:HG2	1.98	0.46
1:D:986:LYS:O	1:D:990:GLN:HG2	2.16	0.45
1:C:867:ARG:HB3	1:C:870:ALA:HA	1.97	0.45
1:B:695:ILE:HG13	1:B:696:GLY:N	2.30	0.45
1:D:852:ALA:HA	1:D:885:LEU:HD11	1.98	0.45
1:A:507:HIS:NE2	1:A:681:GLN:HG2	2.31	0.45
1:B:434:ASN:HB2	1:B:437:GLU:CG	2.46	0.45
1:D:467:CYS:SG	1:D:876:ILE:HD11	2.56	0.45
1:D:805:ASN:ND2	1:D:805:ASN:H	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:994:SER:HB2	1:D:995:PRO:HD2	1.98	0.45
1:A:778:GLU:OE2	1:A:782:ARG:HD3	2.17	0.45
1:A:434:ASN:HB2	1:A:437:GLU:HG2	1.98	0.45
1:D:408:TYR:CZ	1:D:424:ASN:HB3	2.52	0.44
1:A:952:CYS:SG	1:A:995:PRO:HG2	2.56	0.44
1:B:678:VAL:HB	1:B:681:GLN:HG3	1.98	0.44
1:D:855:LEU:HD23	1:D:861:SER:OG	2.17	0.44
1:D:325:ASN:O	1:D:329:GLU:HG2	2.18	0.44
1:A:719:ILE:CG2	1:A:719:ILE:O	2.63	0.44
1:C:374:TYR:O	1:C:378:ILE:HG12	2.18	0.44
1:D:704:HIS:O	1:D:727:ASN:HB3	2.17	0.44
1:C:644:ARG:CG	1:C:644:ARG:NH1	2.80	0.44
1:D:746:MET:HG3	1:D:763:ASN:HA	2.00	0.44
1:A:561:SER:O	1:A:565:GLN:HB3	2.17	0.44
1:B:507:HIS:ND1	1:B:507:HIS:O	2.51	0.44
1:B:655:TYR:HA	1:B:656:PRO:HD3	1.91	0.44
1:A:507:HIS:NE2	1:A:681:GLN:OE1	2.45	0.44
1:D:885:LEU:HA	1:D:886:PRO:HD2	1.89	0.43
1:A:994:SER:HB2	1:A:995:PRO:HD2	2.00	0.43
1:A:986:LYS:O	1:A:990:GLN:HG2	2.18	0.43
1:B:426:ALA:HB2	1:B:441:SER:CB	2.48	0.43
1:C:952:CYS:SG	1:C:995:PRO:HG2	2.58	0.43
1:D:581:TYR:CE1	1:D:603:ILE:HD13	2.54	0.43
1:C:340:TYR:CZ	1:C:356:ASN:HB3	2.54	0.43
1:D:930:GLY:HA2	1:D:987:VAL:HG12	1.99	0.43
2:E:2:VAL:HG22	2:E:3:THR:HG22	2.00	0.43
1:B:546:LEU:HD21	1:B:625:ILE:HD12	2.00	0.43
1:C:442:TYR:CZ	1:C:458:ASN:HB3	2.54	0.43
1:B:704:HIS:O	1:B:727:ASN:HB3	2.18	0.42
1:C:695:ILE:HG13	1:C:696:GLY:N	2.34	0.42
1:D:695:ILE:HG13	1:D:696:GLY:N	2.34	0.42
2:E:2:VAL:HG23	2:E:3:THR:HG22	2.01	0.42
1:C:509:PHE:O	1:C:513:ILE:HG13	2.19	0.42
1:C:678:VAL:HB	1:C:681:GLN:HG3	2.00	0.42
1:A:374:TYR:O	1:A:378:ILE:HG12	2.18	0.42
1:A:408:TYR:CE1	1:A:424:ASN:HB3	2.55	0.42
