Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:47 AM GMT

PDB ID	:	3FV3
Title	:	Secreted aspartic protease 1 from Candida parapsilosis in complex with pepstatin A
Authors	:	Dostal, J.; Brynda, J.; Hruskova-Heidingsfeldova, O.; Sieglova, I.; Pichova, I.; Rezacova, P.
Deposited on	:	2009-01-15
Resolution	:	1.85 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:

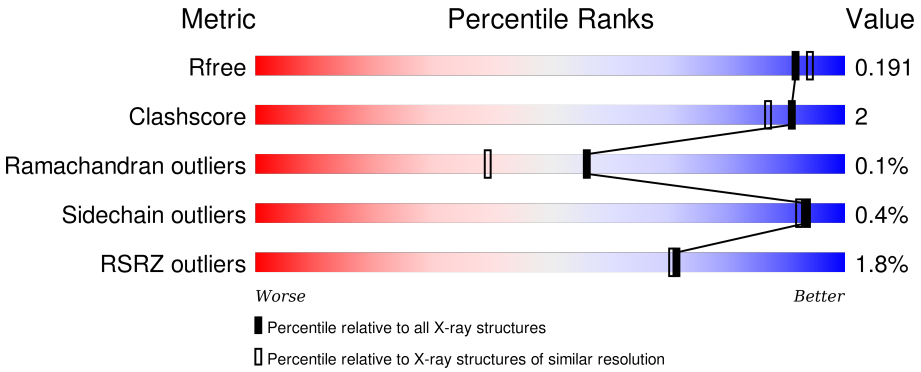
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	339	3% 97%
1	B	339	2% 94% 5%
1	C	339	3% 96%
1	D	339	3% 94% 5%
1	E	339	% 98%

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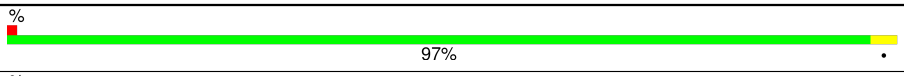
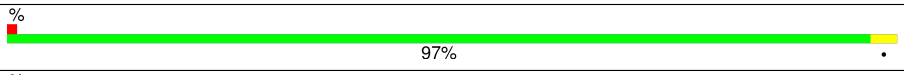
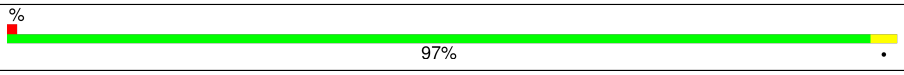
Mol	Chain	Length	Quality of chain
1	F	339	
1	G	339	
1	H	339	
2	I	6	
2	J	6	
2	K	6	
2	L	6	
2	M	6	
2	N	6	
2	O	6	
2	P	6	

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
3	SO4	D	341	-	-	-	X
3	SO4	E	341	-	-	-	X
3	SO4	G	340	-	-	-	X
3	SO4	G	341	-	-	-	X
3	SO4	G	344	-	-	-	X
4	GOL	A	341	-	-	-	X
4	GOL	B	343	-	-	-	X
4	GOL	B	344	-	-	-	X
4	GOL	C	340	-	-	-	X
4	GOL	D	343	-	-	-	X
4	GOL	E	344	-	-	-	X
4	GOL	E	345	-	-	-	X
4	GOL	F	342	-	-	-	X
4	GOL	G	345	-	-	-	X
4	GOL	H	342	-	-	-	X
4	GOL	H	343	-	-	-	X
4	GOL	H	344	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23564 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 Sapp1p-secreted aspartic protease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	5	14	0
			2585	1614	422	545	4			
1	B	339	Total	C	N	O	S	5	16	0
			2596	1620	423	549	4			
1	C	339	Total	C	N	O	S	5	17	0
			2598	1623	422	549	4			
1	D	338	Total	C	N	O	S	6	12	0
			2569	1603	420	542	4			
1	E	339	Total	C	N	O	S	5	22	0
			2621	1639	424	554	4			
1	F	339	Total	C	N	O	S	5	17	0
			2598	1623	421	550	4			
1	G	339	Total	C	N	O	S	5	20	0
			2609	1629	424	552	4			
1	H	339	Total	C	N	O	S	5	22	0
			2620	1637	426	553	4			

- Molecule 2 is a protein called pepstatin A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	6	Total	C	N	O	0	0	0
			48	34	5	9			
2	J	6	Total	C	N	O	0	0	0
			48	34	5	9			
2	K	6	Total	C	N	O	0	0	0
			48	34	5	9			
2	L	6	Total	C	N	O	0	0	0
			48	34	5	9			
2	M	6	Total	C	N	O	0	0	0
			48	34	5	9			
2	N	6	Total	C	N	O	0	0	0
			48	34	5	9			

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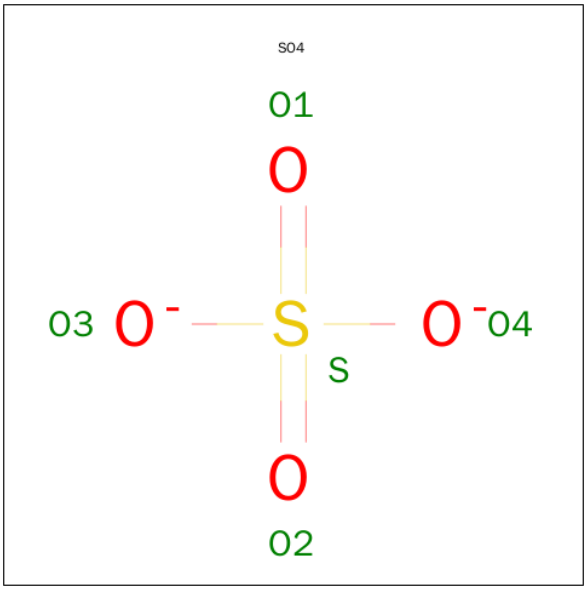
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	O	6	Total C N O 48 34 5 9	0	0	0
2	P	6	Total C N O 48 34 5 9	0	0	0

