Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:38 PM GMT

PDB ID	:	1PVJ
Title	:	Crystal structure of the Streptococcal pyrogenic exotoxin B (SpeB)- inhibitor complex
Authors	:	Ziomek, E.; Sivaraman, J.; Doran, J.; Menard, R.; Cygler, M.
Deposited on	:	2003-06-27
Resolution	:	3.00 Å(reported)

The following versions of software and data (see references (i)) 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 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.
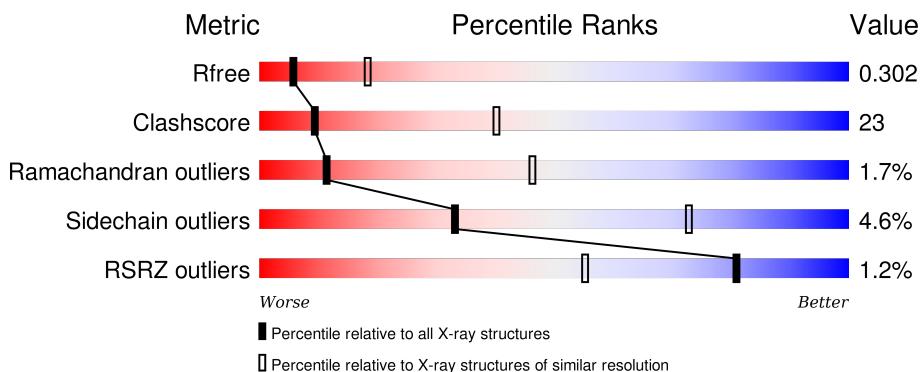
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 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	368	2% 55% 33% • 8%
1	B	368	% 59% 29% 5% 8%
1	C	368	60% 29% • 8%
1	D	368	2% 54% 34% • 8%
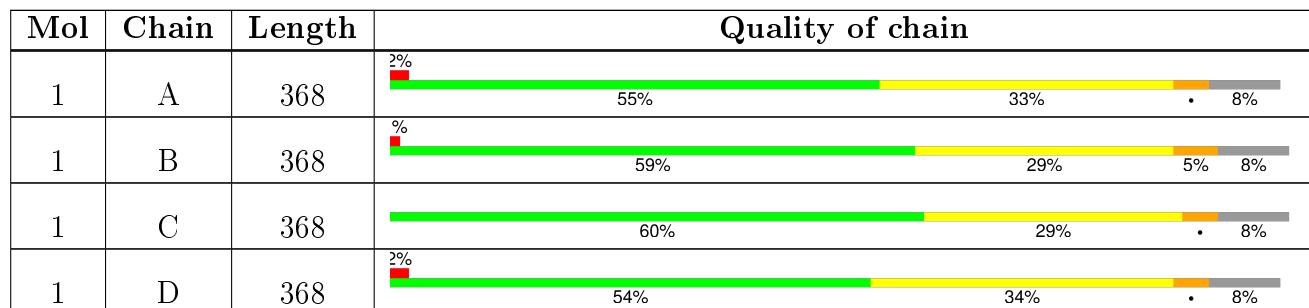
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZFB	A	450	-	-	X	X
2	ZFB	B	450	-	-	X	X
2	ZFB	C	450	-	-	X	X
2	ZFB	D	450	-	-	X	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11052 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 pyrogenic exotoxin B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total 2603	C 1644	N 450	O 502	S 7	0	0	0
1	B	339	Total 2603	C 1644	N 450	O 502	S 7	0	0	0
1	C	339	Total 2603	C 1644	N 450	O 502	S 7	0	0	0
1	D	339	Total 2603	C 1644	N 450	O 502	S 7	0	0	0

- Molecule 2 is (3R)-3-{[(BENZYLOXY)CARBONYL]AMINO}-2-OXO-4-PHENYLBUTAN E-1-DIAZONIUM (three-letter code: ZFB) (formula: $C_{18}H_{18}N_3O_3$).
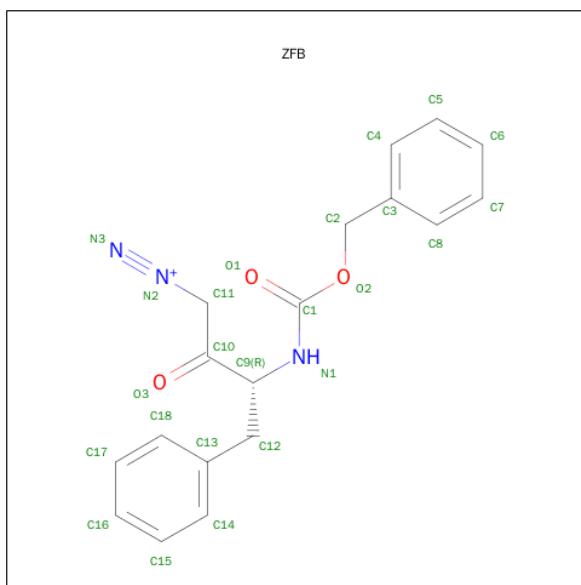
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 22	C 18	N 1	O 3	0	0
2	B	1	Total 22	C 18	N 1	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total 22	C 18	N 1	O 3	0	0
2	D	1	Total 22	C 18	N 1	O 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	156	Total 156	O 156	0	0
3	B	128	Total 128	O 128	0	0
3	C	124	Total 124	O 124	0	0
3	D	144	Total 144	O 144	0	0