1:B:461:HIS:O	1:B:465:ILE:HG13	2.19	0.42
1:B:729:ILE:HA	1:B:729:ILE:HD13	1.88	0.42
1:A:655:TYR:HA	1:A:656:PRO:HD3	1.93	0.42
1:D:596:MET:HG2	1:D:602:PHE:CD1	2.55	0.41
1:C:381:SER:O	1:C:384:PHE:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:855:LEU:O	1:C:889:ARG:NH2	2.50	0.41
1:D:430:LYS:NZ	1:D:461:HIS:CD2	2.85	0.41
2:F:5:VAL:HG22	2:F:7:THR:HG23	2.01	0.41
1:A:327:LYS:HD2	1:A:335:GLU:HG2	2.03	0.41
1:A:581:TYR:CE1	1:A:603:ILE:HD13	2.56	0.41
1:D:461:HIS:O	1:D:465:ILE:HG13	2.20	0.41
1:D:655:TYR:HA	1:D:656:PRO:HD3	1.87	0.41
1:A:408:TYR:CZ	1:A:424:ASN:HB3	2.55	0.41
1:B:719:ILE:O	1:B:719:ILE:CG2	2.67	0.41
1:D:694:PHE:CZ	1:D:920:HIS:HB3	2.55	0.41
1:A:426:ALA:HB2	1:A:441:SER:CB	2.51	0.41
1:D:678:VAL:HB	1:D:681:GLN:HG3	2.03	0.41
1:D:855:LEU:O	1:D:889:ARG:NH2	2.52	0.41
1:D:952:CYS:SG	1:D:995:PRO:HG2	2.61	0.41
1:A:805:ASN:HD22	1:A:805:ASN:H	1.67	0.41
1:B:724:ILE:HG23	1:B:821:THR:HG22	2.03	0.41
1:C:729:ILE:HA	1:C:729:ILE:HD13	1.89	0.41
1:B:852:ALA:HA	1:B:885:LEU:HD11	2.03	0.41
1:C:352:ALA:HB1	3:C:2029:SO4:O1	2.21	0.41
1:C:408:TYR:CZ	1:C:424:ASN:HB3	2.56	0.41
1:D:724:ILE:HG23	1:D:821:THR:HG22	2.03	0.41
1:D:911:CYS:O	1:D:933:MET:HA	2.21	0.41
1:B:566:SER:HB2	1:B:697:ASP:OD1	2.21	0.40
1:D:719:ILE:CG2	1:D:719:ILE:O	2.68	0.40
1:A:457:CYS:SG	1:A:479:LEU:CD2	3.09	0.40
1:B:644:ARG:NH2	1:B:665:ASP:OD1	2.54	0.40
1:A:678:VAL:HB	1:A:681:GLN:HG3	2.04	0.40
1:A:729:ILE:HA	1:A:729:ILE:HD13	1.95	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	692/723 (96%)	665 (96%)	27 (4%)	0	100 100
1	B	692/723 (96%)	665 (96%)	27 (4%)	0	100 100
1	C	692/723 (96%)	670 (97%)	22 (3%)	0	100 100
1	D	692/723 (96%)	665 (96%)	26 (4%)	1 (0%)	56 90
2	E	6/9 (67%)	5 (83%)	0	1 (17%)	0 1
2	F	6/9 (67%)	5 (83%)	0	1 (17%)	0 1
2	G	6/9 (67%)	5 (83%)	0	1 (17%)	0 1
2	H	6/9 (67%)	5 (83%)	0	1 (17%)	0 1
All	All	2792/2928 (95%)	2685 (96%)	102 (4%)	5 (0%)	52 88