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



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

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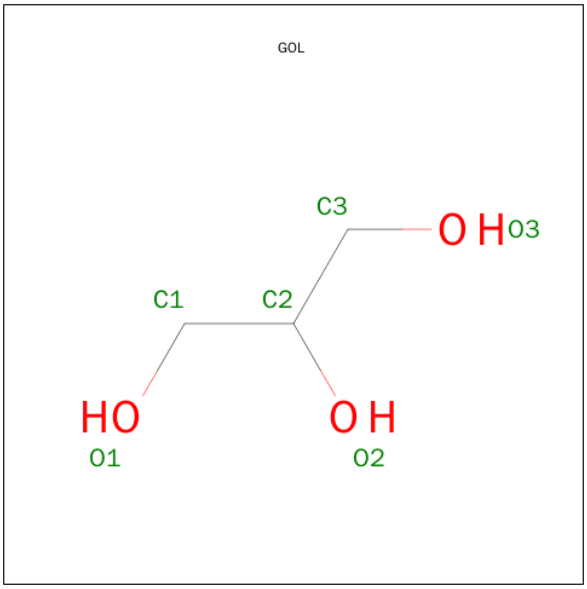
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

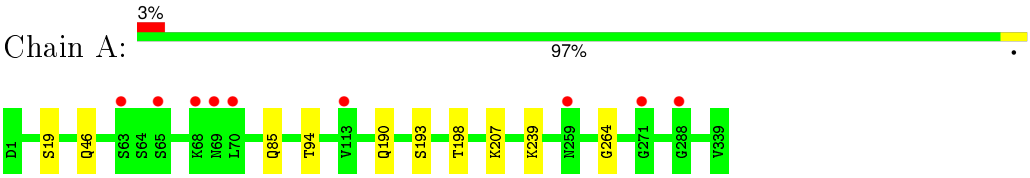
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	228	Total O 228 228	0	0
5	I	2	Total O 2 2	0	0
5	B	283	Total O 283 283	0	0
5	J	3	Total O 3 3	0	0
5	C	151	Total O 151 151	0	0
5	K	1	Total O 1 1	0	0
5	D	239	Total O 239 239	0	0
5	L	6	Total O 6 6	0	0
5	E	326	Total O 326 326	0	0
5	M	5	Total O 5 5	0	0
5	F	309	Total O 309 309	0	0
5	N	3	Total O 3 3	0	0
5	G	295	Total O 295 295	0	0
5	O	4	Total O 4 4	0	0
5	H	301	Total O 301 301	0	0
5	P	3	Total O 3 3	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.

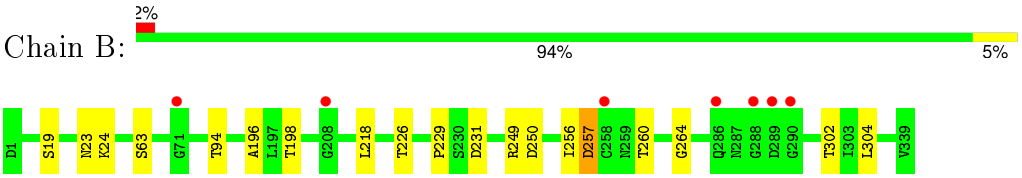
- Molecule 1: Sapp1p-secreted aspartic protease 1

Chain A:



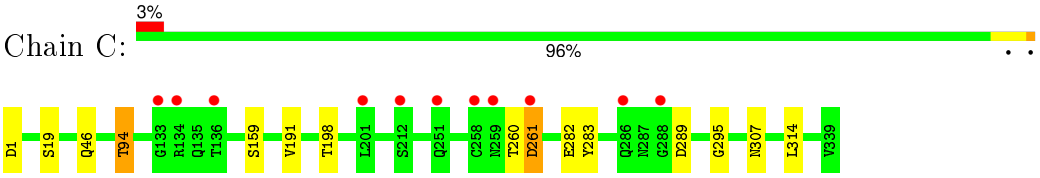
- Molecule 1: Sapp1p-secreted aspartic protease 1

Chain B:



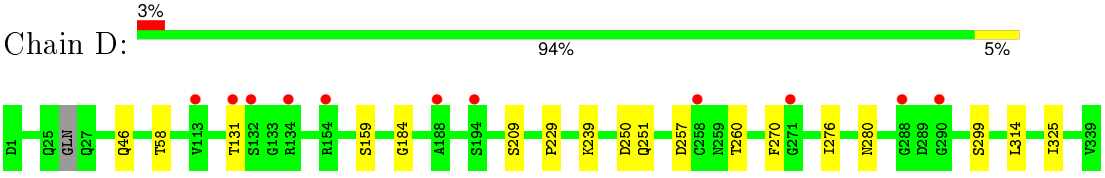
- Molecule 1: Sapp1p-secreted aspartic protease 1

Chain C:



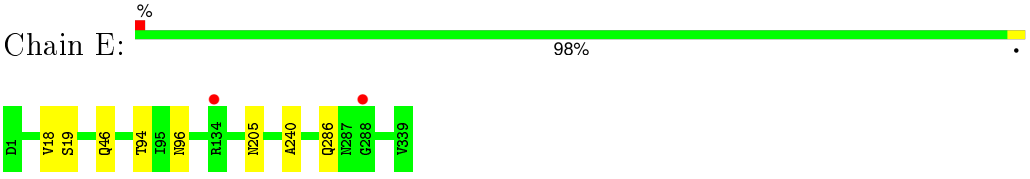
- Molecule 1: Sapp1p-secreted aspartic protease 1

Chain D:



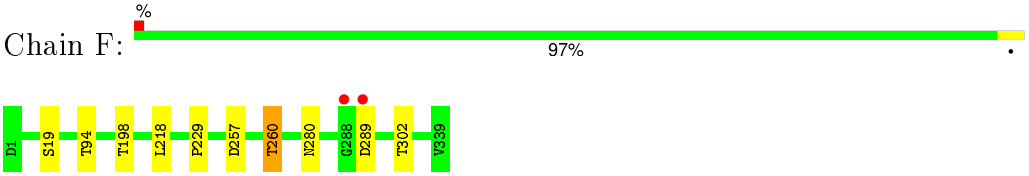
- Molecule 1: Sapp1p-secreted aspartic protease 1