3 Residue-property plots ⓘ

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: pyrogenic exotoxin B

• Molecule 1: pyrogenic exotoxin B

• Molecule 1: pyrogenic exotoxin B

• Molecule 1: pyrogenic exotoxin B

Chain D:
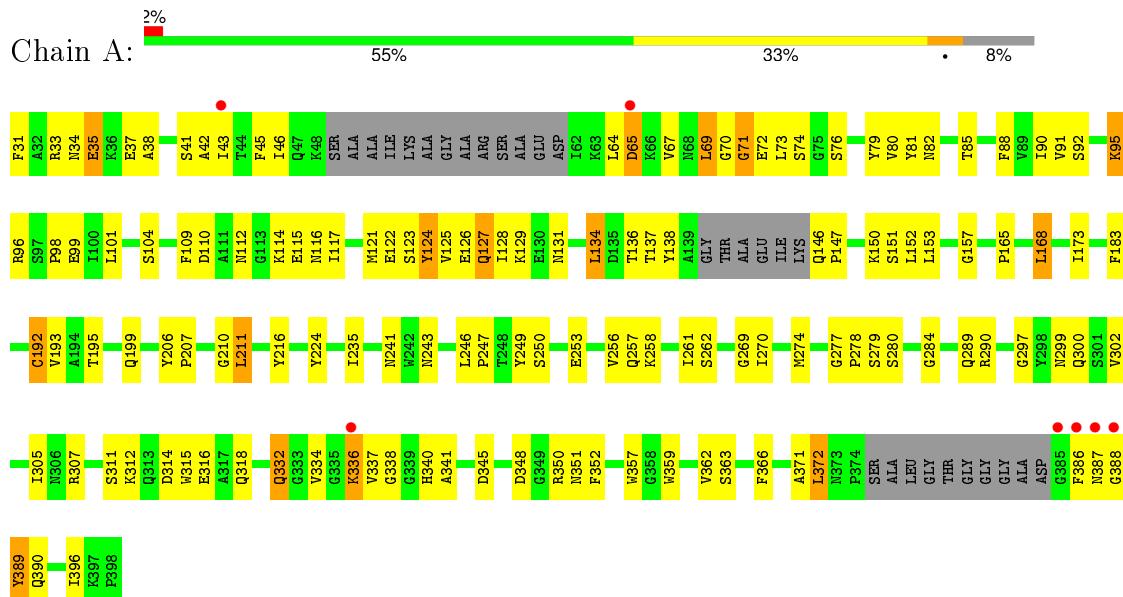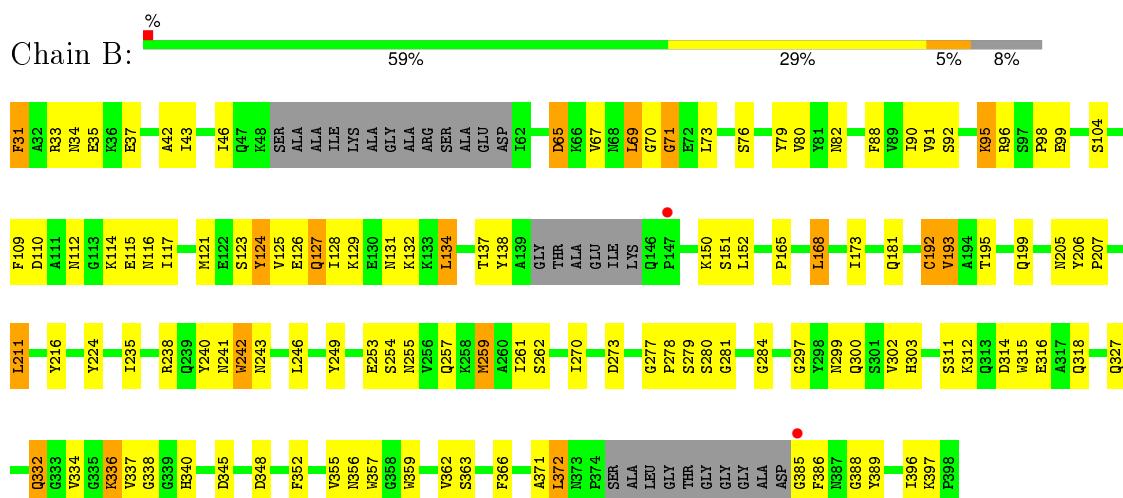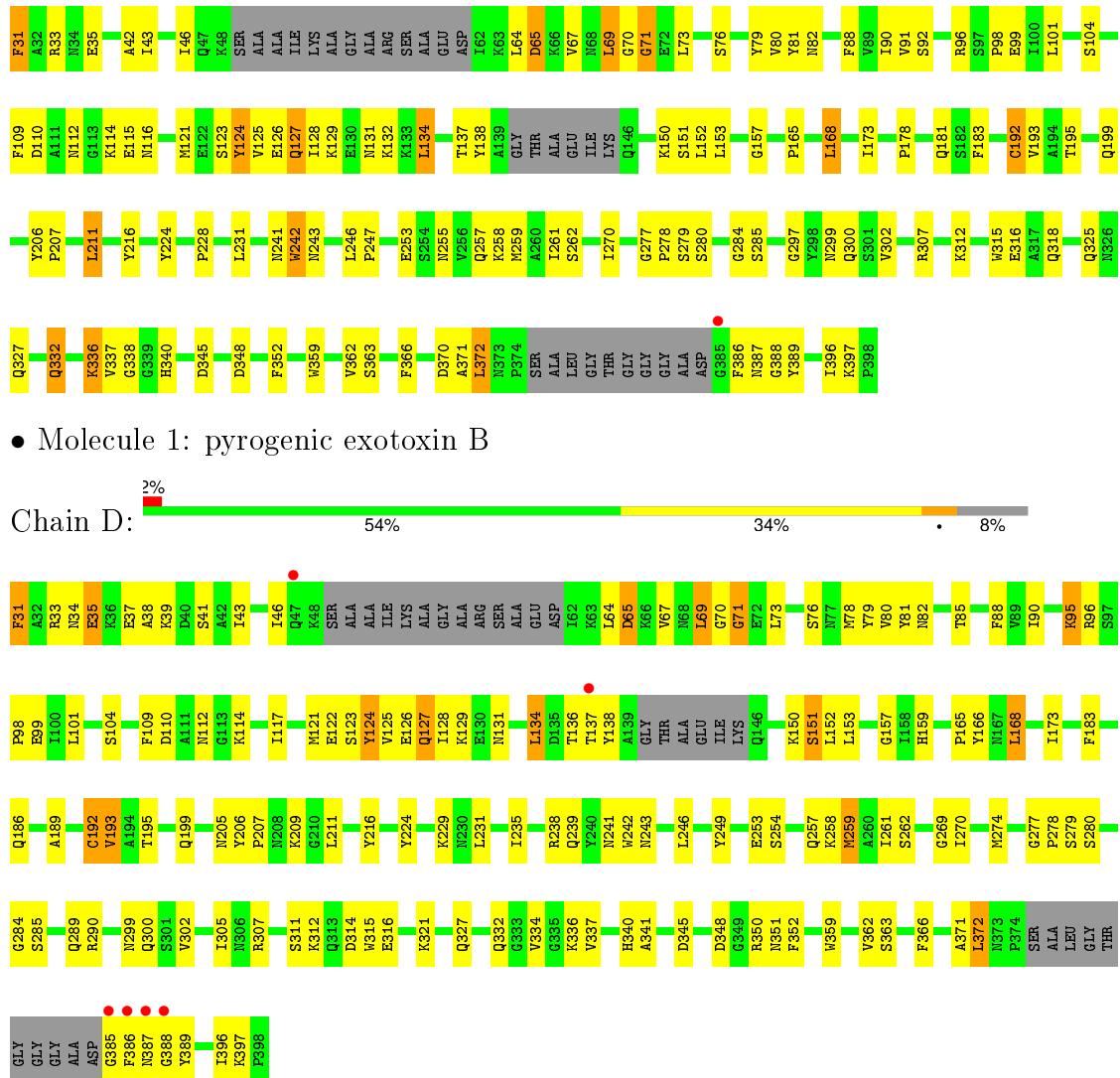
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.77Å 119.50Å 144.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 3.00 47.82 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (45.00-3.00) 88.5 (47.82-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.288 0.250 , 0.302	Depositor DCC
R_{free} test set	1613 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.882	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 40.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	7 of 29801 reflections (0.023%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	11052	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.75 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.1847e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1   Standard geometry (i)

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

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	0.85	1/2662 (0.0%)	0.83	1/3598 (0.0%)
1	B	0.75	1/2662 (0.0%)	0.82	1/3598 (0.0%)
1	C	0.77	1/2662 (0.0%)	0.82	2/3598 (0.1%)
1	D	0.81	1/2662 (0.0%)	0.82	1/3598 (0.0%)
All	All	0.80	4/10648 (0.0%)	0.82	5/14392 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	CYS	CB-SG	-13.56	1.59	1.82
1	C	192	CYS	CB-SG	-11.49	1.62	1.82
1	D	192	CYS	CB-SG	-10.34	1.64	1.82
1	B	192	CYS	CB-SG	-9.49	1.66	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	192	CYS	CA-CB-SG	8.15	128.67	114.00
1	D	192	CYS	CA-CB-SG	7.83	128.10	114.00
1	C	192	CYS	CA-CB-SG	7.18	126.92	114.00
1	A	192	CYS	CA-CB-SG	7.14	126.86	114.00
1	C	192	CYS	CB-CA-C	-5.19	100.02	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2603	0	2472	120	0
1	B	2603	0	2472	105	0
1	C	2603	0	2472	101	0
1	D	2603	0	2472	126	0
2	A	22	0	13	18	0
2	B	22	0	13	16	0
2	C	22	0	13	17	0
2	D	22	0	12	17	0
3	A	156	0	0	3	0
3	B	128	0	0	4	0
3	C	124	0	0	4	0
3	D	144	0	0	9	0
All	All	11052	0	9939	464	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 23.

