



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:16 pm GMT

PDB ID : 2XQ2  
Title : STRUCTURE OF THE K294A MUTANT OF VSGLT  
Authors : Watanabe, A.; Choe, S.; Chaptal, V.; Rosenberg, J.M.; Wright, E.M.; Grabe, M.; Abramson, J.  
Deposited on : 2010-09-01  
Resolution : 2.73 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

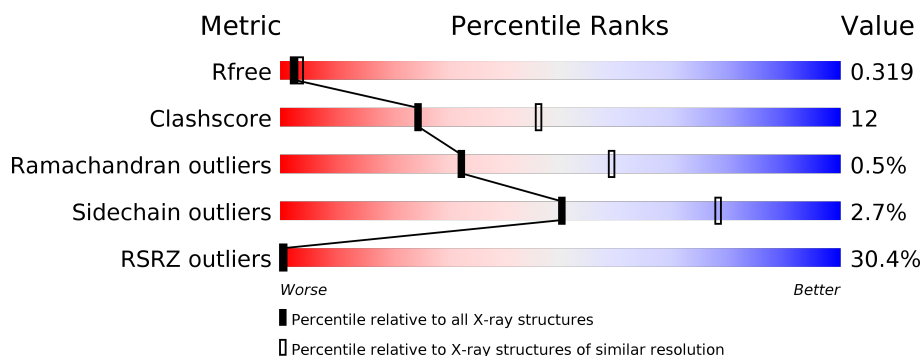
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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))
$R_{free}$	100719	3342 (2.78-2.70)
Clashscore	112137	3731 (2.78-2.70)
Ramachandran outliers	110173	3670 (2.78-2.70)
Sidechain outliers	110143	3671 (2.78-2.70)
RSRZ outliers	101464	3362 (2.78-2.70)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	593	
2	B	593	

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	PEG	A	1574	-	-	-	X
3	PEG	A	1575	-	-	-	X
3	PEG	A	1576	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8090 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 SODIUM/GLUCOSE COTRANSPORTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4107	2762	612	711	22			

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	ALA	LYS	ENGINEERED MUTATION	UNP P96169
A	411	ALA	CYS	ENGINEERED MUTATION	UNP P96169
A	423	CYS	ALA	ENGINEERED MUTATION	UNP P96169
A	544	VAL	-	EXPRESSION TAG	UNP P96169
A	545	ASN	-	EXPRESSION TAG	UNP P96169
A	546	ALA	-	EXPRESSION TAG	UNP P96169
A	547	ASP	-	EXPRESSION TAG	UNP P96169
A	548	ALA	-	EXPRESSION TAG	UNP P96169
A	549	GLU	-	EXPRESSION TAG	UNP P96169
A	550	ILE	-	EXPRESSION TAG	UNP P96169
A	551	THR	-	EXPRESSION TAG	UNP P96169
A	552	LEU	-	EXPRESSION TAG	UNP P96169
A	553	ILE	-	EXPRESSION TAG	UNP P96169
A	554	ILE	-	EXPRESSION TAG	UNP P96169
A	555	PHE	-	EXPRESSION TAG	UNP P96169
A	556	GLY	-	EXPRESSION TAG	UNP P96169
A	557	VAL	-	EXPRESSION TAG	UNP P96169
A	558	MET	-	EXPRESSION TAG	UNP P96169
A	559	ALA	-	EXPRESSION TAG	UNP P96169
A	560	GLY	-	EXPRESSION TAG	UNP P96169
A	561	VAL	-	EXPRESSION TAG	UNP P96169
A	562	ILE	-	EXPRESSION TAG	UNP P96169
A	563	GLY	-	EXPRESSION TAG	UNP P96169
A	564	THR	-	EXPRESSION TAG	UNP P96169
A	565	ILE	-	EXPRESSION TAG	UNP P96169
A	566	LEU	-	EXPRESSION TAG	UNP P96169
A	567	LEU	-	EXPRESSION TAG	UNP P96169

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	568	ILE	-	EXPRESSION TAG	UNP P96169
A	569	SER	-	EXPRESSION TAG	UNP P96169
A	570	TYR	-	EXPRESSION TAG	UNP P96169
A	571	GLY	-	EXPRESSION TAG	UNP P96169
A	572	ILE	-	EXPRESSION TAG	UNP P96169
A	573	LYS	-	EXPRESSION TAG	UNP P96169
A	574	LYS	-	EXPRESSION TAG	UNP P96169
A	575	LEU	-	EXPRESSION TAG	UNP P96169
A	576	ILE	-	EXPRESSION TAG	UNP P96169
A	577	LYS	-	EXPRESSION TAG	UNP P96169
A	578	ALA	-	EXPRESSION TAG	UNP P96169
A	579	SER	-	EXPRESSION TAG	UNP P96169
A	580	TYR	-	EXPRESSION TAG	UNP P96169
A	581	LYS	-	EXPRESSION TAG	UNP P96169
A	582	SER	-	EXPRESSION TAG	UNP P96169
A	583	GLY	-	EXPRESSION TAG	UNP P96169
A	584	GLY	-	EXPRESSION TAG	UNP P96169
A	585	SER	-	EXPRESSION TAG	UNP P96169
A	586	PRO	-	EXPRESSION TAG	UNP P96169
A	587	GLY	-	EXPRESSION TAG	UNP P96169
A	588	HIS	-	EXPRESSION TAG	UNP P96169
A	589	HIS	-	EXPRESSION TAG	UNP P96169
A	590	HIS	-	EXPRESSION TAG	UNP P96169
A	591	HIS	-	EXPRESSION TAG	UNP P96169
A	592	HIS	-	EXPRESSION TAG	UNP P96169
A	593	HIS	-	EXPRESSION TAG	UNP P96169