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	2	VAL
2	H	2	VAL
2	E	2	VAL
1	D	506	SER
2	F	2	VAL

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	600/618 (97%)	571 (95%)	29 (5%)	31 71
1	B	600/618 (97%)	575 (96%)	25 (4%)	36 74
1	C	600/618 (97%)	574 (96%)	26 (4%)	35 74
1	D	600/618 (97%)	572 (95%)	28 (5%)	32 72
2	E	5/5 (100%)	3 (60%)	2 (40%)	0 0
2	F	5/5 (100%)	2 (40%)	3 (60%)	0 0
2	G	5/5 (100%)	4 (80%)	1 (20%)	1 8
2	H	5/5 (100%)	4 (80%)	1 (20%)	1 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2420/2492 (97%)	2305 (95%)	115 (5%)	31 71

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	315	THR
1	A	338	ARG
1	A	381	SER
1	A	384	PHE
1	A	401	VAL
1	A	434	ASN
1	A	452	PHE
1	A	481	SER
1	A	501	MET
1	A	523	ASP
1	A	566	SER
1	A	620	GLN
1	A	630	ASN
1	A	634	LYS
1	A	644	ARG
1	A	680	GLU
1	A	694	PHE
1	A	706	LYS
1	A	713	PHE
1	A	771	THR
1	A	778	GLU
1	A	793	SER
1	A	846	SER
1	A	860	ASN
1	A	868	PHE
1	A	882	ASN
1	A	911	CYS
1	A	926	VAL
1	A	991	ARG
1	B	315	THR
1	B	338	ARG
1	B	381	SER
1	B	384	PHE
1	B	401	VAL
1	B	434	ASN
1	B	452	PHE
1	B	481	SER

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Mol	Chain	Res	Type
1	B	501	MET
1	B	523	ASP
1	B	630	ASN
1	B	644	ARG
1	B	671	GLN
1	B	680	GLU
1	B	694	PHE
1	B	706	LYS
1	B	713	PHE
1	B	771	THR
1	B	778	GLU
1	B	793	SER
1	B	846	SER
1	B	860	ASN
1	B	868	PHE
1	B	926	VAL
1	B	991	ARG
1	C	315	THR
1	C	338	ARG
1	C	381	SER
1	C	384	PHE
1	C	401	VAL
1	C	434	ASN
1	C	452	PHE
1	C	481	SER
1	C	501	MET
1	C	523	ASP
1	C	566	SER
1	C	630	ASN
1	C	634	LYS
1	C	644	ARG
1	C	680	GLU
1	C	694	PHE
1	C	713	PHE
1	C	771	THR
1	C	778	GLU
1	C	793	SER
1	C	860	ASN
1	C	868	PHE
1	C	911	CYS
1	C	926	VAL
1	C	981	LYS

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Mol	Chain	Res	Type
1	C	991	ARG
1	D	315	THR
1	D	338	ARG
1	D	381	SER
1	D	384	PHE
1	D	401	VAL
1	D	434	ASN
1	D	452	PHE
1	D	481	SER
1	D	501	MET
1	D	523	ASP
1	D	566	SER
1	D	620	GLN
1	D	630	ASN
1	D	634	LYS
1	D	644	ARG
1	D	671	GLN
1	D	680	GLU
1	D	694	PHE
1	D	706	LYS
1	D	713	PHE
1	D	771	THR
1	D	778	GLU
1	D	793	SER
1	D	846	SER
1	D	860	ASN
1	D	868	PHE
1	D	911	CYS
1	D	926	VAL
2	E	2	VAL
2	E	3	THR
2	F	2	VAL
2	F	3	THR
2	F	5	VAL
2	G	3	THR
2	H	3	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	424	ASN
1	A	434	ASN

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Mol	Chain	Res	Type
1	A	461	HIS
1	A	784	GLN
1	A	805	ASN
1	A	839	GLN
1	A	860	ASN
1	A	990	GLN
1	B	424	ASN
1	B	434	ASN
1	B	461	HIS
1	B	784	GLN
1	B	805	ASN
1	B	990	GLN
1	C	424	ASN
1	C	434	ASN
1	C	461	HIS
1	C	784	GLN
1	C	805	ASN
1	C	839	GLN
1	C	990	GLN
1	D	424	ASN
1	D	434	ASN
1	D	461	HIS
1	D	784	GLN
1	D	805	ASN
1	D	839	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	SRZ	E	6	2,4	6,8,10	0.41	0	5,8,11	1.41	1 (20%)
2	SRZ	F	6	2,4	6,8,10	0.55	0	5,8,11	0.89	0
2	SRZ	G	6	2,4	6,8,10	0.56	0	5,8,11	1.06	0
2	SRZ	H	6	2,4	6,8,10	0.64	0	5,8,11	1.21	1 (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	SRZ	E	6	2,4	-	0/5/7/10	0/0/0/0
2	SRZ	F	6	2,4	-	0/5/7/10	0/0/0/0
2	SRZ	G	6	2,4	-	0/5/7/10	0/0/0/0
2	SRZ	H	6	2,4	-	0/5/7/10	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	6	SRZ	O-C-CA	-2.41	119.26	125.72
2	H	6	SRZ	O-C-CA	-2.01	120.34	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

35 ligands are modelled in this entry.