All (464) 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:280:SER:H	2:B:450:ZFB:H15	1.03	1.14
1:C:280:SER:H	2:C:450:ZFB:H15	0.98	1.13
1:D:280:SER:H	2:D:450:ZFB:H15	1.04	1.12
1:A:280:SER:H	2:A:450:ZFB:H15	1.00	1.06
1:B:246:LEU:HD11	1:B:257:GLN:HG2	1.46	0.98
1:A:127:GLN:HG2	1:A:372:LEU:HD13	1.44	0.97
1:D:127:GLN:HG2	1:D:372:LEU:HD13	1.47	0.95
1:B:127:GLN:HG2	1:B:372:LEU:HD13	1.47	0.93
1:B:284:GLY:HA3	1:B:332:GLN:HE22	1.32	0.93
1:D:123:SER:O	1:D:127:GLN:HB2	1.69	0.93
1:C:280:SER:N	2:C:450:ZFB:H15	1.83	0.92
1:D:284:GLY:HA3	1:D:332:GLN:HE22	1.33	0.92
1:A:123:SER:O	1:A:127:GLN:HB2	1.69	0.91
1:C:192:CYS:HB3	2:C:450:ZFB:O3	1.70	0.91
1:C:280:SER:H	2:C:450:ZFB:C15	1.84	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:SER:N	2:A:450:ZFB:H15	1.86	0.89
1:A:246:LEU:HD11	1:A:257:GLN:HG2	1.53	0.89
1:C:127:GLN:HG2	1:C:372:LEU:HD13	1.51	0.89
1:C:178:PRO:HG3	3:C:459:HOH:O	1.73	0.88
1:B:280:SER:N	2:B:450:ZFB:H15	1.88	0.87
1:D:280:SER:N	2:D:450:ZFB:H15	1.89	0.87
1:B:280:SER:H	2:B:450:ZFB:C15	1.88	0.86
1:B:192:CYS:HB3	2:B:450:ZFB:O3	1.76	0.85
1:A:280:SER:H	2:A:450:ZFB:C15	1.88	0.85
1:D:246:LEU:HD11	1:D:257:GLN:HG2	1.58	0.85
1:D:280:SER:H	2:D:450:ZFB:C15	1.88	0.84
1:C:173:ILE:HG23	1:C:224:TYR:HB3	1.60	0.84
1:C:123:SER:O	1:C:127:GLN:HB2	1.78	0.83
1:D:173:ILE:HG23	1:D:224:TYR:HB3	1.58	0.82
1:D:192:CYS:HB3	2:D:450:ZFB:O3	1.78	0.82
1:B:173:ILE:HG23	1:B:224:TYR:HB3	1.61	0.82
1:C:284:GLY:HA3	1:C:332:GLN:HE22	1.46	0.81
1:A:192:CYS:HB3	2:A:450:ZFB:O3	1.81	0.80
1:C:246:LEU:HD11	1:C:257:GLN:HG2	1.63	0.80
1:B:123:SER:O	1:B:127:GLN:HB2	1.81	0.80
1:A:173:ILE:HG23	1:A:224:TYR:HB3	1.66	0.77
1:C:80:VAL:HG22	1:C:90:ILE:HG23	1.66	0.76
1:A:348:ASP:CG	1:A:352:PHE:HB2	2.06	0.75
1:C:302:VAL:HG22	1:C:396:ILE:HA	1.68	0.75
1:D:340:HIS:ND1	2:D:450:ZFB:O1	2.23	0.72
1:A:312:LYS:O	1:A:316:GLU:HG3	1.89	0.72
1:D:112:ASN:O	1:D:114:LYS:NZ	2.23	0.72
1:A:340:HIS:ND1	2:A:450:ZFB:O1	2.24	0.71
1:B:206:TYR:CD1	1:B:207:PRO:HA	2.25	0.71
1:C:340:HIS:ND1	2:C:450:ZFB:O1	2.23	0.71
1:A:284:GLY:HA3	1:A:332:GLN:HE22	1.55	0.71
1:A:348:ASP:OD2	1:A:352:PHE:HB2	1.92	0.69
1:B:340:HIS:ND1	2:B:450:ZFB:O1	2.23	0.69
1:B:348:ASP:CG	1:B:352:PHE:HB2	2.14	0.68
1:A:279:SER:HA	2:A:450:ZFB:C16	2.24	0.68
1:D:312:LYS:O	1:D:316:GLU:HG3	1.93	0.68
1:B:327:GLN:OE1	1:B:397:LYS:HD3	1.93	0.68
1:D:73:LEU:HD11	1:D:121:MET:HB2	1.76	0.67
1:D:31:PHE:HE2	1:D:137:THR:HG1	1.43	0.67
1:B:80:VAL:HG22	1:B:90:ILE:HG23	1.74	0.67
1:B:137:THR:HG22	1:B:138:TYR:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:SER:HA	2:B:450:ZFB:C16	2.25	0.66
1:D:348:ASP:CG	1:D:352:PHE:HB2	2.16	0.66
1:C:348:ASP:CG	1:C:352:PHE:HB2	2.16	0.66
1:D:152:LEU:HB2	1:D:345:ASP:HB2	1.77	0.65
1:B:312:LYS:O	1:B:316:GLU:HG3	1.97	0.64
1:B:302:VAL:HG22	1:B:396:ILE:HA	1.79	0.64
1:C:312:LYS:O	1:C:316:GLU:HG3	1.98	0.64
1:C:110:ASP:OD1	1:C:114:LYS:NZ	2.31	0.63
1:C:279:SER:HA	2:C:450:ZFB:C16	2.29	0.63
1:D:206:TYR:CD1	1:D:207:PRO:HA	2.34	0.62
1:D:80:VAL:HG22	1:D:90:ILE:HG23	1.81	0.62
1:C:327:GLN:OE1	1:C:397:LYS:HD3	1.99	0.62
2:B:450:ZFB:C11	2:B:450:ZFB:C1	2.74	0.62
1:D:43:ILE:HA	1:D:46:ILE:HD12	1.82	0.62
1:A:302:VAL:HG22	1:A:396:ILE:HA	1.83	0.61
1:C:73:LEU:HD11	1:C:121:MET:HB2	1.82	0.61
1:C:206:TYR:CD1	1:C:207:PRO:HA	2.35	0.61
2:C:450:ZFB:C1	2:C:450:ZFB:C11	2.76	0.61
2:D:450:ZFB:C11	2:D:450:ZFB:C1	2.78	0.61
1:B:279:SER:HA	2:B:450:ZFB:H16	1.83	0.61
1:D:302:VAL:HG22	1:D:396:ILE:HA	1.83	0.61
1:C:137:THR:HG22	1:C:138:TYR:N	2.16	0.61
1:C:31:PHE:HE2	1:C:137:THR:HG1	1.49	0.61
1:D:279:SER:HA	2:D:450:ZFB:C16	2.32	0.60
1:A:311:SER:OG	1:A:314:ASP:HB2	2.01	0.60
1:C:67:VAL:CG2	1:C:82:ASN:ND2	2.64	0.60
1:B:137:THR:CG2	1:B:138:TYR:N	2.64	0.60
1:B:33:ARG:NH2	1:B:99:GLU:HG3	2.17	0.60
1:C:152:LEU:HB2	1:C:345:ASP:HB2	1.82	0.60
2:C:450:ZFB:H22	2:C:450:ZFB:H14	1.84	0.60
1:A:80:VAL:HG22	1:A:90:ILE:HG23	1.84	0.60
1:B:131:ASN:O	1:B:134:LEU:HD22	2.02	0.60
1:A:279:SER:HA	2:A:450:ZFB:H16	1.83	0.60
1:D:76:SER:HB2	1:D:79:TYR:CZ	2.37	0.60
1:A:241:ASN:OD1	1:A:243:ASN:HB2	2.02	0.59
1:C:386:PHE:CZ	1:C:388:GLY:HA2	2.38	0.59
1:D:192:CYS:CB	2:D:450:ZFB:O3	2.48	0.59
1:B:69:LEU:HD12	1:B:73:LEU:HB3	1.84	0.59
1:D:348:ASP:OD2	1:D:352:PHE:HB2	2.02	0.59
1:D:124:TYR:O	1:D:128:ILE:HG13	2.02	0.59
1:C:67:VAL:HG22	1:C:82:ASN:ND2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:PHE:HB3	1:B:366:PHE:HB3	1.85	0.58
1:A:91:VAL:HG12	1:A:92:SER:O	2.04	0.58
2:A:450:ZFB:C11	2:A:450:ZFB:C1	2.81	0.58
1:B:116:ASN:N	2:B:450:ZFB:HN1	2.02	0.58
1:C:116:ASN:N	2:C:450:ZFB:HN1	2.02	0.58
1:D:76:SER:HB2	1:D:79:TYR:CE2	2.38	0.58
1:A:127:GLN:CG	1:A:372:LEU:HD13	2.29	0.58
1:C:348:ASP:OD2	1:C:352:PHE:HB2	2.04	0.58
1:A:112:ASN:O	1:A:114:LYS:NZ	2.36	0.58
1:C:280:SER:C	2:C:450:ZFB:H8	2.24	0.57
1:A:67:VAL:HG22	1:A:82:ASN:ND2	2.18	0.57
1:B:195:THR:O	1:B:199:GLN:HG3	2.04	0.57
1:B:348:ASP:OD2	1:B:352:PHE:HB2	2.04	0.57
1:C:352:PHE:HB3	1:C:366:PHE:HB3	1.86	0.57
1:B:246:LEU:CD1	1:B:257:GLN:HG2	2.28	0.57
1:A:33:ARG:NH2	1:A:99:GLU:HG3	2.20	0.57
1:D:88:PHE:CD1	1:D:109:PHE:HB2	2.39	0.57
1:A:124:TYR:O	1:A:128:ILE:HG13	2.05	0.56
1:A:73:LEU:HD11	1:A:121:MET:HB2	1.86	0.56
1:C:131:ASN:O	1:C:134:LEU:HD22	2.06	0.56
1:A:334:VAL:HG23	1:A:389:TYR:O	2.04	0.56
1:B:193:VAL:HG13	3:B:500:HOH:O	2.04	0.56
1:A:280:SER:C	2:A:450:ZFB:H8	2.25	0.56
1:D:137:THR:HG22	1:D:138:TYR:N	2.21	0.56
1:C:88:PHE:CD1	1:C:109:PHE:HB2	2.40	0.56
1:B:98:PRO:HD2	1:B:371:ALA:O	2.05	0.56
1:C:279:SER:HA	2:C:450:ZFB:H16	1.88	0.55
1:A:152:LEU:HB2	1:A:345:ASP:HB2	1.87	0.55
1:C:43:ILE:HA	1:C:46:ILE:HD12	1.87	0.55
1:B:205:ASN:OD1	1:B:242:TRP:HB3	2.06	0.55
1:B:280:SER:C	2:B:450:ZFB:H8	2.26	0.55
1:D:125:VAL:O	1:D:127:GLN:N	2.34	0.55
1:D:352:PHE:HB3	1:D:366:PHE:HB3	1.87	0.55
1:B:43:ILE:HA	1:B:46:ILE:HD12	1.88	0.55
1:C:98:PRO:HD2	1:C:371:ALA:O	2.07	0.55
1:D:280:SER:C	2:D:450:ZFB:H8	2.27	0.55
1:A:206:TYR:CD1	1:A:207:PRO:HA	2.42	0.55
1:C:150:LYS:O	1:C:151:SER:C	2.45	0.55
1:C:33:ARG:NH2	1:C:99:GLU:HG3	2.22	0.55
2:C:450:ZFB:H22	2:C:450:ZFB:C14	2.37	0.55
1:D:332:GLN:HA	1:D:341:ALA:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:LYS:O	1:C:338:GLY:N	2.40	0.55
1:D:153:LEU:HB2	1:D:345:ASP:OD2	2.07	0.54
1:A:33:ARG:HH21	1:A:99:GLU:HG3	1.72	0.54
1:A:67:VAL:CG2	1:A:82:ASN:ND2	2.70	0.54
1:D:253:GLU:O	1:D:258:LYS:HE3	2.07	0.54
1:C:69:LEU:HD12	1:C:73:LEU:HB3	1.88	0.54
1:B:110:ASP:OD1	1:B:114:LYS:NZ	2.40	0.54
2:B:450:ZFB:H22	2:B:450:ZFB:H14	1.90	0.54
1:A:125:VAL:O	1:A:127:GLN:N	2.35	0.54
1:A:352:PHE:HB3	1:A:366:PHE:HB3	1.88	0.54
1:C:137:THR:CG2	1:C:138:TYR:N	2.70	0.54
1:C:192:CYS:CB	2:C:450:ZFB:O3	2.46	0.54
1:C:91:VAL:HG12	1:C:92:SER:O	2.07	0.54
1:A:192:CYS:CB	2:A:450:ZFB:O3	2.53	0.53
1:D:165:PRO:O	1:D:168:LEU:HB2	2.09	0.53
1:A:165:PRO:CB	1:A:168:LEU:HD22	2.37	0.53
2:D:450:ZFB:H14	2:D:450:ZFB:H22	1.90	0.53
