Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:02 AM GMT

PDB ID	:	2ZA5
Title	:	Crystal Structure of human tryptase with potent non-peptide inhibitor
Authors	:	Spurlino, J.C.; Barnakov, S.A.; Lewandowski, F.; Milligan, C.
Deposited on	:	2007-10-02
Resolution	:	2.30 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 (i)) were used in the production of this report:

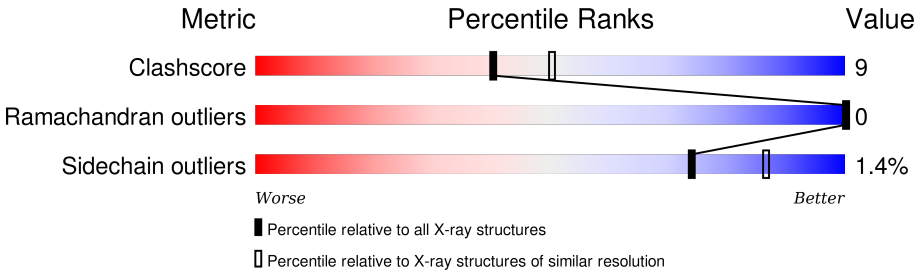
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	245	83% 16%
1	B	245	83% 16%
1	C	245	80% 18%
1	D	245	82% 16%

2 Entry composition

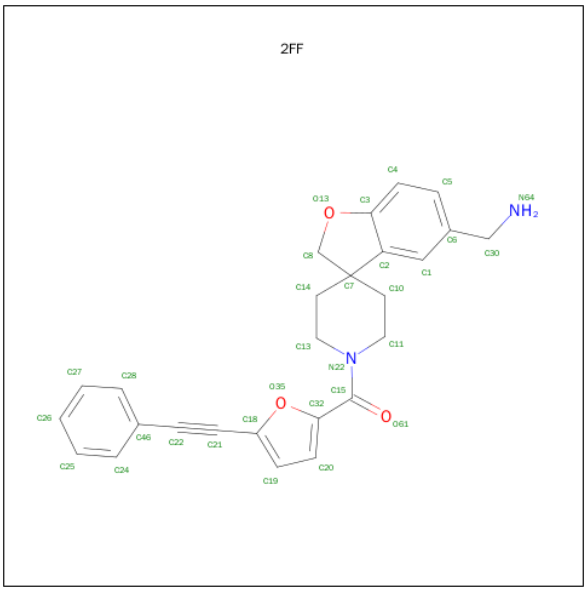
There are 3 unique types of molecules in this entry. The entry contains 8202 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tryptase beta 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	1
			1912	1224	337	339	12			
1	B	243	Total	C	N	O	S	0	0	1
			1912	1224	337	339	12			
1	C	243	Total	C	N	O	S	0	0	1
			1912	1224	337	339	12			
1	D	243	Total	C	N	O	S	0	0	1
			1911	1224	336	339	12			

- Molecule 2 is (5-(AMINOMETHYL)-2H-SPIRO[BENZOFURAN-3,4'-PIPERIDINE]-1'-YL)(5-(PHENYLETHYNYL)FURAN-2-YL)METHANONE (three-letter code: 2FF) (formula: $C_{26}H_{24}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	26	2	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			31	26	2	3		
2	C	1	Total	C	N	O	0	0
			31	26	2	3		
2	D	1	Total	C	N	O	0	0
			31	26	2	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	93	Total	O	0	0
			93	93		
3	B	108	Total	O	0	0
			108	108		
3	C	108	Total	O	0	0
			108	108		
3	D	122	Total	O	0	0
			122	122		

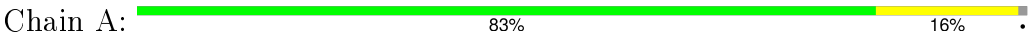
3 Residue-property plots (i)

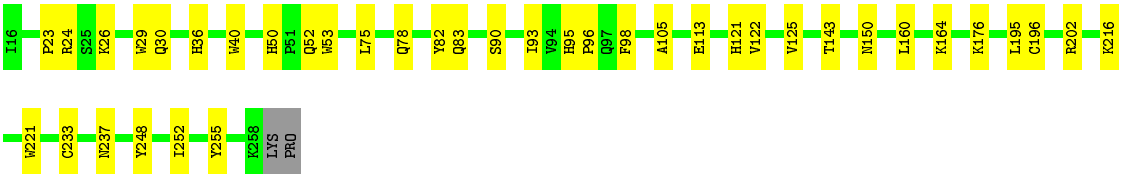
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: Tryptase beta 2