Chain E:



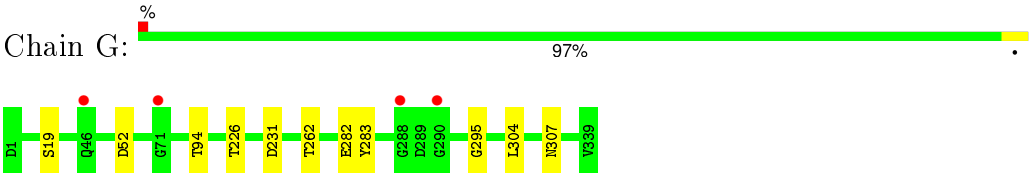
- Molecule 1: Sapp1p-secreted aspartic protease 1

Chain F:



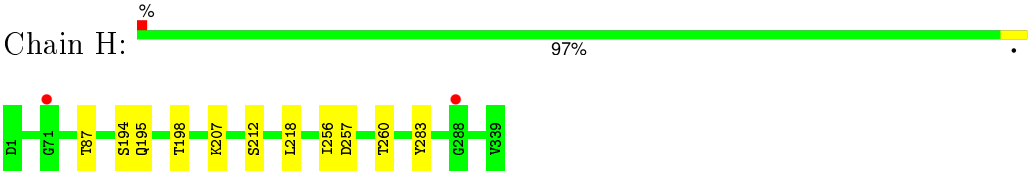
- Molecule 1: Sapp1p-secreted aspartic protease 1

Chain G:



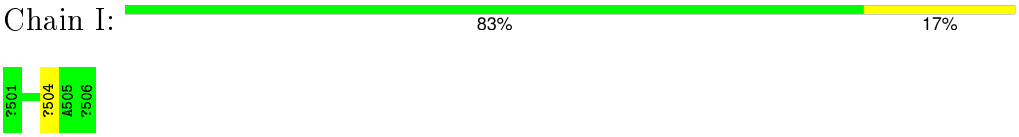
- Molecule 1: Sapp1p-secreted aspartic protease 1

Chain H:



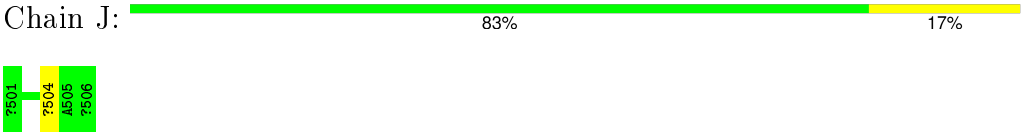
- Molecule 2: pepstatin A

Chain I:



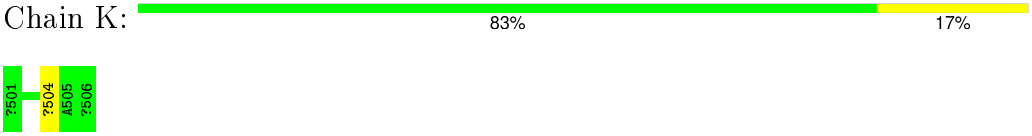
- Molecule 2: pepstatin A

Chain J:



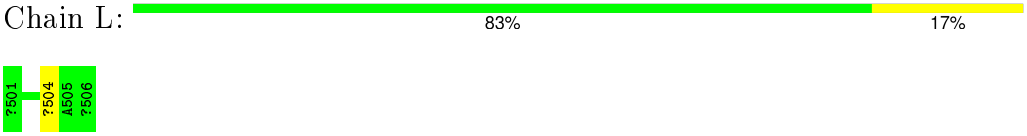
- Molecule 2: pepstatin A

Chain K:



- Molecule 2: pepstatin A

Chain L:



- Molecule 2: pepstatin A

Chain M:

• Molecule 2: pepstatin A

Chain N:

• Molecule 2: pepstatin A

Chain O:

• Molecule 2: pepstatin A

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.49Å 194.25Å 97.15Å 90.00° 91.52° 90.00°	Depositor
Resolution (Å)	46.03 – 1.85 46.03 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.03-1.85) 99.1 (46.03-1.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.166 , 0.190 0.167 , 0.191	Depositor DCC
R_{free} test set	1363 reflections (0.51%)	DCC
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.4	EDS
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 271028 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	23564	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: GOL, SO4, IVA, STA

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	0.50	0/2667	0.57	0/3630
1	B	0.56	0/2687	0.61	0/3657
1	C	0.46	0/2692	0.57	0/3664
1	D	0.59	0/2644	0.61	0/3597
1	E	0.62	0/2727	0.63	0/3711
1	F	0.61	0/2689	0.63	0/3660
1	G	0.59	0/2706	0.60	0/3683
1	H	0.58	0/2726	0.61	0/3709
2	I	0.50	0/17	1.02	0/21
2	J	0.58	0/17	1.04	0/21
2	K	0.41	0/17	0.78	0/21
2	L	0.64	0/17	1.07	0/21
2	M	0.70	0/17	2.06	2/21 (9.5%)
2	N	0.59	0/17	1.02	0/21
2	O	0.62	0/17	1.01	0/21
2	P	0.53	0/17	0.94	0/21
All	All	0.57	0/21674	0.61	2/29479 (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
2	I	0	2
2	J	0	2
2	K	0	2
2	L	0	2
2	M	0	2
2	N	0	2
2	O	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	2
All	All	0	16

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	M	503	VAL	CA-CB-CG1	6.32	120.38	110.90
2	M	503	VAL	CA-CB-CG2	5.07	118.51	110.90