1:B:165:PRO:CB	1:B:168:LEU:HD22	2.39	0.53
1:B:192:CYS:CB	2:B:450:ZFB:O3	2.46	0.53
1:A:88:PHE:CD1	1:A:109:PHE:HB2	2.43	0.53
1:B:67:VAL:CG2	1:B:82:ASN:ND2	2.71	0.53
1:B:112:ASN:O	1:B:114:LYS:NZ	2.41	0.53
1:B:88:PHE:CD1	1:B:109:PHE:HB2	2.43	0.53
1:D:299:ASN:OD1	1:D:300:GLN:N	2.42	0.53
1:D:150:LYS:O	1:D:151:SER:C	2.46	0.53
2:D:450:ZFB:C14	2:D:450:ZFB:H22	2.39	0.53
1:A:153:LEU:HB2	1:A:345:ASP:OD2	2.09	0.53
1:B:211:LEU:HD12	1:B:297:GLY:HA2	1.91	0.53
1:B:67:VAL:HG22	1:B:82:ASN:ND2	2.24	0.53
1:D:165:PRO:CB	1:D:168:LEU:HD22	2.39	0.52
1:C:157:GLY:O	1:C:247:PRO:HB2	2.08	0.52
1:D:321:LYS:HD3	3:D:533:HOH:O	2.10	0.52
1:A:98:PRO:HD2	1:A:371:ALA:O	2.08	0.52
1:B:33:ARG:HH21	1:B:99:GLU:HG3	1.73	0.52
1:A:80:VAL:HG13	1:A:90:ILE:HG12	1.92	0.52
1:C:183:PHE:CE2	1:D:254:SER:HA	2.45	0.52
1:A:137:THR:HG22	1:A:138:TYR:N	2.25	0.52
2:B:450:ZFB:H22	2:B:450:ZFB:C14	2.40	0.52
2:A:450:ZFB:H22	2:A:450:ZFB:H14	1.91	0.52
1:A:299:ASN:OD1	1:A:300:GLN:N	2.43	0.52
1:D:67:VAL:HG22	1:D:82:ASN:ND2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:PHE:CZ	1:A:388:GLY:HA2	2.44	0.52
1:A:76:SER:HB2	1:A:79:TYR:CZ	2.45	0.52
1:C:253:GLU:O	1:C:258:LYS:HE3	2.10	0.52
1:C:261:ILE:HG23	1:C:262:SER:N	2.25	0.52
1:B:127:GLN:CG	1:B:372:LEU:HD13	2.31	0.51
1:D:277:GLY:C	1:D:279:SER:N	2.61	0.51
1:A:224:TYR:CE2	1:A:278:PRO:HD3	2.45	0.51
1:A:76:SER:HB2	1:A:79:TYR:CE2	2.45	0.51
2:A:450:ZFB:O3	2:A:450:ZFB:C14	2.59	0.51
1:B:277:GLY:C	1:B:279:SER:N	2.61	0.51
2:A:450:ZFB:C14	2:A:450:ZFB:H22	2.41	0.51
1:B:150:LYS:O	1:B:151:SER:C	2.48	0.51
1:D:131:ASN:O	1:D:134:LEU:HD22	2.11	0.51
1:C:165:PRO:CB	1:C:168:LEU:HD22	2.41	0.51
1:A:253:GLU:O	1:A:258:LYS:HE3	2.10	0.51
1:D:311:SER:OG	1:D:314:ASP:HB2	2.09	0.51
1:B:303:HIS:HE1	3:B:452:HOH:O	1.93	0.51
1:C:359:TRP:HH2	2:C:450:ZFB:C18	2.23	0.51
1:C:127:GLN:CG	1:C:372:LEU:HD13	2.33	0.51
1:C:124:TYR:O	1:C:128:ILE:HG13	2.10	0.51
1:C:76:SER:HB2	1:C:79:TYR:OH	2.11	0.51
1:C:76:SER:HB2	1:C:79:TYR:CZ	2.46	0.51
1:D:137:THR:CG2	1:D:138:TYR:N	2.73	0.51
1:C:112:ASN:HB3	3:C:552:HOH:O	2.09	0.51
1:B:386:PHE:CZ	1:B:388:GLY:HA2	2.46	0.51
1:B:31:PHE:O	1:B:95:LYS:HG3	2.11	0.51
1:B:241:ASN:OD1	1:B:243:ASN:HB2	2.11	0.50
1:B:216:TYR:HE2	1:B:270:ILE:HG12	1.77	0.50
1:A:150:LYS:O	1:A:151:SER:C	2.50	0.50
1:A:348:ASP:OD1	1:A:352:PHE:HB2	2.11	0.50
1:A:43:ILE:HA	1:A:46:ILE:HD12	1.94	0.50
1:D:153:LEU:N	1:D:345:ASP:OD2	2.37	0.50
1:D:76:SER:HB2	1:D:79:TYR:OH	2.10	0.50
1:B:70:GLY:O	1:B:71:GLY:C	2.50	0.50
1:D:386:PHE:CZ	1:D:388:GLY:HA2	2.47	0.50
1:C:70:GLY:O	1:C:71:GLY:C	2.50	0.50
1:A:116:ASN:N	2:A:450:ZFB:HN1	2.09	0.50
1:D:216:TYR:CE2	1:D:270:ILE:HG23	2.47	0.50
1:B:91:VAL:HG12	1:B:92:SER:O	2.12	0.50
1:D:70:GLY:O	1:D:71:GLY:C	2.50	0.49
1:C:362:VAL:O	1:C:363:SER:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ARG:HB3	1:D:387:ASN:HD22	1.76	0.49
1:D:65:ASP:N	1:D:65:ASP:OD2	2.45	0.49
1:C:277:GLY:C	1:C:279:SER:N	2.63	0.49
1:A:195:THR:O	1:A:199:GLN:HG3	2.12	0.49
1:D:241:ASN:OD1	1:D:243:ASN:HB2	2.11	0.49
1:D:165:PRO:CA	1:D:168:LEU:HD22	2.42	0.49
1:B:261:ILE:HG23	1:B:262:SER:N	2.27	0.49
1:C:195:THR:O	1:C:199:GLN:HG3	2.12	0.49
1:A:210:GLY:HA3	1:A:235:ILE:O	2.13	0.49
1:B:206:TYR:CG	1:B:207:PRO:HA	2.47	0.49
1:D:80:VAL:HG13	1:D:90:ILE:HG12	1.94	0.49
1:B:125:VAL:O	1:B:127:GLN:N	2.39	0.49
1:C:112:ASN:O	1:C:114:LYS:NZ	2.45	0.49
1:A:359:TRP:HH2	2:A:450:ZFB:C18	2.26	0.49
1:A:88:PHE:CE2	1:A:104:SER:HB3	2.48	0.49
1:A:76:SER:HB2	1:A:79:TYR:OH	2.12	0.49
1:A:125:VAL:HG12	1:A:129:LYS:HE3	1.95	0.48
1:C:125:VAL:O	1:C:127:GLN:N	2.46	0.48
1:C:67:VAL:HG22	1:C:82:ASN:HD22	1.77	0.48
1:B:165:PRO:CA	1:B:168:LEU:HD22	2.44	0.48
1:D:67:VAL:CG2	1:D:82:ASN:ND2	2.76	0.48
1:D:98:PRO:HD2	1:D:371:ALA:O	2.14	0.48
1:A:65:ASP:N	1:A:65:ASP:OD2	2.46	0.48
1:D:229:LYS:HD3	3:D:510:HOH:O	2.12	0.48
1:A:85:THR:CG2	3:A:459:HOH:O	2.61	0.48
1:D:359:TRP:HH2	2:D:450:ZFB:C18	2.26	0.48
1:B:42:ALA:O	1:B:46:ILE:HG13	2.14	0.48
1:C:126:GLU:O	1:C:126:GLU:HG3	2.14	0.48
1:A:249:TYR:CD2	1:A:253:GLU:HG2	2.48	0.48
1:A:261:ILE:HG23	1:A:262:SER:N	2.29	0.48
1:C:299:ASN:OD1	1:C:300:GLN:N	2.47	0.47
1:D:279:SER:HA	2:D:450:ZFB:H16	1.94	0.47
1:D:209:LYS:HE2	1:D:239:GLN:OE1	2.15	0.47
1:D:189:ALA:CB	2:D:450:ZFB:H16	2.44	0.47
1:D:69:LEU:HD12	1:D:73:LEU:HB3	1.95	0.47
1:D:216:TYR:CD2	1:D:270:ILE:HG23	2.49	0.47
1:D:195:THR:O	1:D:199:GLN:HG3	2.14	0.47
1:A:69:LEU:HD12	1:A:73:LEU:HB3	1.96	0.47
1:A:216:TYR:CE2	1:A:270:ILE:HG23	2.48	0.47
1:C:211:LEU:HD12	1:C:297:GLY:HA2	1.96	0.47
1:A:224:TYR:CE2	1:A:278:PRO:CD	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:THR:CG2	1:A:138:TYR:N	2.77	0.47
1:A:38:ALA:O	1:A:41:SER:HB2	2.15	0.47
1:D:34:ASN:O	1:D:37:GLU:N	2.47	0.47
1:D:327:GLN:OE1	1:D:397:LYS:HD3	2.15	0.47
1:A:332:GLN:HA	1:A:341:ALA:HA	1.97	0.47
1:D:261:ILE:HG23	1:D:262:SER:N	2.29	0.47
1:A:250:SER:HB3	3:A:602:HOH:O	2.15	0.47
1:C:33:ARG:HH21	1:C:99:GLU:HG3	1.78	0.47
1:B:152:LEU:HB2	1:B:345:ASP:HB2	1.96	0.47
1:A:121:MET:O	1:A:125:VAL:HG23	2.14	0.46
1:A:305:ILE:HD12	1:A:315:TRP:CZ3	2.50	0.46
1:B:312:LYS:HE2	3:B:498:HOH:O	2.15	0.46
1:B:362:VAL:O	1:B:363:SER:HB2	2.15	0.46
1:A:131:ASN:O	1:A:134:LEU:HD22	2.16	0.46
1:A:146:GLN:OE1	1:A:351:ASN:N	2.48	0.46
1:B:73:LEU:HD11	1:B:121:MET:HB2	1.97	0.46
1:D:38:ALA:O	1:D:41:SER:HB2	2.16	0.46
1:D:31:PHE:HE2	1:D:137:THR:OG1	1.98	0.46
1:D:67:VAL:HG22	1:D:82:ASN:HD22	1.80	0.46
1:A:117:ILE:HG12	1:A:357:TRP:CE3	2.50	0.46
1:D:334:VAL:HG23	1:D:389:TYR:O	2.15	0.46
1:C:126:GLU:CG	1:C:126:GLU:O	2.64	0.46
1:D:259:MET:HE2	1:D:259:MET:HA	1.96	0.46
1:A:110:ASP:OD1	1:A:114:LYS:NZ	2.47	0.46
1:B:165:PRO:O	1:B:168:LEU:HB2	2.14	0.46
1:A:307:ARG:HB3	1:A:387:ASN:HD22	1.81	0.46
1:A:246:LEU:CD1	1:A:257:GLN:HG2	2.35	0.46
1:C:207:PRO:O	1:C:242:TRP:NE1	2.30	0.46
1:D:205:ASN:OD1	1:D:242:TRP:HB3	2.16	0.46
1:C:165:PRO:CA	1:C:168:LEU:HD22	2.46	0.45
1:B:255:ASN:O	1:B:259:MET:HB3	2.15	0.45
1:A:34:ASN:O	1:A:35:GLU:C	2.54	0.45
1:B:299:ASN:OD1	1:B:300:GLN:N	2.49	0.45
2:D:450:ZFB:O3	2:D:450:ZFB:C14	2.65	0.45
1:D:224:TYR:CE2	1:D:278:PRO:HD3	2.51	0.45
1:A:387:ASN:O	1:A:390:GLN:HG3	2.16	0.45
1:D:117:ILE:HD11	1:D:359:TRP:CD1	2.51	0.45
1:A:64:LEU:HB3	1:A:81:TYR:HB3	1.99	0.45
1:A:42:ALA:O	1:A:46:ILE:HG13	2.16	0.45
1:C:241:ASN:OD1	1:C:243:ASN:HB2	2.16	0.45
1:D:231:LEU:HD12	1:D:231:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ASP:OD1	1:B:352:PHE:HB2	2.16	0.45
1:D:206:TYR:CG	1:D:207:PRO:HA	2.51	0.45
1:B:336:LYS:O	1:B:338:GLY:N	2.50	0.45
1:A:289:GLN:HG3	1:A:290:ARG:N	2.31	0.45
1:D:289:GLN:HG3	1:D:290:ARG:N	2.32	0.45
1:B:311:SER:OG	1:B:314:ASP:HB2	2.16	0.45
1:D:117:ILE:HD11	1:D:359:TRP:HD1	1.82	0.45
1:C:125:VAL:HG12	1:C:129:LYS:HE3	1.97	0.45
1:B:117:ILE:HD11	1:B:359:TRP:CD1	2.51	0.45
2:B:450:ZFB:O3	2:B:450:ZFB:C14	2.64	0.45
1:C:206:TYR:CG	1:C:207:PRO:HA	2.51	0.45