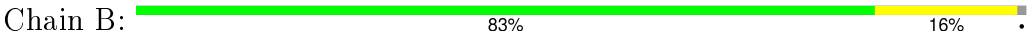
Chain A:

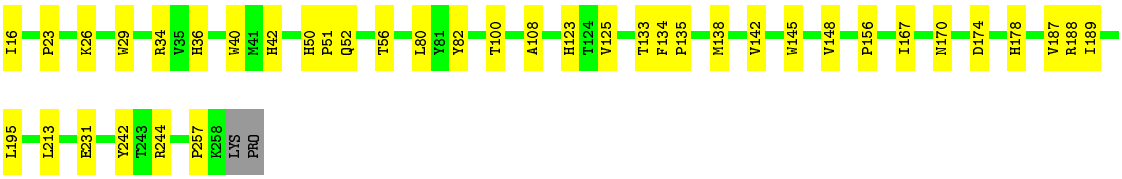




- Molecule 1: Tryptase beta 2

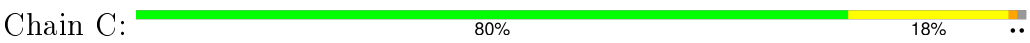
Chain B:

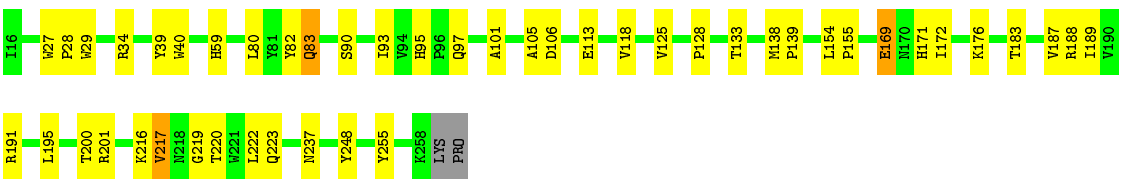




- Molecule 1: Tryptase beta 2

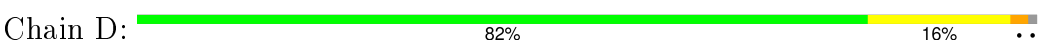
Chain C:

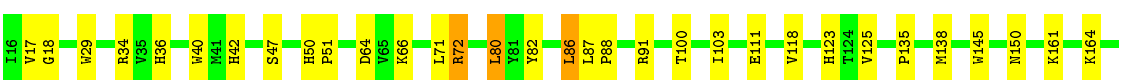




- Molecule 1: Tryptase beta 2

Chain D:






K176
Y177
H178
L179
R202
P212
Y227
C233
P239
Y242
H253
K258
LYS
PRO

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	82.68Å 82.68Å 170.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.30	Depositor
% Data completeness (in resolution range)	97.9 (19.91-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX	Depositor
R, R_{free}	0.181 , 0.233	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8202	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2FF

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	0.42	0/1977	0.59	0/2711
1	B	0.44	0/1977	0.60	0/2711
1	C	0.44	0/1977	0.60	0/2711
1	D	0.44	0/1975	0.61	1/2707 (0.0%)
All	All	0.43	0/7906	0.60	1/10840 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	80	LEU	CA-CB-CG	5.86	128.78	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1912	0	1842	27	0
1	B	1912	0	1842	33	0
1	C	1912	0	1842	38	0
1	D	1911	0	1839	35	0
2	A	31	0	24	0	0
2	B	31	0	24	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	0	24	2	0
2	D	31	0	24	1	0
3	A	93	0	0	1	0
3	B	108	0	0	5	0
3	C	108	0	0	4	0
3	D	122	0	0	3	0
All	All	8202	0	7461	132	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 9.