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	SO4	A	2029	-	4,4,4	0.18	0	6,6,6	0.24	0
3	SO4	A	2030	-	4,4,4	0.16	0	6,6,6	0.30	0
3	SO4	A	2031	-	4,4,4	0.12	0	6,6,6	0.08	0
3	SO4	A	2032	-	4,4,4	0.10	0	6,6,6	0.11	0
3	SO4	A	2033	-	4,4,4	0.13	0	6,6,6	0.44	0
3	SO4	A	2034	-	4,4,4	0.19	0	6,6,6	0.53	0
3	SO4	A	2035	-	4,4,4	0.13	0	6,6,6	0.40	0
3	SO4	A	2036	-	4,4,4	0.23	0	6,6,6	0.49	0
3	SO4	B	2029	-	4,4,4	0.23	0	6,6,6	0.53	0
3	SO4	B	2030	-	4,4,4	0.25	0	6,6,6	0.61	0
3	SO4	B	2031	-	4,4,4	0.13	0	6,6,6	0.29	0
3	SO4	B	2032	-	4,4,4	0.12	0	6,6,6	0.45	0
3	SO4	B	2033	-	4,4,4	0.15	0	6,6,6	0.38	0
3	SO4	B	2034	-	4,4,4	0.19	0	6,6,6	0.13	0
3	SO4	B	2035	-	4,4,4	0.17	0	6,6,6	0.15	0
3	SO4	C	2029	-	4,4,4	0.25	0	6,6,6	0.36	0
3	SO4	C	2030	-	4,4,4	0.21	0	6,6,6	0.51	0
3	SO4	C	2031	-	4,4,4	0.19	0	6,6,6	0.25	0
3	SO4	C	2032	-	4,4,4	0.15	0	6,6,6	0.15	0
3	SO4	C	2033	-	4,4,4	0.17	0	6,6,6	0.16	0
3	SO4	C	2034	-	4,4,4	0.12	0	6,6,6	0.12	0
3	SO4	D	2029	-	4,4,4	0.11	0	6,6,6	0.24	0
3	SO4	D	2030	-	4,4,4	0.16	0	6,6,6	0.26	0
3	SO4	D	2031	-	4,4,4	0.12	0	6,6,6	0.24	0
3	SO4	D	2032	-	4,4,4	0.19	0	6,6,6	0.12	0
3	SO4	D	2033	-	4,4,4	0.21	0	6,6,6	0.13	0
3	SO4	D	2034	-	4,4,4	0.15	0	6,6,6	0.26	0
3	SO4	D	2035	-	4,4,4	0.16	0	6,6,6	0.13	0
4	UDP	E	1001	2	20,26,26	1.67	4 (20%)	24,40,40	1.37	3 (12%)
3	SO4	E	1009	-	4,4,4	0.14	0	6,6,6	0.21	0
4	UDP	F	1001	2	20,26,26	1.55	4 (20%)	24,40,40	1.63	3 (12%)
3	SO4	F	1009	-	4,4,4	0.15	0	6,6,6	0.19	0
4	UDP	G	1001	2	20,26,26	1.61	3 (15%)	24,40,40	1.79	4 (16%)
4	UDP	H	1001	2	20,26,26	1.68	5 (25%)	24,40,40	1.66	2 (8%)
3	SO4	H	1009	-	4,4,4	0.06	0	6,6,6	0.34	0