1:B:65:ASP:OD2	1:B:65:ASP:N	2.50	0.45
1:A:70:GLY:O	1:A:71:GLY:C	2.55	0.45
1:A:101:LEU:HD11	1:A:128:ILE:HD11	1.98	0.45
1:D:123:SER:O	1:D:124:TYR:C	2.54	0.45
1:B:117:ILE:HD11	1:B:359:TRP:HD1	1.81	0.45
1:C:228:PRO:HA	3:C:456:HOH:O	2.16	0.45
1:B:334:VAL:HB	1:B:389:TYR:HB2	1.99	0.45
1:C:315:TRP:O	1:C:318:GLN:HB2	2.17	0.45
1:A:72:GLU:CB	1:A:122:GLU:HG2	2.48	0.44
1:D:311:SER:O	1:D:312:LYS:C	2.52	0.44
1:D:34:ASN:O	1:D:35:GLU:C	2.54	0.44
1:D:334:VAL:HB	1:D:389:TYR:HB2	2.00	0.44
1:D:96:ARG:HG2	1:D:136:THR:O	2.17	0.44
1:C:325:GLN:O	1:C:327:GLN:HG3	2.17	0.44
1:D:350:ARG:O	1:D:351:ASN:HB2	2.17	0.44
1:C:64:LEU:HB3	1:C:81:TYR:HB3	1.99	0.44
1:B:69:LEU:HB2	1:B:73:LEU:HB2	1.99	0.44
1:D:246:LEU:CD1	1:D:257:GLN:HG2	2.39	0.44
1:A:289:GLN:HG3	1:A:290:ARG:H	1.82	0.44
1:D:159:HIS:HE1	3:D:457:HOH:O	2.00	0.44
1:C:65:ASP:N	1:C:65:ASP:OD2	2.50	0.44
1:D:235:ILE:HA	1:D:238:ARG:HG3	2.00	0.44
1:B:96:ARG:NH1	1:B:132:LYS:O	2.51	0.44
1:A:34:ASN:O	1:A:37:GLU:N	2.50	0.44
1:A:269:GLY:O	1:A:274:MET:HB2	2.18	0.44
1:B:126:GLU:O	1:B:126:GLU:HG3	2.17	0.44
1:C:216:TYR:OH	1:C:231:LEU:HD22	2.18	0.44
1:C:216:TYR:CD2	1:C:270:ILE:HG23	2.52	0.44
1:C:224:TYR:CE2	1:C:278:PRO:HD3	2.52	0.44
1:A:183:PHE:CE2	1:B:254:SER:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ASN:O	1:C:259:MET:HB3	2.17	0.44
1:A:256:VAL:HG21	1:B:181:GLN:HE21	1.83	0.44
1:C:359:TRP:CH2	2:C:450:ZFB:C18	3.00	0.44
1:A:307:ARG:HG2	1:A:387:ASN:HB2	1.99	0.44
1:D:39:LYS:HE2	3:D:488:HOH:O	2.18	0.44
1:A:96:ARG:HG2	1:A:136:THR:O	2.18	0.44
1:B:115:GLU:HB3	2:B:450:ZFB:C12	2.48	0.43
1:C:115:GLU:HB3	2:C:450:ZFB:C12	2.48	0.43
1:D:125:VAL:C	1:D:127:GLN:N	2.71	0.43
1:D:249:TYR:CD2	1:D:253:GLU:HG2	2.52	0.43
1:D:300:GLN:N	3:D:451:HOH:O	2.45	0.43
1:D:39:LYS:HD2	3:D:568:HOH:O	2.17	0.43
1:B:235:ILE:HA	1:B:238:ARG:HG3	2.00	0.43
1:D:290:ARG:HG3	1:D:290:ARG:HH21	1.83	0.43
1:B:355:VAL:CG1	1:B:356:ASN:N	2.81	0.43
1:B:124:TYR:O	1:B:128:ILE:HG13	2.17	0.43
1:C:80:VAL:HG13	1:C:90:ILE:HG12	2.00	0.43
1:A:243:ASN:HD22	1:A:243:ASN:HA	1.48	0.43
1:A:206:TYR:CG	1:A:207:PRO:HA	2.52	0.43
1:D:125:VAL:HG12	1:D:129:LYS:HE3	2.01	0.43
1:B:123:SER:O	1:B:124:TYR:C	2.56	0.43
1:D:307:ARG:HG2	1:D:387:ASN:HB2	2.00	0.43
1:B:281:GLY:HA2	3:B:454:HOH:O	2.18	0.43
1:B:131:ASN:O	1:B:134:LEU:CD2	2.66	0.43
1:D:88:PHE:CE2	1:D:104:SER:HB3	2.53	0.43
1:C:76:SER:HB2	1:C:79:TYR:CE2	2.53	0.43
1:D:64:LEU:HB3	1:D:81:TYR:HB3	2.01	0.43
1:A:126:GLU:HG3	1:A:126:GLU:O	2.19	0.43
1:B:246:LEU:HD12	1:B:249:TYR:CE2	2.53	0.43
1:A:123:SER:O	1:A:124:TYR:C	2.56	0.43
1:A:165:PRO:CA	1:A:168:LEU:HD22	2.48	0.43
1:A:88:PHE:CG	1:A:109:PHE:HB2	2.53	0.43
1:C:388:GLY:C	1:C:389:TYR:CD1	2.92	0.43
1:A:165:PRO:O	1:A:168:LEU:HB2	2.18	0.43
1:B:88:PHE:CE2	1:B:104:SER:HB3	2.54	0.43
1:B:259:MET:HA	1:B:259:MET:HE2	2.00	0.43
1:A:211:LEU:HD12	1:A:297:GLY:HA2	2.00	0.43
1:A:95:LYS:HD3	3:A:606:HOH:O	2.18	0.43
1:B:246:LEU:HD21	1:B:257:GLN:HG2	2.01	0.43
1:D:372:LEU:HD21	1:D:385:GLY:CA	2.49	0.43
1:D:31:PHE:O	1:D:95:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:LYS:NZ	1:C:370:ASP:OD2	2.46	0.43
1:A:216:TYR:CD2	1:A:270:ILE:HG23	2.54	0.43
1:C:181:GLN:HG2	3:C:521:HOH:O	2.18	0.43
1:D:126:GLU:HG3	1:D:126:GLU:O	2.19	0.43
1:D:101:LEU:HD11	1:D:128:ILE:HD11	2.00	0.42
1:B:241:ASN:OD1	1:B:241:ASN:C	2.57	0.42
1:C:216:TYR:HE2	1:C:270:ILE:HG12	1.84	0.42
1:B:315:TRP:O	1:B:318:GLN:HB2	2.19	0.42
1:B:121:MET:O	1:B:125:VAL:HG23	2.18	0.42
1:B:137:THR:CG2	1:B:138:TYR:H	2.32	0.42
1:C:359:TRP:CH2	2:C:450:ZFB:H18	2.54	0.42
1:A:42:ALA:O	1:A:45:PHE:HB3	2.19	0.42
1:D:362:VAL:O	1:D:363:SER:HB2	2.19	0.42
1:D:88:PHE:CG	1:D:109:PHE:HB2	2.54	0.42
1:A:362:VAL:O	1:A:363:SER:HB2	2.20	0.42
1:C:88:PHE:CE2	1:C:104:SER:HB3	2.55	0.42
1:B:67:VAL:HG22	1:B:82:ASN:HD22	1.83	0.42
1:D:334:VAL:HG13	3:D:539:HOH:O	2.18	0.42
1:D:362:VAL:HG13	1:D:362:VAL:O	2.19	0.42
1:C:96:ARG:NH1	1:C:132:LYS:O	2.53	0.42
1:A:277:GLY:C	1:A:279:SER:N	2.71	0.42
1:A:125:VAL:C	1:A:127:GLN:N	2.72	0.42
1:C:241:ASN:C	1:C:241:ASN:OD1	2.57	0.42
1:C:307:ARG:HG2	1:C:387:ASN:HB2	2.01	0.42
1:A:334:VAL:HB	1:A:389:TYR:HB2	2.02	0.42
1:D:254:SER:O	1:D:258:LYS:HG3	2.19	0.42
1:A:350:ARG:O	1:A:351:ASN:HB2	2.19	0.42
1:B:334:VAL:HG23	1:B:389:TYR:O	2.19	0.42
1:D:168:LEU:HA	1:D:168:LEU:HD12	1.81	0.42
1:C:101:LEU:HD11	1:C:128:ILE:HD11	2.02	0.42
1:C:216:TYR:CE2	1:C:270:ILE:HG23	2.55	0.42
1:B:76:SER:HB2	1:B:79:TYR:CZ	2.55	0.42
1:B:125:VAL:HG12	1:B:129:LYS:HE3	2.01	0.42
1:B:372:LEU:HD21	1:B:385:GLY:CA	2.50	0.42
1:B:238:ARG:HD2	1:B:240:TYR:CE2	2.55	0.42
1:A:359:TRP:CH2	2:A:450:ZFB:C18	3.03	0.42
1:A:69:LEU:HB2	1:A:73:LEU:HB2	2.00	0.42
1:D:224:TYR:CE2	1:D:278:PRO:CD	3.03	0.42
1:D:33:ARG:NH2	1:D:99:GLU:HG3	2.34	0.42
1:B:34:ASN:O	1:B:37:GLU:N	2.53	0.42
1:A:359:TRP:CH2	2:A:450:ZFB:H18	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:TYR:O	1:D:262:SER:HA	2.20	0.41
1:D:183:PHE:O	1:D:186:GLN:HB2	2.20	0.41
1:D:193:VAL:HG13	3:D:541:HOH:O	2.20	0.41
1:B:277:GLY:O	1:B:278:PRO:C	2.59	0.41
1:B:249:TYR:CD2	1:B:253:GLU:HG2	2.55	0.41
1:B:125:VAL:C	1:B:127:GLN:N	2.74	0.41
1:B:165:PRO:HA	1:B:168:LEU:HD22	2.02	0.41
1:B:340:HIS:HA	2:B:450:ZFB:O1	2.20	0.41
1:C:42:ALA:O	1:C:46:ILE:HG13	2.20	0.41
1:A:165:PRO:HB2	1:A:168:LEU:HD22	2.02	0.41
1:A:318:GLN:HE21	1:A:318:GLN:HB3	1.70	0.41
1:D:78:MET:HE2	1:D:78:MET:HB3	1.89	0.41
1:D:359:TRP:CH2	2:D:450:ZFB:C18	3.03	0.41
1:C:336:LYS:C	1:C:338:GLY:H	2.24	0.41
1:C:165:PRO:HA	1:C:168:LEU:HD22	2.03	0.41
1:A:70:GLY:O	1:A:74:SER:N	2.54	0.41
1:D:284:GLY:O	1:D:285:SER:C	2.59	0.41
1:D:73:LEU:HD21	1:D:122:GLU:N	2.36	0.41
1:A:115:GLU:HB3	2:A:450:ZFB:HN1	1.86	0.41
1:D:110:ASP:OD1	1:D:114:LYS:NZ	2.51	0.41
1:D:165:PRO:HA	1:D:168:LEU:HD22	2.02	0.41
1:C:307:ARG:HB3	1:C:387:ASN:HD22	1.85	0.41
1:A:157:GLY:O	1:A:247:PRO:HB2	2.20	0.41
1:D:269:GLY:O	1:D:274:MET:HB2	2.21	0.41
1:A:311:SER:O	1:A:312:LYS:C	2.60	0.41
1:A:388:GLY:C	1:A:389:TYR:CD1	2.95	0.41
1:A:388:GLY:C	1:A:389:TYR:HD1	2.24	0.41
1:D:134:LEU:N	1:D:134:LEU:HD13	2.35	0.41
1:D:127:GLN:CG	1:D:372:LEU:HD13	2.32	0.40
1:C:246:LEU:CD1	1:C:257:GLN:HG2	2.43	0.40
1:A:224:TYR:CZ	1:A:278:PRO:CD	3.04	0.40
1:A:336:LYS:O	1:A:338:GLY:N	2.54	0.40
1:D:359:TRP:CH2	2:D:450:ZFB:H18	2.56	0.40
1:C:31:PHE:HE2	1:C:137:THR:OG1	2.02	0.40
1:D:305:ILE:HD12	1:D:315:TRP:CZ3	2.57	0.40
1:B:80:VAL:HG13	1:B:90:ILE:HG12	2.03	0.40
1:D:157:GLY:HA2	3:D:457:HOH:O	2.21	0.40
1:C:69:LEU:HB2	1:C:73:LEU:HB2	2.02	0.40
1:B:355:VAL:HG11	1:B:357:TRP:CE2	2.57	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	331/368 (90%)	306 (92%)	20 (6%)	5 (2%)	13	50
1	B	331/368 (90%)	301 (91%)	24 (7%)	6 (2%)	11	45
1	C	331/368 (90%)	300 (91%)	25 (8%)	6 (2%)	11	45
1	D	331/368 (90%)	300 (91%)	25 (8%)	6 (2%)	11	45
All	All	1324/1472 (90%)	1207 (91%)	94 (7%)	23 (2%)	11	46