All (132) 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:108:ALA:HB3	3:B:335:HOH:O	1.55	1.07
1:B:56:THR:HG23	3:B:335:HOH:O	1.60	1.00
1:C:217:VAL:HG13	1:C:222:LEU:HD23	1.44	0.99
1:A:150:ASN:HD21	1:A:233:CYS:H	1.13	0.90
1:C:101:ALA:HA	3:C:341:HOH:O	1.74	0.87
1:D:17:VAL:C	1:D:18:GLY:CA	2.44	0.86
1:C:106:ASP:HB2	3:C:341:HOH:O	1.76	0.85
1:D:150:ASN:HD21	1:D:233:CYS:H	1.29	0.81
1:B:50:HIS:HD2	1:B:52:GLN:H	1.32	0.76
1:B:123:HIS:HB2	3:B:270:HOH:O	1.87	0.74
1:D:176:LYS:HA	1:D:179:LEU:HD22	1.68	0.74
1:D:135:PRO:HD2	1:D:138:MET:SD	2.30	0.72
1:B:174:ASP:O	1:B:178:HIS:HD2	1.74	0.70
1:B:50:HIS:CD2	1:B:52:GLN:H	2.09	0.70
1:A:150:ASN:HD21	1:A:233:CYS:N	1.89	0.69
1:D:118:VAL:HG13	1:D:123:HIS:HB3	1.73	0.69
1:C:95:HIS:HD2	1:C:97:GLN:H	1.39	0.68
1:D:72:ARG:HG3	1:D:86:LEU:HB3	1.76	0.67
1:D:72:ARG:CG	1:D:86:LEU:HB3	2.25	0.67
1:C:138:MET:HG3	1:C:139:PRO:HD2	1.78	0.66
1:A:36:HIS:HB2	1:A:40:TRP:CH2	2.31	0.66
1:D:123:HIS:HB2	3:D:290:HOH:O	1.97	0.65
1:D:253:HIS:CD2	3:D:314:HOH:O	2.52	0.63
1:C:217:VAL:HG13	1:C:222:LEU:CD2	2.26	0.62
1:B:142:VAL:HG21	1:B:242:TYR:OH	2.00	0.61
1:C:59:HIS:HD2	1:C:106:ASP:OD2	1.84	0.61
1:C:138:MET:HG3	1:C:139:PRO:CD	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:THR:HG23	1:D:103:ILE:H	1.65	0.60
2:B:1:2FF:C20	2:B:1:2FF:H111	2.32	0.60
1:A:50:HIS:CD2	1:A:52:GLN:H	2.19	0.60
1:B:50:HIS:CE1	1:B:257:PRO:HG2	2.37	0.59
1:B:189:ILE:HD13	2:B:1:2FF:H25	1.83	0.59
1:A:176:LYS:HE2	1:A:237:ASN:HA	1.86	0.57
1:C:95:HIS:CD2	1:C:97:GLN:H	2.22	0.56
1:D:100:THR:HG22	1:D:103:ILE:HD12	1.88	0.55
1:B:170:ASN:HD21	1:B:244:ARG:HH21	1.54	0.54
1:C:82:TYR:CD2	1:C:83:GLN:HB2	2.42	0.54
1:B:142:VAL:HG22	1:B:213:LEU:HD13	1.90	0.54
1:D:164:LYS:O	1:D:202:ARG:HD3	2.07	0.54
1:C:188:ARG:HG2	1:C:188:ARG:HH11	1.73	0.54
1:B:195:LEU:HD23	1:B:195:LEU:C	2.27	0.54
1:D:253:HIS:HD2	3:D:314:HOH:O	1.86	0.54
1:A:50:HIS:HD2	1:A:52:GLN:H	1.55	0.54
1:D:36:HIS:HB2	1:D:40:TRP:CH2	2.42	0.54
1:C:82:TYR:CE2	1:C:83:GLN:HB2	2.43	0.53
1:C:169:GLU:OE1	1:C:171:HIS:HB2	2.08	0.53
1:D:150:ASN:HD21	1:D:233:CYS:N	2.03	0.53
1:D:135:PRO:O	1:D:138:MET:HG3	2.08	0.53
1:D:64:ASP:O	1:D:66:LYS:HD2	2.09	0.53
1:B:29:TRP:CG	1:B:125:VAL:HB	2.43	0.53
1:D:29:TRP:CG	1:D:125:VAL:HB	2.45	0.52
1:D:177:TYR:CE1	1:D:239:PRO:HD2	2.44	0.52
1:C:220:THR:O	1:C:222:LEU:HD22	2.10	0.52
1:A:82:TYR:HB2	1:D:82:TYR:CE1	2.45	0.52
1:B:36:HIS:HB2	1:B:40:TRP:CH2	2.46	0.51
1:C:217:VAL:CG1	1:C:222:LEU:HD23	2.31	0.50
1:A:216:LYS:HE3	1:A:221:TRP:CE2	2.46	0.50
1:A:82:TYR:CD2	1:A:83:GLN:HB2	2.46	0.50
1:D:72:ARG:HG2	1:D:86:LEU:HB3	1.93	0.50
1:B:56:THR:C	3:B:335:HOH:O	2.51	0.49
1:D:50:HIS:CG	1:D:51:PRO:HD2	2.46	0.49
1:A:24:ARG:NH1	1:A:78:GLN:HG2	2.27	0.49
1:B:29:TRP:CD2	1:B:125:VAL:HB	2.48	0.48
1:C:27:TRP:N	1:C:28:PRO:CD	2.76	0.48
1:A:164:LYS:O	1:A:202:ARG:HD3	2.14	0.48
1:D:80:LEU:HG	1:D:145:TRP:CD1	2.49	0.48
1:A:29:TRP:CD2	1:A:125:VAL:HB	2.48	0.48
2:C:2:2FF:H111	2:C:2:2FF:C20	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:TYR:HE1	1:D:239:PRO:HD2	1.78	0.47