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	SO4	A	2029	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2030	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2031	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2032	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2033	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2034	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2035	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2036	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2029	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2030	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2031	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2032	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2033	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2034	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2035	-	-	0/0/0/0	0/0/0/0
3	SO4	C	2029	-	-	0/0/0/0	0/0/0/0
3	SO4	C	2030	-	-	0/0/0/0	0/0/0/0
3	SO4	C	2031	-	-	0/0/0/0	0/0/0/0
3	SO4	C	2032	-	-	0/0/0/0	0/0/0/0
3	SO4	C	2033	-	-	0/0/0/0	0/0/0/0
3	SO4	C	2034	-	-	0/0/0/0	0/0/0/0
3	SO4	D	2029	-	-	0/0/0/0	0/0/0/0
3	SO4	D	2030	-	-	0/0/0/0	0/0/0/0
3	SO4	D	2031	-	-	0/0/0/0	0/0/0/0
3	SO4	D	2032	-	-	0/0/0/0	0/0/0/0
3	SO4	D	2033	-	-	0/0/0/0	0/0/0/0
3	SO4	D	2034	-	-	0/0/0/0	0/0/0/0
3	SO4	D	2035	-	-	0/0/0/0	0/0/0/0
4	UDP	E	1001	2	-	0/12/32/32	0/2/2/2
3	SO4	E	1009	-	-	0/0/0/0	0/0/0/0
4	UDP	F	1001	2	-	0/12/32/32	0/2/2/2
3	SO4	F	1009	-	-	0/0/0/0	0/0/0/0
4	UDP	G	1001	2	-	0/12/32/32	0/2/2/2
4	UDP	H	1001	2	-	0/12/32/32	0/2/2/2
3	SO4	H	1009	-	-	0/0/0/0	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1001	UDP	C2'-C1'	-4.43	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1001	UDP	C2'-C1'	-3.14	1.48	1.53
4	E	1001	UDP	C2'-C1'	-2.58	1.49	1.53
4	H	1001	UDP	C4-N3	2.09	1.36	1.33
4	G	1001	UDP	O4'-C1'	2.18	1.44	1.41
4	F	1001	UDP	PB-O3B	2.28	1.62	1.54
4	H	1001	UDP	PB-O3B	2.36	1.62	1.54
4	H	1001	UDP	C6-N1	2.65	1.39	1.35
4	E	1001	UDP	C4-N3	2.77	1.38	1.33
4	G	1001	UDP	C4-N3	2.78	1.38	1.33
4	F	1001	UDP	C6-N1	2.95	1.39	1.35
4	H	1001	UDP	O4'-C1'	3.12	1.45	1.41
4	E	1001	UDP	O4'-C1'	3.28	1.45	1.41
4	F	1001	UDP	C4-N3	3.67	1.39	1.33
4	E	1001	UDP	C6-N1	4.59	1.41	1.35
4	G	1001	UDP	C6-N1	4.97	1.42	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1001	UDP	C4'-O4'-C1'	-3.00	106.46	109.64
4	F	1001	UDP	O4'-C1'-N1	-2.96	102.47	108.10
4	G	1001	UDP	O4'-C1'-N1	-2.93	102.53	108.10
4	G	1001	UDP	C2'-C1'-N1	2.12	119.14	113.46
4	E	1001	UDP	O2B-PB-O1B	2.20	117.80	110.63
4	F	1001	UDP	O2B-PB-O1B	2.26	117.99	110.63
4	G	1001	UDP	O2B-PB-O1B	2.83	119.86	110.63
4	H	1001	UDP	O2B-PB-O1B	2.83	119.86	110.63
4	E	1001	UDP	C4-N3-C2	4.08	118.50	114.21
4	F	1001	UDP	C4-N3-C2	5.44	119.94	114.21
4	H	1001	UDP	C4-N3-C2	5.54	120.04	114.21
4	G	1001	UDP	C4-N3-C2	6.13	120.66	114.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2029	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	698/723 (96%)	-0.39	1 (0%)	95	95	37, 52, 75, 114	0
1	B	698/723 (96%)	-0.37	3 (0%)	93	90	37, 52, 75, 114	0
1	C	698/723 (96%)	-0.38	2 (0%)	94	92	37, 52, 75, 114	0
1	D	698/723 (96%)	-0.39	3 (0%)	93	90	37, 52, 75, 114	0
2	E	6/9 (66%)	-0.47	0	100	100	42, 47, 58, 66	0
2	F	6/9 (66%)	-0.74	0	100	100	42, 45, 52, 59	0
2	G	6/9 (66%)	-0.79	0	100	100	41, 49, 54, 61	0
2	H	6/9 (66%)	-0.87	0	100	100	50, 58, 66, 70	0
All	All	2816/2928 (96%)	-0.38	9 (0%)	94	92	37, 52, 75, 114	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	312	SER	4.1
1	D	488	GLU	2.5
1	B	881	GLN	2.4
1	D	312	SER	2.3
1	D	506	SER	2.3
1	C	312	SER	2.1
1	B	314	PRO	2.1
1	C	488	GLU	2.0
1	A	745	LYS	2.0