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	337	VAL
1	B	35	GLU
1	B	337	VAL
1	C	35	GLU
1	D	35	GLU
1	D	337	VAL
1	A	71	GLY
1	B	71	GLY
1	B	95	LYS
1	C	71	GLY
1	C	127	GLN
1	C	337	VAL
1	D	71	GLY
1	A	95	LYS
1	A	127	GLN
1	B	127	GLN
1	B	242	TRP
1	C	242	TRP
1	D	95	LYS
1	C	285	SER
1	D	127	GLN
1	D	151	SER

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	272/297 (92%)	259 (95%)	13 (5%)	31	71
1	B	272/297 (92%)	259 (95%)	13 (5%)	31	71
1	C	272/297 (92%)	260 (96%)	12 (4%)	35	74
1	D	272/297 (92%)	260 (96%)	12 (4%)	35	74
All	All	1088/1188 (92%)	1038 (95%)	50 (5%)	33	73

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	PHE
1	A	65	ASP
1	A	69	LEU
1	A	124	TYR
1	A	134	LEU
1	A	147	PRO
1	A	168	LEU
1	A	193	VAL
1	A	211	LEU
1	A	332	GLN
1	A	336	LYS
1	A	372	LEU
1	A	389	TYR
1	B	31	PHE
1	B	65	ASP
1	B	69	LEU
1	B	124	TYR
1	B	134	LEU
1	B	168	LEU
1	B	193	VAL
1	B	211	LEU
1	B	259	MET
1	B	273	ASP
1	B	332	GLN