1:B:82:TYR:CE1	1:C:82:TYR:HB2	2.49	0.47
2:D:3:2FF:H111	2:D:3:2FF:C20	2.45	0.47
1:A:93:ILE:HD13	1:A:255:TYR:CD1	2.49	0.47
1:D:71:LEU:O	1:D:72:ARG:HD3	2.15	0.47
1:B:34:ARG:HD3	1:B:42:HIS:HA	1.98	0.46
1:C:138:MET:O	3:C:292:HOH:O	2.20	0.46
1:C:216:LYS:HE2	1:C:219:GLY:HA2	1.97	0.46
1:A:195:LEU:HD23	1:A:195:LEU:C	2.35	0.46
1:A:23:PRO:HG2	1:A:26:LYS:HE2	1.98	0.46
1:B:50:HIS:CG	1:B:51:PRO:HD2	2.52	0.45
1:A:75:LEU:HD13	1:A:122:VAL:HG11	1.97	0.45
1:A:30:GLN:NE2	1:A:143:THR:OG1	2.49	0.45
1:D:100:THR:CG2	1:D:103:ILE:HD12	2.46	0.45
1:B:231:GLU:OE1	2:B:1:2FF:H28	2.17	0.45
1:C:95:HIS:HE1	3:C:358:HOH:O	2.00	0.45
1:C:188:ARG:HH12	1:C:191:ARG:HA	1.81	0.45
1:B:134:PHE:O	1:B:167:ILE:HG21	2.17	0.45
1:D:227:VAL:HG22	1:D:242:TYR:CE2	2.53	0.44
1:C:201:ARG:CZ	1:C:201:ARG:HB2	2.47	0.44
1:C:189:ILE:HD13	2:C:2:2FF:H25	1.99	0.44
1:A:29:TRP:CG	1:A:125:VAL:HB	2.52	0.44
1:D:176:LYS:O	1:D:179:LEU:HB2	2.18	0.44
1:D:118:VAL:CG1	1:D:123:HIS:HB3	2.47	0.44
1:B:23:PRO:HD2	1:B:26:LYS:HE2	1.98	0.44
1:A:98:PHE:HB2	1:A:105:ALA:O	2.17	0.43
1:C:188:ARG:NH1	1:C:191:ARG:HA	2.33	0.43
1:B:135:PRO:HG2	1:B:138:MET:CE	2.48	0.43
1:D:47:SER:HB3	1:D:212:PRO:HG3	2.01	0.43
1:B:142:VAL:CG2	1:B:213:LEU:HD13	2.47	0.43
1:B:156:PRO:HG2	1:C:39:TYR:CE2	2.53	0.43
1:B:178:HIS:CE1	1:B:187:VAL:O	2.71	0.43
1:C:93:ILE:HD13	1:C:255:TYR:CD1	2.53	0.43
1:D:17:VAL:O	1:D:18:GLY:CA	2.66	0.43
1:B:80:LEU:HG	1:B:145:TRP:CD1	2.54	0.42
1:A:24:ARG:HH11	1:A:78:GLN:HG2	1.84	0.42
1:D:34:ARG:HD3	1:D:42:HIS:HA	2.00	0.42
1:B:188:ARG:NH1	3:B:288:HOH:O	2.51	0.42
1:A:78:GLN:NE2	3:A:341:HOH:O	2.53	0.42
1:A:50:HIS:CD2	1:A:53:TRP:HD1	2.37	0.42
1:A:248:TYR:O	1:A:252:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ALA:HA	1:C:248:TYR:OH	2.20	0.42
1:D:161:LYS:HB3	1:D:161:LYS:HE2	1.80	0.42
1:C:128:PRO:HD3	1:C:223:GLN:O	2.19	0.41
1:C:176:LYS:HE2	1:C:237:ASN:HD22	1.84	0.41
1:B:133:THR:CG2	1:B:133:THR:O	2.68	0.41
1:D:87:LEU:HA	1:D:88:PRO:HD2	1.95	0.41
1:C:154:LEU:HA	1:C:155:PRO:HD3	1.90	0.41
1:C:80:LEU:HA	1:C:80:LEU:HD12	1.93	0.41
1:B:82:TYR:CD1	1:C:82:TYR:HB2	2.56	0.41
1:B:189:ILE:HD13	2:B:1:2FF:C25	2.50	0.41
1:A:50:HIS:HB3	1:A:53:TRP:HB2	2.02	0.41
1:A:195:LEU:HD23	1:A:196:CYS:N	2.36	0.41
1:C:90:SER:HB3	1:C:113:GLU:OE2	2.20	0.41
1:A:95:HIS:HA	1:A:96:PRO:HD2	1.90	0.41
1:C:34:ARG:HD2	1:C:40:TRP:O	2.21	0.41
1:C:29:TRP:CG	1:C:125:VAL:HB	2.55	0.41
1:C:195:LEU:HD23	1:C:195:LEU:C	2.41	0.41
1:C:169:GLU:HG3	1:C:172:ILE:HG12	2.02	0.40
1:B:16:ILE:O	1:B:148:VAL:HA	2.21	0.40
1:B:174:ASP:O	1:B:178:HIS:CD2	2.64	0.40
1:C:183:THR:HG22	1:C:187:VAL:HB	2.03	0.40
1:A:90:SER:HB3	1:A:113:GLU:HG2	2.04	0.40
1:D:91:ARG:HB2	1:D:111:GLU:HB3	2.03	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	241/245 (98%)	230 (95%)	11 (5%)	0	100	100
1	B	241/245 (98%)	230 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	241/245 (98%)	225 (93%)	16 (7%)	0	100 100
1	D	239/245 (98%)	230 (96%)	9 (4%)	0	100 100
All	All	962/980 (98%)	915 (95%)	47 (5%)	0	100 100

