Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:53 AM GMT

PDB ID	:	2V8I
Title	:	STRUCTURE OF A FAMILY 2 PECTATE LYASE IN A NATIVE FORM
Authors	:	Abbott, D.W.; Boraston, A.B.
Deposited on	:	2007-08-08
Resolution	:	1.50 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:

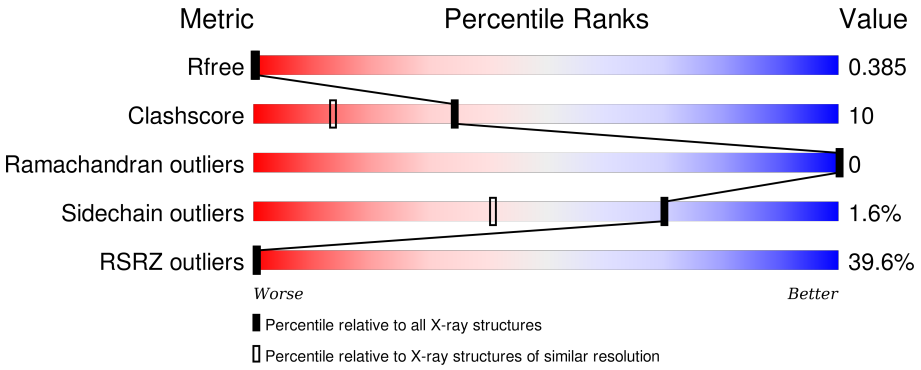
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.50 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	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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	543	40% 89% 11%

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	IOD	A	1547	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IOD	A	1549	-	-	X	X
2	IOD	A	1550	-	-	-	X
2	IOD	A	1552	-	-	X	-
2	IOD	A	1554	-	-	X	-
2	IOD	A	1555	-	-	X	X
2	IOD	A	1558	-	-	-	X
2	IOD	A	1560	-	-	X	-
2	IOD	A	1563	-	-	X	-
2	IOD	A	1564	-	-	X	X
2	IOD	A	1567	-	-	X	-
2	IOD	A	1568	-	-	X	X
2	IOD	A	1569	-	-	X	-
2	IOD	A	1572	-	-	X	-
2	IOD	A	1573	-	-	X	-
2	IOD	A	1574	-	-	-	X
2	IOD	A	1576	-	-	X	-
2	IOD	A	1588	-	-	X	-
2	IOD	A	1589	-	-	X	-
2	IOD	A	1592	-	-	X	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5172 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 PECTATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	543	4362	2766	756	827	13	0	5	0

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	I		
2	A	51	51	51	0	0

- Molecule 3 is water.

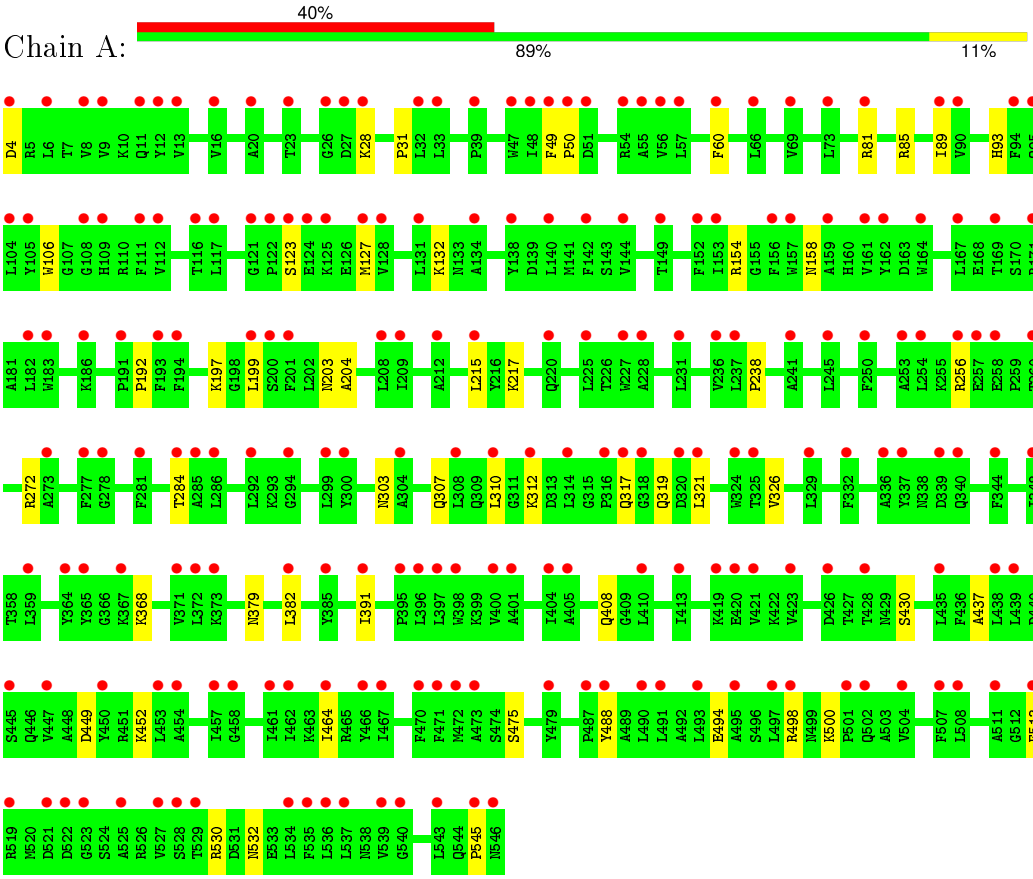
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	759	759	759	0	0