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	504	STA	Mainchain,Peptide
2	J	504	STA	Mainchain,Peptide
2	K	504	STA	Mainchain,Peptide
2	L	504	STA	Mainchain,Peptide
2	M	504	STA	Mainchain,Peptide
2	N	504	STA	Mainchain,Peptide
2	O	504	STA	Mainchain,Peptide
2	P	504	STA	Mainchain,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	2585	0	2526	7	0
1	B	2596	0	2540	19	0
1	C	2598	0	2546	14	0
1	D	2569	0	2503	12	0
1	E	2621	0	2579	13	0
1	F	2598	0	2542	8	0
1	G	2609	0	2558	9	0
1	H	2620	0	2578	9	0
2	I	48	0	60	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	48	0	60	0	0
2	K	48	0	60	0	0
2	L	48	0	60	0	0
2	M	48	0	60	0	0
2	N	48	0	60	0	0
2	O	48	0	60	0	0
2	P	48	0	60	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	D	10	0	0	1	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
3	G	25	0	0	0	0
3	H	10	0	0	0	0
4	A	18	0	24	1	0
4	B	24	0	32	2	0
4	C	18	0	24	0	0
4	D	18	0	24	2	0
4	E	24	0	32	4	0
4	F	6	0	8	1	0
4	G	12	0	16	1	0
4	H	30	0	40	3	0
5	A	228	0	0	2	0
5	B	283	0	0	5	0
5	C	151	0	0	1	0
5	D	239	0	0	3	0
5	E	326	0	0	6	0
5	F	309	0	0	1	0
5	G	295	0	0	2	0
5	H	301	0	0	4	0
5	I	2	0	0	0	0
5	J	3	0	0	0	0
5	K	1	0	0	0	0
5	L	6	0	0	0	0
5	M	5	0	0	0	0
5	N	3	0	0	0	0
5	O	4	0	0	0	0
5	P	3	0	0	0	0
All	All	23564	0	21052	92	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 2.