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

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
2	SRZ	G	6	9/11	0.95	0.14	-	45,47,48,49	0
2	SRZ	E	6	9/11	0.96	0.12	-	43,45,46,47	0
2	SRZ	H	6	9/11	0.96	0.12	-	57,59,60,62	0
2	SRZ	F	6	9/11	0.94	0.16	-	40,44,46,47	0

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^{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	SO4	C	2030	5/5	0.96	0.14	-0.29	60,60,62,62	0
4	UDP	H	1001	25/25	0.98	0.14	-0.32	48,50,60,62	0
4	UDP	F	1001	25/25	0.98	0.13	-0.83	33,37,42,42	0
3	SO4	H	1009	5/5	0.96	0.11	-0.92	76,76,77,77	0
4	UDP	G	1001	25/25	0.98	0.13	-0.94	34,37,41,41	0
4	UDP	E	1001	25/25	0.98	0.11	-1.62	37,39,42,43	0
3	SO4	A	2036	5/5	0.95	0.13	-1.76	82,84,84,84	0
3	SO4	B	2032	5/5	0.95	0.15	-1.82	65,67,67,68	0
3	SO4	F	1009	5/5	0.98	0.10	-1.88	66,67,67,68	0
3	SO4	E	1009	5/5	0.98	0.10	-5.17	59,59,60,61	0
3	SO4	B	2031	5/5	0.94	0.14	-	107,107,107,108	0
3	SO4	A	2035	5/5	0.96	0.29	-	79,79,80,81	0
3	SO4	B	2035	5/5	0.94	0.27	-	94,94,94,94	0
3	SO4	A	2034	5/5	0.91	0.16	-	81,81,82,84	0
3	SO4	C	2029	5/5	0.96	0.16	-	66,66,67,68	0
3	SO4	C	2034	5/5	0.92	0.23	-	102,103,104,104	0
3	SO4	A	2033	5/5	0.92	0.17	-	103,103,104,104	0
3	SO4	B	2029	5/5	0.97	0.14	-	64,66,67,67	0
3	SO4	A	2030	5/5	0.95	0.16	-	78,78,78,79	0
3	SO4	A	2032	5/5	0.97	0.17	-	85,85,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	B	2030	5/5	0.95	0.18	-	73,74,75,75	0
3	SO4	D	2031	5/5	0.85	0.26	-	119,119,120,120	0
3	SO4	A	2031	5/5	0.94	0.19	-	102,102,102,102	0
3	SO4	A	2029	5/5	0.97	0.16	-	65,66,67,67	0
3	SO4	D	2029	5/5	0.98	0.10	-	58,58,58,60	0
3	SO4	C	2032	5/5	0.94	0.17	-	111,111,111,112	0
3	SO4	D	2034	5/5	0.85	0.29	-	124,125,125,126	0
3	SO4	D	2032	5/5	0.77	0.36	-	145,145,145,145	0
3	SO4	D	2035	5/5	0.87	0.22	-	129,129,129,130	0
3	SO4	D	2033	5/5	0.95	0.13	-	99,99,100,100	0
3	SO4	D	2030	5/5	0.96	0.19	-	78,78,78,79	0
3	SO4	C	2031	5/5	0.98	0.15	-	72,72,73,73	0
3	SO4	B	2034	5/5	0.92	0.23	-	96,97,97,97	0
3	SO4	B	2033	5/5	0.94	0.17	-	85,86,86,86	0
3	SO4	C	2033	5/5	0.95	0.13	-	98,98,98,98	0

6.5 Other polymers (i)

There are no such residues in this entry.