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: PECTATE LYASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.49Å 95.64Å 126.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.59 – 1.50 19.31 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.59-1.50) 97.4 (19.31-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.243 0.381 , 0.385	Depositor DCC
R_{free} test set	5569 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 111165 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	5172	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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: IOD

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	0.49	0/4477	0.59	0/6061

There are no bond length outliers.

There are no bond angle outliers.

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	4362	0	4224	56	0
2	A	51	0	0	60	0
3	A	759	0	0	31	0
All	All	5172	0	4224	86	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 10.

All (86) 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)
2:A:1555:IOD:I	3:A:2357:HOH:O	2.21	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1576:IOD:I	3:A:2726:HOH:O	2.28	1.19
2:A:1565:IOD:I	2:A:1591:IOD:I	3.06	1.13
2:A:1588:IOD:I	3:A:2713:HOH:O	2.40	1.06
1:A:199:LEU:HB2	2:A:1555:IOD:I	2.33	0.99
1:A:199:LEU:N	2:A:1555:IOD:I	2.67	0.97
2:A:1549:IOD:I	2:A:1552:IOD:I	3.23	0.97
2:A:1552:IOD:I	3:A:2726:HOH:O	2.52	0.96
2:A:1587:IOD:I	3:A:2537:HOH:O	2.56	0.94
2:A:1572:IOD:I	3:A:2323:HOH:O	2.56	0.92
2:A:1558:IOD:I	3:A:2627:HOH:O	2.56	0.92
2:A:1552:IOD:I	2:A:1576:IOD:I	3.27	0.92
2:A:1563:IOD:I	3:A:2486:HOH:O	2.58	0.91
1:A:312:LYS:HE2	2:A:1563:IOD:I	2.41	0.90
2:A:1572:IOD:I	3:A:2107:HOH:O	2.61	0.88
2:A:1556:IOD:I	3:A:2652:HOH:O	2.61	0.88
1:A:81[B]:ARG:NH2	2:A:1569:IOD:I	2.75	0.88
2:A:1560:IOD:I	3:A:2041:HOH:O	2.61	0.87
2:A:1554:IOD:I	3:A:2290:HOH:O	2.62	0.86
1:A:317:GLN:HA	2:A:1568:IOD:I	2.46	0.85
2:A:1560:IOD:I	3:A:2333:HOH:O	2.62	0.85
1:A:49:PHE:HB3	1:A:50:PRO:HD2	1.59	0.84
2:A:1593:IOD:I	3:A:2556:HOH:O	2.65	0.84
1:A:197:LYS:HB2	1:A:256:ARG:HH22	1.45	0.81
2:A:1592:IOD:I	3:A:2494:HOH:O	2.68	0.81
2:A:1557:IOD:I	3:A:2519:HOH:O	2.69	0.80
1:A:199:LEU:CB	2:A:1555:IOD:I	3.01	0.79
2:A:1554:IOD:I	3:A:2315:HOH:O	2.72	0.78
2:A:1570:IOD:I	3:A:2247:HOH:O	2.74	0.75
2:A:1567:IOD:I	3:A:2742:HOH:O	2.73	0.75
1:A:4:ASP:N	2:A:1561:IOD:I	2.91	0.74
1:A:326:VAL:HG21	1:A:391:ILE:HD11	1.71	0.72
1:A:530:ARG:HD3	2:A:1567:IOD:I	2.60	0.72