All (92) 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:E:286[A]:GLN:OE1	5:E:2136:HOH:O	1.66	1.11
1:H:257:ASP:O	1:H:260[B]:THR:HG23	1.69	0.93
1:C:19:SER:HB2	1:C:94[A]:THR:HG23	1.53	0.88
1:F:198[A]:THR:HG21	5:F:632:HOH:O	1.74	0.85
1:E:19:SER:HB2	1:E:94[A]:THR:CG2	2.06	0.84
1:A:85[A]:GLN:OE1	5:A:1738:HOH:O	1.95	0.83
1:G:19:SER:HB2	1:G:94[A]:THR:CG2	2.07	0.83
1:F:19:SER:HB2	1:F:94[A]:THR:HG23	1.60	0.83
1:H:256:ILE:HG12	1:H:260[B]:THR:HG21	1.60	0.82
1:D:250:ASP:HB3	1:D:251:GLN:OE1	1.81	0.81
1:E:286[B]:GLN:NE2	5:E:1374:HOH:O	1.91	0.81
1:C:260:THR:CG2	1:C:261:ASP:HB3	2.11	0.81
1:F:257:ASP:O	1:F:260:THR:HG22	1.83	0.79
1:F:19:SER:HB2	1:F:94[A]:THR:CG2	2.13	0.79
1:C:260:THR:HA	1:C:261:ASP:HB2	1.64	0.78
1:C:260:THR:HG22	1:C:261:ASP:HB3	1.66	0.77
1:E:46[A]:GLN:HG2	5:E:2137:HOH:O	1.84	0.77
1:B:249[A]:ARG:HD2	5:B:1710:HOH:O	1.32	0.76
1:C:260:THR:HA	1:C:261:ASP:CB	2.16	0.75
1:G:19:SER:HB2	1:G:94[A]:THR:HG23	1.73	0.71
1:A:19:SER:HB2	1:A:94[A]:THR:HG23	1.72	0.70
1:D:46[B]:GLN:HG2	5:D:2144:HOH:O	1.92	0.68
1:B:19:SER:HB2	1:B:94[A]:THR:CG2	2.24	0.68
1:D:131:THR:HG22	5:D:815:HOH:O	1.94	0.66
1:A:19:SER:HB2	1:A:94[A]:THR:CG2	2.25	0.66
1:E:19:SER:HB2	1:E:94[A]:THR:HG22	1.80	0.64
1:G:52:ASP:OD1	5:G:2135:HOH:O	2.15	0.63
1:C:19:SER:HB2	1:C:94[A]:THR:CG2	2.28	0.63
1:B:264:GLY:HA3	4:B:341:GOL:H11	1.82	0.62
1:B:249[B]:ARG:HD3	1:B:250:ASP:OD1	2.01	0.61
1:F:280:ASN:HB3	4:F:342:GOL:H31	1.83	0.61
1:G:231:ASP:HB3	5:G:1678:HOH:O	2.01	0.61
1:B:257:ASP:HB2	1:B:260[B]:THR:HG23	1.82	0.61
1:E:18[B]:VAL:HA	4:E:344:GOL:H32	1.83	0.60
1:F:198[A]:THR:HG22	1:F:218:LEU:HA	1.83	0.60
1:E:205[B]:ASN:ND2	5:E:1276:HOH:O	2.35	0.59
1:H:198:THR:HG21	5:H:1310:HOH:O	2.03	0.58
1:B:19:SER:HB2	1:B:94[A]:THR:HG22	1.87	0.57
1:A:207:LYS:HB2	1:A:239:LYS:HE3	1.86	0.57
1:C:283:TYR:HA	1:C:295:GLY:HA3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94[A]:THR:HG23	4:E:344:GOL:H11	1.87	0.57
1:B:256:ILE:HG12	1:B:260[B]:THR:HG21	1.87	0.57
1:B:198:THR:HG21	5:B:691:HOH:O	2.05	0.57
1:D:276:ILE:HD11	1:D:325[A]:ILE:HG22	1.88	0.55
1:B:198:THR:HG22	1:B:218:LEU:HA	1.89	0.55
1:D:58:THR:OG1	3:D:341:SO4:O1	2.19	0.55
1:H:207:LYS:HD3	4:H:342:GOL:H31	1.89	0.54
1:H:198:THR:HG22	1:H:218:LEU:HA	1.90	0.54
1:F:198[A]:THR:HG22	1:F:218:LEU:CA	2.38	0.53
1:H:87[B]:THR:HG22	5:H:658:HOH:O	2.09	0.53
1:E:46[B]:GLN:HG2	5:E:2137:HOH:O	2.08	0.53
1:H:283:TYR:HB2	4:H:343:GOL:H31	1.92	0.52
1:C:260:THR:CA	1:C:261:ASP:CB	2.86	0.52
1:D:229:PRO:HA	1:D:299:SER:O	2.10	0.52
1:B:23:ASN:HD21	1:B:63:SER:HB3	1.77	0.50
1:E:19:SER:HB2	1:E:94[A]:THR:HG23	1.89	0.50
1:D:209:SER:HB2	1:D:239:LYS:HE2	1.93	0.49
1:B:231:ASP:HB2	5:B:1670:HOH:O	2.12	0.49
1:H:194[B]:SER:OG	1:H:195[B]:GLN:NE2	2.46	0.48
1:C:260:THR:HG23	1:C:261:ASP:HB3	1.93	0.48
1:A:264:GLY:CA	4:A:343:GOL:H32	2.44	0.48
1:E:286[B]:GLN:CD	5:E:1374:HOH:O	2.43	0.48
1:B:249[A]:ARG:CD	5:B:1710:HOH:O	1.85	0.47
1:B:24:LYS:HD3	1:B:94[A]:THR:HG21	1.97	0.47
1:G:19:SER:HB2	1:G:94[A]:THR:HG22	1.93	0.47
1:G:262:THR:HG22	4:G:345:GOL:O1	2.15	0.47
1:A:193:SER:HB3	1:A:198[A]:THR:HG22	1.96	0.46
4:H:342:GOL:H32	5:H:899:HOH:O	2.16	0.46
1:B:94[A]:THR:HG23	4:B:343:GOL:H11	1.97	0.46
1:C:282:GLU:HB3	1:C:307:ASN:HB2	1.97	0.46
1:D:184:GLY:H	4:D:344:GOL:H2	1.81	0.46
1:D:270:PHE:N	5:D:928:HOH:O	2.48	0.45
1:D:280:ASN:HB3	4:D:343:GOL:H2	1.98	0.45
1:H:87[B]:THR:HG23	5:H:499:HOH:O	2.17	0.44
1:C:159:SER:HA	1:C:314:LEU:O	2.18	0.44
1:G:282:GLU:HB3	1:G:307:ASN:HB2	1.99	0.43
1:G:226:THR:HG23	1:G:304:LEU:HD23	2.00	0.43
1:B:249[B]:ARG:NE	5:B:1710:HOH:O	2.43	0.43
1:B:229:PRO:HD3	1:B:302:THR:OG1	2.18	0.42
1:D:257:ASP:O	1:D:260:THR:HG22	2.19	0.42
1:E:96:ASN:H	4:E:344:GOL:C3	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94[A]:THR:HG22	5:C:1219:HOH:O	2.20	0.42
1:C:191:VAL:HA	1:C:198:THR:O	2.20	0.41
1:B:226:THR:HG23	1:B:304:LEU:HD23	2.03	0.41
1:G:283:TYR:HA	1:G:295:GLY:HA3	2.03	0.41
1:B:196:ALA:HB1	1:B:218:LEU:HD13	2.02	0.41
1:B:198:THR:HG22	1:B:218:LEU:CA	2.50	0.40
1:E:240:ALA:HB1	4:E:345:GOL:H12	2.02	0.40
1:C:260:THR:HA	1:C:261:ASP:HB3	2.02	0.40
1:A:190:GLN:NE2	5:A:1865:HOH:O	2.44	0.40
1:D:159:SER:HA	1:D:314:LEU:O	2.22	0.40
1:F:229:PRO:HD3	1:F:302:THR:OG1	2.22	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	351/339 (104%)	342 (97%)	9 (3%)	0	100	100
1	B	353/339 (104%)	343 (97%)	10 (3%)	0	100	100
1	C	354/339 (104%)	346 (98%)	6 (2%)	2 (1%)	30	13
1	D	346/339 (102%)	339 (98%)	7 (2%)	0	100	100
1	E	359/339 (106%)	352 (98%)	7 (2%)	0	100	100
1	F	354/339 (104%)	348 (98%)	5 (1%)	1 (0%)	46	29
1	G	357/339 (105%)	352 (99%)	5 (1%)	0	100	100
1	H	359/339 (106%)	350 (98%)	9 (2%)	0	100	100
2	I	3/6 (50%)	3 (100%)	0	0	100	100
2	J	3/6 (50%)	3 (100%)	0	0	100	100
2	K	3/6 (50%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
2	M	3/6 (50%)	3 (100%)	0	0	100	100
2	N	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
2	O	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
2	P	3/6 (50%)	3 (100%)	0	0	100	100
All	All	2857/2760 (104%)	2793 (98%)	61 (2%)	3 (0%)	56	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	261	ASP
1	C	289	ASP
1	F	289	ASP

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	294/281 (105%)	293 (100%)	1 (0%)	94	94
1	B	297/281 (106%)	296 (100%)	1 (0%)	94	94
1	C	298/281 (106%)	293 (98%)	5 (2%)	68	54
1	D	292/281 (104%)	292 (100%)	0	100	100
1	E	303/281 (108%)	303 (100%)	0	100	100
1	F	297/281 (106%)	296 (100%)	1 (0%)	94	94
1	G	300/281 (107%)	300 (100%)	0	100	100
1	H	302/281 (108%)	301 (100%)	1 (0%)	94	94
2	I	2/2 (100%)	2 (100%)	0	100	100
2	J	2/2 (100%)	2 (100%)	0	100	100
2	K	2/2 (100%)	2 (100%)	0	100	100
2	L	2/2 (100%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	M	2/2 (100%)	1 (50%)	1 (50%)	0 0
2	N	2/2 (100%)	2 (100%)	0	100 100
2	O	2/2 (100%)	2 (100%)	0	100 100
2	P	2/2 (100%)	2 (100%)	0	100 100
All	All	2399/2264 (106%)	2389 (100%)	10 (0%)	93 92