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Mol	Chain	Res	Type
1	B	336	LYS
1	B	372	LEU
1	C	31	PHE
1	C	65	ASP
1	C	69	LEU
1	C	124	TYR
1	C	134	LEU
1	C	153	LEU
1	C	168	LEU
1	C	193	VAL
1	C	211	LEU
1	C	332	GLN
1	C	336	LYS
1	C	372	LEU
1	D	31	PHE
1	D	65	ASP
1	D	69	LEU
1	D	85	THR
1	D	124	TYR
1	D	134	LEU
1	D	168	LEU
1	D	193	VAL
1	D	211	LEU
1	D	259	MET
1	D	336	LYS
1	D	372	LEU

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

Mol	Chain	Res	Type
1	A	243	ASN
1	A	304	GLN
1	A	318	GLN
1	A	332	GLN
1	A	387	ASN
1	B	208	ASN
1	B	243	ASN
1	B	304	GLN
1	B	318	GLN
1	B	325	GLN
1	B	332	GLN
1	C	181	GLN

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Mol	Chain	Res	Type
1	C	243	ASN
1	C	304	GLN
1	C	318	GLN
1	C	325	GLN
1	C	332	GLN
1	D	208	ASN
1	D	243	ASN
1	D	304	GLN
1	D	318	GLN
1	D	332	GLN
1	D	387	ASN

5.3.3　RNA (i)

There are no RNA molecules in this entry.

5.4　Non-standard residues in protein, DNA, RNA chains (i)

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

5.5　Carbohydrates (i)

There are no carbohydrates in this entry.