1:A:174:GLU:OE2	2:A:1564:IOD:I	2.78	0.71
1:A:284:THR:HG21	3:A:2205:HOH:O	1.91	0.71
1:A:530:ARG:CD	2:A:1567:IOD:I	3.09	0.70
2:A:1560:IOD:I	3:A:2133:HOH:O	2.78	0.70
2:A:1574:IOD:I	3:A:2640:HOH:O	2.78	0.70
2:A:1564:IOD:I	3:A:2221:HOH:O	2.79	0.69
1:A:317:GLN:C	2:A:1568:IOD:I	3.02	0.68
1:A:379:ASN:HD21	1:A:408:GLN:HG3	1.61	0.65
1:A:215:LEU:HD21	2:A:1589:IOD:I	2.68	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:GLN:CA	2:A:1568:IOD:I	3.17	0.62
1:A:530:ARG:NH1	2:A:1567:IOD:I	2.95	0.61
1:A:530:ARG:HD2	2:A:1567:IOD:I	2.70	0.61
2:A:1589:IOD:I	3:A:2092:HOH:O	2.86	0.61
2:A:1592:IOD:I	3:A:2242:HOH:O	2.87	0.60
1:A:449:ASP:HA	1:A:452:LYS:HE3	1.85	0.58
1:A:500:LYS:HE3	2:A:1588:IOD:I	2.74	0.58
1:A:268:LYS:HB3	2:A:1580:IOD:I	2.74	0.58
1:A:430:SER:OG	1:A:464:ILE:HD11	2.04	0.58
1:A:192:PRO:HB3	1:A:238:PRO:HB3	1.86	0.57
1:A:49:PHE:CB	1:A:50:PRO:HD2	2.32	0.56
1:A:132:LYS:HG3	1:A:203:ASN:HB2	1.88	0.56
1:A:545:PRO:HA	2:A:1548:IOD:I	2.76	0.56
1:A:443:HIS:HD2	2:A:1547:IOD:I	2.58	0.55
1:A:123:SER:HA	3:A:2726:HOH:O	2.07	0.54
1:A:31:PRO:HG3	2:A:1573:IOD:I	2.78	0.54
1:A:89:ILE:O	1:A:93:HIS:HD2	1.91	0.54
2:A:1569:IOD:I	3:A:2136:HOH:O	2.89	0.53
1:A:530:ARG:HD2	2:A:1572:IOD:I	2.78	0.53
1:A:494:GLU:OE2	1:A:498:ARG:NE	2.41	0.53
1:A:199:LEU:CA	2:A:1555:IOD:I	3.26	0.52
2:A:1573:IOD:I	3:A:2018:HOH:O	2.89	0.52
1:A:197:LYS:HG3	1:A:256:ARG:HH12	1.75	0.52
1:A:379:ASN:ND2	1:A:408:GLN:HG3	2.25	0.52
1:A:310:LEU:HD23	1:A:321:LEU:HD21	1.93	0.50
1:A:154:ARG:HD3	2:A:1589:IOD:I	2.83	0.49
1:A:158:ASN:ND2	1:A:180:GLY:H	2.12	0.48
1:A:60:PHE:HB2	1:A:93:HIS:CE1	2.48	0.48
1:A:532:ASN:CG	2:A:1567:IOD:I	3.22	0.48
1:A:532:ASN:OD1	2:A:1567:IOD:I	3.02	0.47
1:A:49:PHE:HB3	1:A:50:PRO:CD	2.38	0.47
1:A:382:LEU:HG	1:A:437:ALA:HB1	1.96	0.46
1:A:85:ARG:NH1	2:A:1569:IOD:I	3.14	0.46
1:A:217:LYS:HB2	1:A:217:LYS:HE2	1.81	0.46
1:A:204:ALA:HB2	3:A:2228:HOH:O	2.16	0.45
1:A:317:GLN:O	2:A:1568:IOD:I	3.05	0.45
2:A:1551:IOD:I	3:A:2599:HOH:O	2.92	0.45
1:A:303:ASN:HD21	1:A:307:GLN:NE2	2.15	0.44
1:A:132:LYS:HE3	1:A:513:PHE:CE2	2.54	0.43
1:A:368:LYS:NZ	2:A:1553:IOD:I	3.18	0.42
1:A:123:SER:OG	2:A:1549:IOD:I	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LYS:CB	1:A:256:ARG:HH22	2.23	0.42
1:A:319:GLN:NE2	3:A:2497:HOH:O	2.53	0.40
1:A:443:HIS:CD2	2:A:1547:IOD:I	3.42	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	546/543 (101%)	537 (98%)	9 (2%)	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	454/449 (101%)	446 (98%)	8 (2%)	66 35