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	B	257	ASP
1	C	1	ASP
1	C	46[A]	GLN
1	C	46[B]	GLN
1	C	94[A]	THR
1	C	94[B]	THR
2	M	503	VAL
1	F	260	THR
1	H	212	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	115	GLN
1	C	287	ASN
1	F	115	GLN
1	F	287	ASN
1	H	46	GLN
1	H	115	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)

16 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	STA	I	504	2	10,10,11	0.44	0	10,12,14	0.80	0
2	STA	I	506	2	8,11,11	0.28	0	8,14,14	0.84	0
2	STA	J	504	2	10,10,11	0.67	0	10,12,14	0.94	0
2	STA	J	506	2	8,11,11	0.52	0	8,14,14	0.92	0
2	STA	K	504	2	10,10,11	0.60	0	10,12,14	1.04	1 (10%)
2	STA	K	506	2	8,11,11	0.33	0	8,14,14	0.51	0
2	STA	L	504	2	10,10,11	0.82	0	10,12,14	0.87	0
2	STA	L	506	2	8,11,11	0.28	0	8,14,14	0.55	0
2	STA	M	504	2	10,10,11	0.53	0	10,12,14	0.70	0
2	STA	M	506	2	8,11,11	0.60	0	8,14,14	0.70	0
2	STA	N	504	2	10,10,11	0.83	0	10,12,14	0.89	0
2	STA	N	506	2	8,11,11	0.61	0	8,14,14	1.14	1 (12%)
2	STA	O	504	2	10,10,11	0.60	0	10,12,14	0.83	0
2	STA	O	506	2	8,11,11	0.48	0	8,14,14	0.90	0
2	STA	P	504	2	10,10,11	0.51	0	10,12,14	0.69	0
2	STA	P	506	2	8,11,11	0.61	0	8,14,14	1.62	3 (37%)

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	STA	I	504	2	-	0/11/11/12	0/0/0/0
2	STA	I	506	2	-	0/10/12/12	0/0/0/0
2	STA	J	504	2	-	0/11/11/12	0/0/0/0
2	STA	J	506	2	-	0/10/12/12	0/0/0/0
2	STA	K	504	2	-	0/11/11/12	0/0/0/0
2	STA	K	506	2	-	0/10/12/12	0/0/0/0
2	STA	L	504	2	-	0/11/11/12	0/0/0/0
2	STA	L	506	2	-	0/10/12/12	0/0/0/0
2	STA	M	504	2	-	0/11/11/12	0/0/0/0
2	STA	M	506	2	-	0/10/12/12	0/0/0/0
2	STA	N	504	2	-	0/11/11/12	0/0/0/0
2	STA	N	506	2	-	0/10/12/12	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	STA	O	504	2	-	0/11/11/12	0/0/0/0
2	STA	O	506	2	-	0/10/12/12	0/0/0/0
2	STA	P	504	2	-	0/11/11/12	0/0/0/0
2	STA	P	506	2	-	0/10/12/12	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	506	STA	OH-CH-CM	-2.79	104.88	109.73
2	P	506	STA	OH-CH-CA	-2.41	105.91	109.49
2	K	504	STA	OH-CH-CA	-2.35	106.00	109.49
2	N	506	STA	CM-CH-CA	-2.25	109.25	112.68
2	P	506	STA	CM-CH-CA	2.55	116.56	112.68

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)