There are no Ramachandran outliers to report.

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	207/210 (99%)	205 (99%)	2 (1%)	82 91
1	B	207/210 (99%)	206 (100%)	1 (0%)	92 97
1	C	207/210 (99%)	201 (97%)	6 (3%)	50 66
1	D	207/210 (99%)	204 (99%)	3 (1%)	74 86
All	All	828/840 (99%)	816 (99%)	12 (1%)	74 86

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	HIS
1	A	160	LEU
1	B	100	THR
1	C	83	GLN
1	C	118	VAL
1	C	133	THR
1	C	169	GLU
1	C	200	THR
1	C	217	VAL
1	D	72	ARG
1	D	86	LEU
1	D	179	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	50	HIS
1	A	52	GLN
1	A	85	GLN
1	A	123	HIS
1	A	150	ASN
1	A	171	HIS
1	A	218	ASN
1	A	223	GLN
1	B	50	HIS
1	B	52	GLN
1	B	85	GLN
1	B	170	ASN
1	B	178	HIS
1	C	30	GLN
1	C	59	HIS
1	C	83	GLN
1	C	95	HIS
1	C	170	ASN
1	C	218	ASN
1	C	223	GLN
1	C	237	ASN
1	C	254	HIS
1	D	30	GLN
1	D	52	GLN
1	D	150	ASN
1	D	237	ASN
1	D	253	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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	2FF	A	4	-	31,35,35	2.25	9 (29%)	31,50,50	2.18	6 (19%)
2	2FF	B	1	-	31,35,35	2.24	9 (29%)	31,50,50	2.09	6 (19%)
2	2FF	C	2	-	31,35,35	2.20	8 (25%)	31,50,50	2.09	8 (25%)
2	2FF	D	3	-	31,35,35	2.21	10 (32%)	31,50,50	2.09	6 (19%)