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	99	ASP
1	A	106	TRP

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Mol	Chain	Res	Type
1	A	127[A]	MET
1	A	127[B]	MET
1	A	272	ARG
1	A	475	SER
1	A	488	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	75	GLN
1	A	93	HIS
1	A	158	ASN
1	A	307	GLN
1	A	379	ASN
1	A	443	HIS
1	A	499	ASN

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

Of 51 ligands modelled in this entry, 51 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	543/543 (100%)	1.97	215 (39%)	0 0	11, 17, 29, 35	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	ASP	8.7
1	A	199	LEU	7.6
1	A	391	ILE	7.4
1	A	545	PRO	6.4
1	A	27	ASP	6.4
1	A	50	PRO	6.3
1	A	253	ALA	6.2
1	A	316	PRO	6.1
1	A	421	VAL	5.9
1	A	122	PRO	5.3
1	A	28	LYS	5.3
1	A	546	ASN	5.3
1	A	420	GLU	5.2
1	A	527	VAL	4.9
1	A	317	GLN	4.7
1	A	127[A]	MET	4.7
1	A	26	GLY	4.7
1	A	55	ALA	4.7
1	A	9	VAL	4.7
1	A	153	ILE	4.6
1	A	164	TRP	4.6
1	A	144	VAL	4.6
1	A	453	LEU	4.6
1	A	395	PRO	4.5
1	A	312	LYS	4.5
1	A	310	LEU	4.3
1	A	161	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	457	ILE	4.2
1	A	112	VAL	4.1
1	A	441	LEU	4.1
1	A	490	LEU	4.1
1	A	89	ILE	4.1
1	A	400	VAL	3.9
1	A	340	GLN	3.9
1	A	152	PHE	3.9
1	A	324	TRP	3.9
1	A	125	LYS	3.8
1	A	438	LEU	3.8
1	A	521	ASP	3.7
1	A	128	VAL	3.7
1	A	396	LEU	3.7
1	A	321	LEU	3.7
1	A	354	LEU	3.7
1	A	493	LEU	3.7
1	A	191	PRO	3.6
1	A	314	LEU	3.6
1	A	447	VAL	3.6
1	A	539	VAL	3.6
1	A	498	ARG	3.6
1	A	227	TRP	3.5
1	A	254	LEU	3.5
1	A	372	LEU	3.5
1	A	339[A]	ASP	3.5
1	A	439	LEU	3.5
1	A	48	ILE	3.5
1	A	47	TRP	3.4
1	A	336	ALA	3.4
1	A	257	GLU	3.4
1	A	308	LEU	3.4
1	A	4	ASP	3.4
1	A	461	ILE	3.3
1	A	534	LEU	3.3
1	A	320	ASP	3.3
1	A	450	TYR	3.3
1	A	69	VAL	3.3
1	A	404	ILE	3.3
1	A	413	ILE	3.3
1	A	294	GLY	3.2
1	A	471	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	49	PHE	3.2
1	A	397	LEU	3.2
1	A	157	TRP	3.2
1	A	193	PHE	3.1
1	A	273	ALA	3.1
1	A	171	ARG	3.1
1	A	32	LEU	3.1
1	A	140	LEU	3.1
1	A	162	TYR	3.1
1	A	256	ARG	3.1
1	A	236	VAL	3.1
1	A	212	ALA	3.1
1	A	220	GLN	3.1
1	A	241	ALA	3.1
1	A	134	ALA	3.0
1	A	13	VAL	3.0
1	A	103	LEU	3.0
1	A	215	LEU	3.0
1	A	258	GLU	3.0
1	A	183	TRP	3.0
1	A	245	LEU	3.0
1	A	348	ILE	3.0
1	A	462	ILE	3.0
1	A	382	LEU	3.0
1	A	398	TRP	3.0
1	A	90	VAL	3.0
1	A	329	LEU	2.9
1	A	537	LEU	2.9