40 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	340	-	4,4,4	0.21	0	6,6,6	0.18	0
4	GOL	A	341	-	5,5,5	0.27	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	A	342	-	5,5,5	0.33	0	5,5,5	0.39	0
4	GOL	A	343	-	5,5,5	0.43	0	5,5,5	0.19	0
3	SO4	B	340	-	4,4,4	0.19	0	6,6,6	0.23	0
4	GOL	B	341	-	5,5,5	0.36	0	5,5,5	0.29	0
4	GOL	B	342	-	5,5,5	0.30	0	5,5,5	0.38	0
4	GOL	B	343	-	5,5,5	0.51	0	5,5,5	0.58	0
4	GOL	B	344	-	5,5,5	0.32	0	5,5,5	0.57	0
4	GOL	C	340	-	5,5,5	0.32	0	5,5,5	0.35	0
4	GOL	C	341	-	5,5,5	0.40	0	5,5,5	0.29	0
4	GOL	C	342	-	5,5,5	0.34	0	5,5,5	0.32	0
3	SO4	D	340	-	4,4,4	0.19	0	6,6,6	0.11	0
3	SO4	D	341	-	4,4,4	0.24	0	6,6,6	0.38	0
4	GOL	D	342	-	5,5,5	0.27	0	5,5,5	0.19	0
4	GOL	D	343	-	5,5,5	0.41	0	5,5,5	0.29	0
4	GOL	D	344	-	5,5,5	0.36	0	5,5,5	0.18	0
3	SO4	E	340	-	4,4,4	0.30	0	6,6,6	0.26	0
3	SO4	E	341	-	4,4,4	0.16	0	6,6,6	0.13	0
4	GOL	E	342	-	5,5,5	0.51	0	5,5,5	0.46	0
4	GOL	E	343	-	5,5,5	0.31	0	5,5,5	0.33	0
4	GOL	E	344	-	5,5,5	0.53	0	5,5,5	0.75	0
4	GOL	E	345	-	5,5,5	0.27	0	5,5,5	0.57	0
3	SO4	F	340	-	4,4,4	0.20	0	6,6,6	0.31	0
3	SO4	F	341	-	4,4,4	0.33	0	6,6,6	0.39	0
4	GOL	F	342	-	5,5,5	0.34	0	5,5,5	0.29	0
3	SO4	G	340	-	4,4,4	0.13	0	6,6,6	0.34	0
3	SO4	G	341	-	4,4,4	0.15	0	6,6,6	0.13	0
3	SO4	G	342	-	4,4,4	0.14	0	6,6,6	0.18	0
3	SO4	G	343	-	4,4,4	0.25	0	6,6,6	0.14	0
3	SO4	G	344	-	4,4,4	0.21	0	6,6,6	0.16	0
4	GOL	G	345	-	5,5,5	0.28	0	5,5,5	0.70	0
4	GOL	G	346	-	5,5,5	0.36	0	5,5,5	0.13	0
3	SO4	H	340	-	4,4,4	0.24	0	6,6,6	0.19	0
3	SO4	H	341	-	4,4,4	0.35	0	6,6,6	0.18	0
4	GOL	H	342	-	5,5,5	0.37	0	5,5,5	0.37	0
4	GOL	H	343	-	5,5,5	0.27	0	5,5,5	0.52	0
4	GOL	H	344	-	5,5,5	0.51	0	5,5,5	0.53	0
4	GOL	H	345	-	5,5,5	0.33	0	5,5,5	0.41	0
4	GOL	H	346	-	5,5,5	0.34	0	5,5,5	0.22	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	340	-	-	0/0/0/0	0/0/0/0
4	GOL	A	341	-	-	0/4/4/4	0/0/0/0
4	GOL	A	342	-	-	0/4/4/4	0/0/0/0
4	GOL	A	343	-	-	0/4/4/4	0/0/0/0
3	SO4	B	340	-	-	0/0/0/0	0/0/0/0
4	GOL	B	341	-	-	0/4/4/4	0/0/0/0
4	GOL	B	342	-	-	0/4/4/4	0/0/0/0
4	GOL	B	343	-	-	0/4/4/4	0/0/0/0
4	GOL	B	344	-	-	0/4/4/4	0/0/0/0
4	GOL	C	340	-	-	0/4/4/4	0/0/0/0
4	GOL	C	341	-	-	0/4/4/4	0/0/0/0
4	GOL	C	342	-	-	0/4/4/4	0/0/0/0
3	SO4	D	340	-	-	0/0/0/0	0/0/0/0
3	SO4	D	341	-	-	0/0/0/0	0/0/0/0
4	GOL	D	342	-	-	0/4/4/4	0/0/0/0
4	GOL	D	343	-	-	0/4/4/4	0/0/0/0
4	GOL	D	344	-	-	0/4/4/4	0/0/0/0
3	SO4	E	340	-	-	0/0/0/0	0/0/0/0
3	SO4	E	341	-	-	0/0/0/0	0/0/0/0
4	GOL	E	342	-	-	0/4/4/4	0/0/0/0
4	GOL	E	343	-	-	0/4/4/4	0/0/0/0
4	GOL	E	344	-	-	0/4/4/4	0/0/0/0
4	GOL	E	345	-	-	0/4/4/4	0/0/0/0
3	SO4	F	340	-	-	0/0/0/0	0/0/0/0
3	SO4	F	341	-	-	0/0/0/0	0/0/0/0
4	GOL	F	342	-	-	0/4/4/4	0/0/0/0
3	SO4	G	340	-	-	0/0/0/0	0/0/0/0
3	SO4	G	341	-	-	0/0/0/0	0/0/0/0
3	SO4	G	342	-	-	0/0/0/0	0/0/0/0
3	SO4	G	343	-	-	0/0/0/0	0/0/0/0
3	SO4	G	344	-	-	0/0/0/0	0/0/0/0
4	GOL	G	345	-	-	0/4/4/4	0/0/0/0
4	GOL	G	346	-	-	0/4/4/4	0/0/0/0
3	SO4	H	340	-	-	0/0/0/0	0/0/0/0
3	SO4	H	341	-	-	0/0/0/0	0/0/0/0
4	GOL	H	342	-	-	0/4/4/4	0/0/0/0
4	GOL	H	343	-	-	0/4/4/4	0/0/0/0
4	GOL	H	344	-	-	0/4/4/4	0/0/0/0
4	GOL	H	345	-	-	0/4/4/4	0/0/0/0
4	GOL	H	346	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	343	GOL	1	0
4	B	341	GOL	1	0
4	B	343	GOL	1	0
3	D	341	SO4	1	0
4	D	343	GOL	1	0
4	D	344	GOL	1	0
4	E	344	GOL	3	0
4	E	345	GOL	1	0
4	F	342	GOL	1	0
4	G	345	GOL	1	0
4	H	342	GOL	2	0
4	H	343	GOL	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	339/339 (100%)	0.13	9 (2%) 58 55	8, 13, 20, 27	2 (0%)
1	B	339/339 (100%)	-0.04	7 (2%) 67 65	8, 13, 21, 29	2 (0%)
1	C	339/339 (100%)	0.43	11 (3%) 51 48	8, 13, 20, 31	0
1	D	338/339 (99%)	0.33	11 (3%) 50 47	7, 12, 21, 30	4 (1%)
1	E	339/339 (100%)	-0.03	2 (0%) 90 90	8, 12, 21, 29	1 (0%)
1	F	339/339 (100%)	-0.04	2 (0%) 90 90	8, 12, 21, 34	4 (1%)
1	G	339/339 (100%)	0.03	4 (1%) 81 81	9, 12, 20, 28	3 (0%)
1	H	339/339 (100%)	0.01	2 (0%) 90 90	7, 12, 19, 30	2 (0%)
2	I	3/6 (50%)	-0.66	0 100 100	12, 12, 14, 15	0
2	J	3/6 (50%)	-0.79	0 100 100	9, 9, 11, 11	0