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	2FF	A	4	-	-	0/8/39/39	0/4/5/5
2	2FF	B	1	-	-	0/8/39/39	0/4/5/5
2	2FF	C	2	-	-	0/8/39/39	0/4/5/5
2	2FF	D	3	-	-	0/8/39/39	0/4/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	2FF	C8-C7	-2.55	1.51	1.54
2	D	3	2FF	O61-C15	-2.20	1.18	1.22
2	D	3	2FF	C8-C7	-2.04	1.51	1.54
2	A	4	2FF	O61-C15	-2.02	1.18	1.22
2	D	3	2FF	C1-C6	2.02	1.42	1.39
2	A	4	2FF	C5-C4	2.03	1.42	1.38
2	A	4	2FF	C1-C6	2.19	1.43	1.39
2	C	2	2FF	C1-C6	2.21	1.43	1.39
2	D	3	2FF	C5-C4	2.24	1.42	1.38
2	C	2	2FF	C5-C4	2.27	1.42	1.38
2	B	1	2FF	C5-C4	2.43	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	2FF	C1-C6	2.44	1.43	1.39
2	B	1	2FF	C46-C22	2.47	1.50	1.44
2	C	2	2FF	C46-C22	2.57	1.50	1.44
2	D	3	2FF	C46-C22	2.83	1.51	1.44
2	D	3	2FF	C5-C6	2.95	1.45	1.38
2	A	4	2FF	C46-C22	3.11	1.52	1.44
2	C	2	2FF	C5-C6	3.19	1.45	1.38
2	A	4	2FF	C5-C6	3.29	1.45	1.38
2	B	1	2FF	C5-C6	3.50	1.46	1.38
2	D	3	2FF	C15-N22	3.83	1.43	1.34
2	C	2	2FF	C15-N22	3.89	1.43	1.34
2	B	1	2FF	C18-C21	4.08	1.50	1.43
2	C	2	2FF	C18-C21	4.08	1.50	1.43
2	A	4	2FF	C15-N22	4.40	1.44	1.34
2	A	4	2FF	C18-C21	4.57	1.51	1.43
2	B	1	2FF	C15-N22	4.66	1.45	1.34
2	D	3	2FF	C18-C21	4.77	1.51	1.43
2	A	4	2FF	C3-C2	5.04	1.47	1.38
2	D	3	2FF	C3-C2	5.17	1.48	1.38
2	B	1	2FF	C3-C2	5.26	1.48	1.38
2	C	2	2FF	O13-C3	5.61	1.46	1.38
2	C	2	2FF	C3-C2	5.71	1.49	1.38
2	B	1	2FF	O13-C3	5.72	1.46	1.38
2	D	3	2FF	O13-C3	5.80	1.46	1.38
2	A	4	2FF	O13-C3	5.86	1.46	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3	2FF	O61-C15-N22	-2.97	117.70	122.42
2	A	4	2FF	C13-N22-C15	-2.67	114.48	122.80
2	D	3	2FF	C13-N22-C15	-2.61	114.64	122.80
2	C	2	2FF	C13-N22-C15	-2.60	114.69	122.80
2	C	2	2FF	C2-C1-C6	-2.47	117.78	122.32
2	B	1	2FF	C13-N22-C15	-2.35	115.47	122.80
2	C	2	2FF	C14-C13-N22	-2.31	105.87	111.11
2	A	4	2FF	C14-C13-N22	-2.02	106.53	111.11
2	C	2	2FF	C24-C46-C28	2.00	122.72	118.94
2	B	1	2FF	O13-C3-C4	2.02	131.17	127.96
2	D	3	2FF	O13-C8-C7	2.17	107.49	104.59
2	C	2	2FF	C8-C7-C2	2.45	104.39	101.51
2	C	2	2FF	C14-C7-C10	2.87	111.66	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	2FF	C8-C7-C2	2.88	104.89	101.51
2	A	4	2FF	C14-C7-C10	3.81	112.56	108.90
2	A	4	2FF	C8-C7-C2	4.05	106.26	101.51
2	D	3	2FF	C8-C7-C2	4.36	106.63	101.51
2	B	1	2FF	C14-C7-C10	4.49	113.20	108.90
2	D	3	2FF	C13-N22-C11	4.53	120.95	112.56
2	B	1	2FF	C13-N22-C11	4.58	121.06	112.56
2	A	4	2FF	C13-N22-C11	4.89	121.63	112.56
2	C	2	2FF	C13-N22-C11	5.14	122.10	112.56
2	C	2	2FF	C1-C2-C7	6.95	133.50	125.36
2	D	3	2FF	C1-C2-C7	7.27	133.89	125.36
2	B	1	2FF	C1-C2-C7	7.38	134.01	125.36
2	A	4	2FF	C1-C2-C7	7.40	134.04	125.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	2FF	4	0
2	C	2	2FF	2	0
2	D	3	2FF	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.