1	A	405	ALA	2.9
1	A	518	TYR	2.9
1	A	131	LEU	2.9
1	A	16	VAL	2.9
1	A	300	TYR	2.9
1	A	373	LYS	2.9
1	A	325	THR	2.8
1	A	318	GLY	2.8
1	A	231	LEU	2.8
1	A	501	PRO	2.8
1	A	12	TYR	2.8
1	A	332	PHE	2.8
1	A	385	TYR	2.8
1	A	470	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	522	ASP	2.8
1	A	60	PHE	2.8
1	A	513	PHE	2.8
1	A	121	GLY	2.8
1	A	228	ALA	2.8
1	A	473	ALA	2.8
1	A	525	ALA	2.8
1	A	6	LEU	2.7
1	A	359	LEU	2.7
1	A	209	ILE	2.7
1	A	142	PHE	2.7
1	A	299	LEU	2.7
1	A	138	TYR	2.7
1	A	479	TYR	2.7
1	A	467	ILE	2.7
1	A	194	PHE	2.7
1	A	108	GLY	2.7
1	A	426	ASP	2.7
1	A	56	VAL	2.7
1	A	284	THR	2.7
1	A	8	VAL	2.7
1	A	454	ALA	2.7
1	A	292	LEU	2.7
1	A	410	LEU	2.7
1	A	435	LEU	2.7
1	A	536	LEU	2.7
1	A	286	LEU	2.6
1	A	508	LEU	2.6
1	A	186	LYS	2.6
1	A	529	THR	2.6
1	A	540	GLY	2.6
1	A	111	PHE	2.6
1	A	423	VAL	2.6
1	A	543	LEU	2.6
1	A	208	LEU	2.6
1	A	428	THR	2.6
1	A	491	LEU	2.6
1	A	23	THR	2.5
1	A	54	ARG	2.5
1	A	528	SER	2.5
1	A	73	LEU	2.5
1	A	497	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	519	ARG	2.5
1	A	401	ALA	2.5
1	A	33	LEU	2.5
1	A	514	THR	2.5
1	A	502	GLN	2.5
1	A	159	ALA	2.5
1	A	277	PHE	2.4
1	A	281	PHE	2.4
1	A	367	LYS	2.4
1	A	444	ALA	2.4
1	A	364	TYR	2.4
1	A	466	TYR	2.4
1	A	167	LEU	2.4
1	A	260	THR	2.4
1	A	117	LEU	2.4
1	A	156	PHE	2.4
1	A	344	PHE	2.4
1	A	535	PHE	2.4
1	A	487	PRO	2.4
1	A	472	MET	2.3
1	A	116	THR	2.3
1	A	182	LEU	2.3
1	A	94	PHE	2.3
1	A	250	PHE	2.3
1	A	337	TYR	2.3
1	A	488	TYR	2.3
1	A	95	GLN	2.3
1	A	169	THR	2.3
1	A	445	SER	2.3
1	A	419	LYS	2.3
1	A	507	PHE	2.3
1	A	523	GLY	2.3
1	A	357	TYR	2.2
1	A	442	TYR	2.2
1	A	495	ALA	2.2
1	A	511	ALA	2.2
1	A	371	VAL	2.2
1	A	149	THR	2.2
1	A	104	LEU	2.2
1	A	124	GLU	2.2
1	A	57	LEU	2.2
1	A	11	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	109	HIS	2.1
1	A	66	LEU	2.1
1	A	265	THR	2.1
1	A	200	SER	2.1
1	A	304	ALA	2.1
1	A	464	ILE	2.1
1	A	20	ALA	2.1
1	A	39	PRO	2.1
1	A	225	LEU	2.1
1	A	81[A]	ARG	2.1
1	A	201	PHE	2.1
1	A	105	TYR	2.1
1	A	504	VAL	2.1
1	A	285	ALA	2.0
1	A	278	GLY	2.0
1	A	365	TYR	2.0
1	A	237	LEU	2.0
1	A	458	GLY	2.0
1	A	517	ALA	2.0
1	A	123	SER	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, 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	IOD	A	1558	1/1	1.00	0.45	11.96	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	IOD	A	1592	1/1	0.99	0.34	7.69	4,4,4,4	0