5.6　Ligand geometry (i)

4 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	#$|Z| > 2$
2	ZFB	A	450	1	22,23,25	4.66	15 (68%)	25,29,31	2.98	7 (28%)
2	ZFB	B	450	1	22,23,25	4.73	17 (77%)	25,29,31	3.00	7 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z|$ > 2	Counts	RMSZ	#$|Z|$ > 2
2	ZFB	C	450	1	22,23,25	4.78	18 (81%)	25,29,31	2.98	8 (32%)
2	ZFB	D	450	1	22,23,25	4.64	16 (72%)	25,29,31	2.93	7 (28%)

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	ZFB	A	450	1	-	0/17/17/20	0/2/2/2
2	ZFB	B	450	1	-	0/17/17/20	0/2/2/2
2	ZFB	C	450	1	-	0/17/17/20	0/2/2/2
2	ZFB	D	450	1	-	0/17/17/20	0/2/2/2

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	450	ZFB	C12-C9	-11.45	1.25	1.54
2	C	450	ZFB	C12-C9	-11.34	1.25	1.54
2	B	450	ZFB	C12-C9	-10.67	1.27	1.54
2	D	450	ZFB	C12-C9	-10.65	1.27	1.54
2	A	450	ZFB	C2-C3	-6.17	1.36	1.50
2	B	450	ZFB	C11-C10	-6.05	1.32	1.49
2	D	450	ZFB	C2-C3	-5.90	1.36	1.50
2	D	450	ZFB	C11-C10	-5.88	1.32	1.49
2	C	450	ZFB	C2-C3	-5.84	1.36	1.50
2	A	450	ZFB	C11-C10	-5.83	1.32	1.49
2	B	450	ZFB	C2-C3	-5.76	1.37	1.50
2	C	450	ZFB	C11-C10	-4.89	1.35	1.49
2	B	450	ZFB	C9-N1	-4.08	1.36	1.45
2	C	450	ZFB	C9-N1	-4.06	1.36	1.45
2	D	450	ZFB	C1-N1	-3.26	1.25	1.34
2	A	450	ZFB	C9-N1	-3.19	1.38	1.45
2	D	450	ZFB	C9-N1	-2.91	1.39	1.45
2	A	450	ZFB	C1-N1	-2.58	1.27	1.34
2	C	450	ZFB	C1-N1	-2.57	1.27	1.34
2	B	450	ZFB	C1-N1	-2.54	1.27	1.34
2	C	450	ZFB	C12-C13	-2.10	1.46	1.51
2	B	450	ZFB	C12-C13	-2.08	1.46	1.51
2	B	450	ZFB	C17-C18	2.06	1.43	1.38
2	A	450	ZFB	C17-C18	2.07	1.43	1.38
2	A	450	ZFB	C4-C3	2.08	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	450	ZFB	C18-C13	2.19	1.43	1.38
2	C	450	ZFB	C16-C15	2.21	1.43	1.38
2	B	450	ZFB	C16-C15	2.21	1.43	1.38
2	D	450	ZFB	C4-C3	2.23	1.43	1.38
2	D	450	ZFB	C17-C18	2.26	1.43	1.38
2	D	450	ZFB	C17-C16	2.28	1.43	1.38
2	C	450	ZFB	C4-C3	2.30	1.43	1.38
2	B	450	ZFB	C17-C16	2.37	1.44	1.38
2	C	450	ZFB	C18-C13	2.45	1.44	1.38
2	C	450	ZFB	C17-C16	2.46	1.44	1.38
2	D	450	ZFB	C18-C13	2.65	1.44	1.38
2	D	450	ZFB	O2-C2	2.69	1.51	1.45
2	C	450	ZFB	C17-C18	2.69	1.44	1.38
2	B	450	ZFB	C18-C13	2.73	1.44	1.38
2	B	450	ZFB	C7-C6	2.76	1.45	1.38
2	A	450	ZFB	C7-C6	2.80	1.45	1.38
2	D	450	ZFB	C7-C6	2.87	1.45	1.38
2	A	450	ZFB	O2-C2	2.90	1.52	1.45
2	C	450	ZFB	C7-C6	2.91	1.45	1.38
2	C	450	ZFB	O2-C2	3.11	1.52	1.45
2	B	450	ZFB	O2-C2	3.55	1.53	1.45
2	A	450	ZFB	C14-C13	3.60	1.46	1.38
2	D	450	ZFB	C14-C13	4.20	1.47	1.38
2	C	450	ZFB	C14-C13	4.43	1.48	1.38
2	B	450	ZFB	C14-C13	4.69	1.48	1.38
2	C	450	ZFB	C6-C5	4.80	1.50	1.38
2	B	450	ZFB	C6-C5	4.89	1.50	1.38
2	D	450	ZFB	C6-C5	4.96	1.50	1.38
2	A	450	ZFB	C6-C5	5.03	1.50	1.38
2	B	450	ZFB	C7-C8	5.81	1.50	1.38
2	C	450	ZFB	C7-C8	6.05	1.51	1.38
2	B	450	ZFB	C5-C4	6.06	1.51	1.38
2	D	450	ZFB	C5-C4	6.10	1.51	1.38
2	D	450	ZFB	C7-C8	6.17	1.51	1.38
2	A	450	ZFB	C5-C4	6.25	1.51	1.38
2	A	450	ZFB	C7-C8	6.32	1.51	1.38
2	C	450	ZFB	C5-C4	6.43	1.52	1.38
2	A	450	ZFB	O2-C1	10.02	1.55	1.35
2	D	450	ZFB	O2-C1	10.25	1.56	1.35
2	C	450	ZFB	O2-C1	10.83	1.57	1.35
2	B	450	ZFB	O2-C1	10.89	1.57	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	450	ZFB	C12-C9-N1	-5.12	100.09	110.80
2	A	450	ZFB	C12-C9-N1	-5.03	100.27	110.80
2	C	450	ZFB	C12-C9-N1	-5.01	100.32	110.80
2	D	450	ZFB	C12-C9-N1	-4.76	100.84	110.80
2	D	450	ZFB	O1-C1-N1	-2.49	120.51	124.86
2	C	450	ZFB	O1-C1-N1	-2.27	120.90	124.86
2	C	450	ZFB	O2-C1-O1	-2.18	119.73	124.22
2	A	450	ZFB	O2-C1-O1	-2.05	120.01	124.22
2	B	450	ZFB	O1-C1-N1	-2.02	121.34	124.86
2	A	450	ZFB	C7-C8-C3	2.41	124.47	120.65
2	C	450	ZFB	C7-C8-C3	2.44	124.52	120.65
2	D	450	ZFB	C7-C8-C3	2.44	124.53	120.65
2	B	450	ZFB	C7-C8-C3	2.55	124.69	120.65
2	A	450	ZFB	O2-C1-N1	3.27	117.79	110.54
2	B	450	ZFB	O2-C1-N1	3.43	118.14	110.54
2	D	450	ZFB	O2-C1-N1	3.44	118.17	110.54
2	C	450	ZFB	O2-C1-N1	3.88	119.15	110.54
2	C	450	ZFB	C13-C12-C9	6.41	132.05	113.41
2	D	450	ZFB	C13-C12-C9	6.46	132.19	113.41
2	B	450	ZFB	C13-C12-C9	6.56	132.47	113.41
2	A	450	ZFB	C13-C12-C9	6.81	133.22	113.41
2	C	450	ZFB	C2-O2-C1	7.09	132.80	115.91
2	D	450	ZFB	C2-O2-C1	7.17	133.00	115.91
2	B	450	ZFB	C2-O2-C1	7.18	133.03	115.91
2	A	450	ZFB	C2-O2-C1	7.21	133.09	115.91
2	A	450	ZFB	O2-C2-C3	7.54	128.32	109.36
2	D	450	ZFB	O2-C2-C3	7.61	128.50	109.36
2	C	450	ZFB	O2-C2-C3	7.66	128.65	109.36
2	B	450	ZFB	O2-C2-C3	7.74	128.83	109.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	450	ZFB	18	0
2	B	450	ZFB	16	0
2	C	450	ZFB	17	0
2	D	450	ZFB	17	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	339/368 (92%)	-0.13	7 (2%)	67	36	9, 17, 25, 29	0
1	B	339/368 (92%)	-0.20	2 (0%)	90	73	9, 17, 25, 29	0
1	C	339/368 (92%)	-0.23	1 (0%)	94	84	9, 17, 25, 29	0
1	D	339/368 (92%)	-0.15	6 (1%)	71	43	9, 17, 25, 29	0
All	All	1356/1472 (92%)	-0.18	16 (1%)	81	55	9, 17, 25, 29	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	387	ASN	6.1
1	A	387	ASN	5.4
1	D	385	GLY	5.0
1	A	386	PHE	4.5
1	A	385	GLY	4.3
1	D	386	PHE	3.9
1	B	385	GLY	2.8
1	A	388	GLY	2.7
1	A	336	LYS	2.6
1	C	385	GLY	2.6
1	D	47	GLN	2.5
1	A	43	ILE	2.4
1	D	388	GLY	2.3
1	D	137	THR	2.2
1	A	65	ASP	2.2
1	B	147	PRO	2.0

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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ZFB	C	450	22/24	0.75	0.43	8.46	23,28,31,31	0
2	ZFB	B	450	22/24	0.76	0.42	6.49	23,28,31,31	0
2	ZFB	D	450	22/24	0.82	0.40	5.21	23,28,31,31	0
2	ZFB	A	450	22/24	0.75	0.50	4.96	23,28,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.