2	K	3/6 (50%)	-0.47	0 100 100	15, 15, 16, 20	0
2	L	3/6 (50%)	-0.77	0 100 100	7, 7, 8, 15	0
2	M	3/6 (50%)	-0.52	0 100 100	9, 9, 9, 10	0
2	N	3/6 (50%)	-0.89	0 100 100	7, 7, 8, 9	0
2	O	3/6 (50%)	-1.19	0 100 100	8, 8, 10, 12	0
2	P	3/6 (50%)	-0.87	0 100 100	8, 8, 8, 10	0
All	All	2735/2760 (99%)	0.10	48 (1%) 71 71	7, 12, 20, 34	18 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	288	GLY	5.0
1	A	288	GLY	4.6
1	C	134	ARG	4.6
1	B	288	GLY	3.7
1	H	288	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	288	GLY	3.6
1	C	258	CYS	3.5
1	G	288	GLY	3.4
1	C	288	GLY	3.1
1	C	261	ASP	3.0
1	B	290	GLY	3.0
1	F	288	GLY	3.0
1	D	290	GLY	2.9
1	A	70	LEU	2.8
1	B	289	ASP	2.7
1	D	134	ARG	2.7
1	A	271	GLY	2.6
1	C	133	GLY	2.5
1	B	71	GLY	2.5
1	C	251[A]	GLN	2.4
1	D	188	ALA	2.4
1	C	212	SER	2.4
1	C	286	GLN	2.4
1	A	65	SER	2.4
1	D	271	GLY	2.4
1	C	136	THR	2.3
1	G	71[A]	GLY	2.3
1	D	194[A]	SER	2.3
1	D	258	CYS	2.3
1	A	113	VAL	2.3
1	D	132	SER	2.2
1	B	208	GLY	2.2
1	D	154[A]	ARG	2.2
1	D	113	VAL	2.2
1	A	63	SER	2.2
1	G	290	GLY	2.2
1	F	289	ASP	2.2
1	B	258	CYS	2.1
1	A	259	ASN	2.1
1	D	131	THR	2.1
1	G	46[A]	GLN	2.1
1	A	68	LYS	2.1
1	E	134	ARG	2.1
1	C	201	LEU	2.0
1	H	71[A]	GLY	2.0
1	A	69	ASN	2.0
1	C	259	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	286	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	STA	P	506	12/12	0.84	0.14	-	11,17,35,37	0
2	STA	I	506	12/12	0.89	0.15	-	15,19,38,39	0
2	STA	J	506	12/12	0.89	0.15	-	11,16,36,37	0
2	STA	O	504	11/12	0.98	0.06	-	5,6,8,8	0
2	STA	I	504	11/12	0.98	0.06	-	8,11,11,12	0
2	STA	N	506	12/12	0.92	0.13	-	8,12,29,32	0
2	STA	L	506	12/12	0.83	0.17	-	14,21,40,40	0
2	STA	M	504	11/12	0.98	0.06	-	5,7,9,9	0
2	STA	P	504	11/12	0.98	0.07	-	5,7,8,9	0
2	STA	K	504	11/12	0.96	0.08	-	12,14,16,16	0
2	STA	M	506	12/12	0.88	0.17	-	10,14,36,36	0
2	STA	J	504	11/12	0.98	0.06	-	5,6,9,10	0
2	STA	K	506	12/12	0.81	0.21	-	24,29,42,44	0
2	STA	L	504	11/12	0.98	0.07	-	6,7,10,10	0
2	STA	N	504	11/12	0.98	0.06	-	4,5,8,8	0
2	STA	O	506	12/12	0.90	0.13	-	11,17,37,38	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
4	GOL	G	345	6/6	0.84	0.26	16.17	26,34,36,40	0
4	GOL	F	342	6/6	0.85	0.23	10.00	34,42,44,45	0
3	SO4	G	340	5/5	0.96	0.19	5.61	43,43,45,45	0
4	GOL	D	343	6/6	0.82	0.31	5.42	35,43,45,49	0
4	GOL	B	343	6/6	0.94	0.21	4.58	24,27,29,29	0
4	GOL	B	344	6/6	0.92	0.26	4.33	30,37,38,39	0
4	GOL	E	345	6/6	0.95	0.15	4.15	18,27,27,28	0
3	SO4	E	341	5/5	0.90	0.25	3.93	65,65,65,66	0
4	GOL	E	344	6/6	0.94	0.21	3.73	19,23,24,26	0
3	SO4	D	341	5/5	0.94	0.21	3.54	51,52,53,53	0
3	SO4	G	341	5/5	0.89	0.25	3.49	76,76,76,76	0
4	GOL	C	340	6/6	0.86	0.34	3.27	54,57,57,58	0
4	GOL	H	344	6/6	0.90	0.22	3.22	26,27,30,30	0
4	GOL	A	341	6/6	0.90	0.20	2.83	38,40,41,41	0
4	GOL	H	343	6/6	0.91	0.17	2.81	32,37,38,40	0
4	GOL	H	342	6/6	0.79	0.15	2.12	46,47,49,49	0
3	SO4	G	344	5/5	0.83	0.21	2.01	73,74,75,75	0
4	GOL	E	342	6/6	0.81	0.16	1.88	36,38,40,40	0
3	SO4	G	342	5/5	0.90	0.15	1.22	75,75,75,76	0
3	SO4	F	341	5/5	0.94	0.13	1.20	14,17,18,19	5
4	GOL	A	342	6/6	0.94	0.18	1.16	40,42,42,43	0
4	GOL	B	342	6/6	0.78	0.15	0.95	40,42,43,44	0
4	GOL	E	343	6/6	0.88	0.14	0.87	36,37,38,38	0
4	GOL	D	342	6/6	0.79	0.14	0.44	35,37,38,40	0
4	GOL	H	345	6/6	0.92	0.12	0.07	39,40,40,41	0
4	GOL	C	341	6/6	0.90	0.12	-0.42	46,46,46,46	0
3	SO4	H	341	5/5	0.97	0.09	-1.32	14,16,17,20	5
4	GOL	C	342	6/6	0.86	0.12	-	56,56,56,56	0
3	SO4	F	340	5/5	0.93	0.17	-	60,61,61,62	0
4	GOL	A	343	6/6	0.84	0.15	-	59,59,59,59	0
3	SO4	A	340	5/5	0.87	0.15	-	93,93,94,94	0
4	GOL	H	346	6/6	0.73	0.21	-	53,54,55,57	0
3	SO4	G	343	5/5	0.97	0.12	-	60,60,60,61	0
3	SO4	E	340	5/5	0.95	0.13	-	46,47,49,49	0
3	SO4	H	340	5/5	0.94	0.14	-	67,67,67,68	0
4	GOL	D	344	6/6	0.81	0.15	-	60,61,62,62	0
3	SO4	D	340	5/5	0.81	0.20	-	91,91,92,92	0
3	SO4	B	340	5/5	0.94	0.15	-	49,51,51,51	0
4	GOL	G	346	6/6	0.88	0.27	-	46,47,48,48	0
4	GOL	B	341	6/6	0.84	0.14	-	42,44,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.