2	IOD	A	1550	1/1	0.99	0.33	7.64	12,12,12,12	0
2	IOD	A	1564	1/1	0.94	0.57	5.84	18,18,18,18	0
2	IOD	A	1549	1/1	0.99	0.34	4.97	10,10,10,10	0
2	IOD	A	1555	1/1	0.96	0.50	3.70	19,19,19,19	0
2	IOD	A	1568	1/1	0.95	0.53	3.47	30,30,30,30	0
2	IOD	A	1574	1/1	0.99	0.28	3.43	6,6,6,6	0
2	IOD	A	1571	1/1	1.00	0.27	1.49	2,2,2,2	0
2	IOD	A	1548	1/1	0.97	0.25	0.12	13,13,13,13	1
2	IOD	A	1569	1/1	0.98	0.53	-	21,21,21,21	0
2	IOD	A	1573	1/1	0.98	0.55	-	22,22,22,22	0
2	IOD	A	1566	1/1	0.96	0.50	-	25,25,25,25	0
2	IOD	A	1584	1/1	0.99	0.35	-	7,7,7,7	0
2	IOD	A	1554	1/1	0.97	0.44	-	16,16,16,16	0
2	IOD	A	1581	1/1	0.97	0.54	-	25,25,25,25	0
2	IOD	A	1547	1/1	0.99	0.25	-	3,3,3,3	0
2	IOD	A	1559	1/1	0.99	0.45	-	21,21,21,21	0
2	IOD	A	1567	1/1	0.97	0.62	-	26,26,26,26	0
2	IOD	A	1578	1/1	0.99	0.49	-	20,20,20,20	0
2	IOD	A	1553	1/1	0.96	0.46	-	17,17,17,17	0
2	IOD	A	1596	1/1	0.99	0.34	-	12,12,12,12	0
2	IOD	A	1594	1/1	0.94	0.52	-	29,29,29,29	0
2	IOD	A	1565	1/1	0.99	0.42	-	19,19,19,19	0
2	IOD	A	1589	1/1	0.98	0.43	-	13,13,13,13	0
2	IOD	A	1597	1/1	0.98	0.38	-	13,13,13,13	1
2	IOD	A	1572	1/1	0.98	0.53	-	20,20,20,20	0
2	IOD	A	1551	1/1	0.99	0.42	-	12,12,12,12	0
2	IOD	A	1576	1/1	0.96	0.56	-	29,29,29,29	0
2	IOD	A	1562	1/1	0.98	0.51	-	18,18,18,18	0
2	IOD	A	1575	1/1	0.96	0.51	-	27,27,27,27	0
2	IOD	A	1583	1/1	0.99	0.35	-	11,11,11,11	0
2	IOD	A	1595	1/1	0.99	0.35	-	15,15,15,15	0
2	IOD	A	1557	1/1	0.99	0.36	-	14,14,14,14	0
2	IOD	A	1591	1/1	0.99	0.31	-	3,3,3,3	0
2	IOD	A	1570	1/1	0.97	0.44	-	24,24,24,24	0
2	IOD	A	1580	1/1	0.99	0.46	-	24,24,24,24	0
2	IOD	A	1585	1/1	0.93	0.47	-	26,26,26,26	0
2	IOD	A	1560	1/1	0.99	0.48	-	15,15,15,15	0
2	IOD	A	1556	1/1	0.98	0.41	-	16,16,16,16	0
2	IOD	A	1590	1/1	0.98	0.48	-	23,23,23,23	0
2	IOD	A	1577	1/1	0.98	0.40	-	14,14,14,14	0
2	IOD	A	1579	1/1	0.99	0.47	-	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	IOD	A	1593	1/1	0.97	0.49	-	19,19,19,19	0
2	IOD	A	1587	1/1	0.98	0.46	-	28,28,28,28	0
2	IOD	A	1582	1/1	0.99	0.27	-	5,5,5,5	0
2	IOD	A	1563	1/1	0.99	0.40	-	12,12,12,12	0
2	IOD	A	1586	1/1	0.97	0.43	-	21,21,21,21	0
2	IOD	A	1588	1/1	0.92	0.37	-	23,23,23,23	0
2	IOD	A	1552	1/1	0.99	0.46	-	18,18,18,18	0
2	IOD	A	1561	1/1	0.98	0.50	-	16,16,16,16	0

6.5 Other polymers

There are no such residues in this entry.