- Molecule 2 is a protein called SODIUM/GLUCOSE COTRANSPORTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			3957	2651	594	691	21			

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	294	ALA	LYS	ENGINEERED MUTATION	UNP P96169
B	411	ALA	CYS	ENGINEERED MUTATION	UNP P96169
B	423	CYS	ALA	ENGINEERED MUTATION	UNP P96169
B	544	VAL	-	EXPRESSION TAG	UNP P96169
B	545	ASN	-	EXPRESSION TAG	UNP P96169
B	546	ALA	-	EXPRESSION TAG	UNP P96169

*Continued on next page...*

*Continued from previous page...*

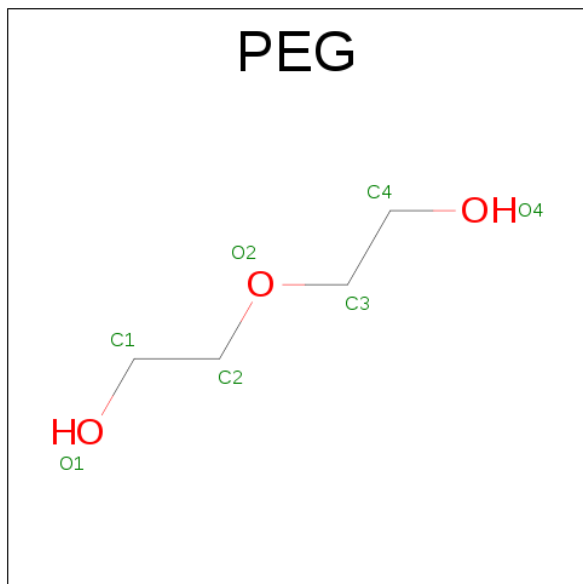
Chain	Residue	Modelled	Actual	Comment	Reference
B	547	ASP	-	EXPRESSION TAG	UNP P96169
B	548	ALA	-	EXPRESSION TAG	UNP P96169
B	549	GLU	-	EXPRESSION TAG	UNP P96169
B	550	ILE	-	EXPRESSION TAG	UNP P96169
B	551	THR	-	EXPRESSION TAG	UNP P96169
B	552	LEU	-	EXPRESSION TAG	UNP P96169
B	553	ILE	-	EXPRESSION TAG	UNP P96169
B	554	ILE	-	EXPRESSION TAG	UNP P96169
B	555	PHE	-	EXPRESSION TAG	UNP P96169
B	556	GLY	-	EXPRESSION TAG	UNP P96169
B	557	VAL	-	EXPRESSION TAG	UNP P96169
B	558	MET	-	EXPRESSION TAG	UNP P96169
B	559	ALA	-	EXPRESSION TAG	UNP P96169
B	560	GLY	-	EXPRESSION TAG	UNP P96169
B	561	VAL	-	EXPRESSION TAG	UNP P96169
B	562	ILE	-	EXPRESSION TAG	UNP P96169
B	563	GLY	-	EXPRESSION TAG	UNP P96169
B	564	THR	-	EXPRESSION TAG	UNP P96169
B	565	ILE	-	EXPRESSION TAG	UNP P96169
B	566	LEU	-	EXPRESSION TAG	UNP P96169
B	567	LEU	-	EXPRESSION TAG	UNP P96169
B	568	ILE	-	EXPRESSION TAG	UNP P96169
B	569	SER	-	EXPRESSION TAG	UNP P96169
B	570	TYR	-	EXPRESSION TAG	UNP P96169
B	571	GLY	-	EXPRESSION TAG	UNP P96169
B	572	ILE	-	EXPRESSION TAG	UNP P96169
B	573	LYS	-	EXPRESSION TAG	UNP P96169
B	574	LYS	-	EXPRESSION TAG	UNP P96169
B	575	LEU	-	EXPRESSION TAG	UNP P96169
B	576	ILE	-	EXPRESSION TAG	UNP P96169
B	577	LYS	-	EXPRESSION TAG	UNP P96169
B	578	ALA	-	EXPRESSION TAG	UNP P96169
B	579	SER	-	EXPRESSION TAG	UNP P96169
B	580	TYR	-	EXPRESSION TAG	UNP P96169
B	581	LYS	-	EXPRESSION TAG	UNP P96169
B	582	SER	-	EXPRESSION TAG	UNP P96169
B	583	GLY	-	EXPRESSION TAG	UNP P96169
B	584	GLY	-	EXPRESSION TAG	UNP P96169
B	585	SER	-	EXPRESSION TAG	UNP P96169
B	586	PRO	-	EXPRESSION TAG	UNP P96169
B	587	GLY	-	EXPRESSION TAG	UNP P96169
B	588	HIS	-	EXPRESSION TAG	UNP P96169

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	589	HIS	-	EXPRESSION TAG	UNP P96169
B	590	HIS	-	EXPRESSION TAG	UNP P96169
B	591	HIS	-	EXPRESSION TAG	UNP P96169
B	592	HIS	-	EXPRESSION TAG	UNP P96169
B	593	HIS	-	EXPRESSION TAG	UNP P96169

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0

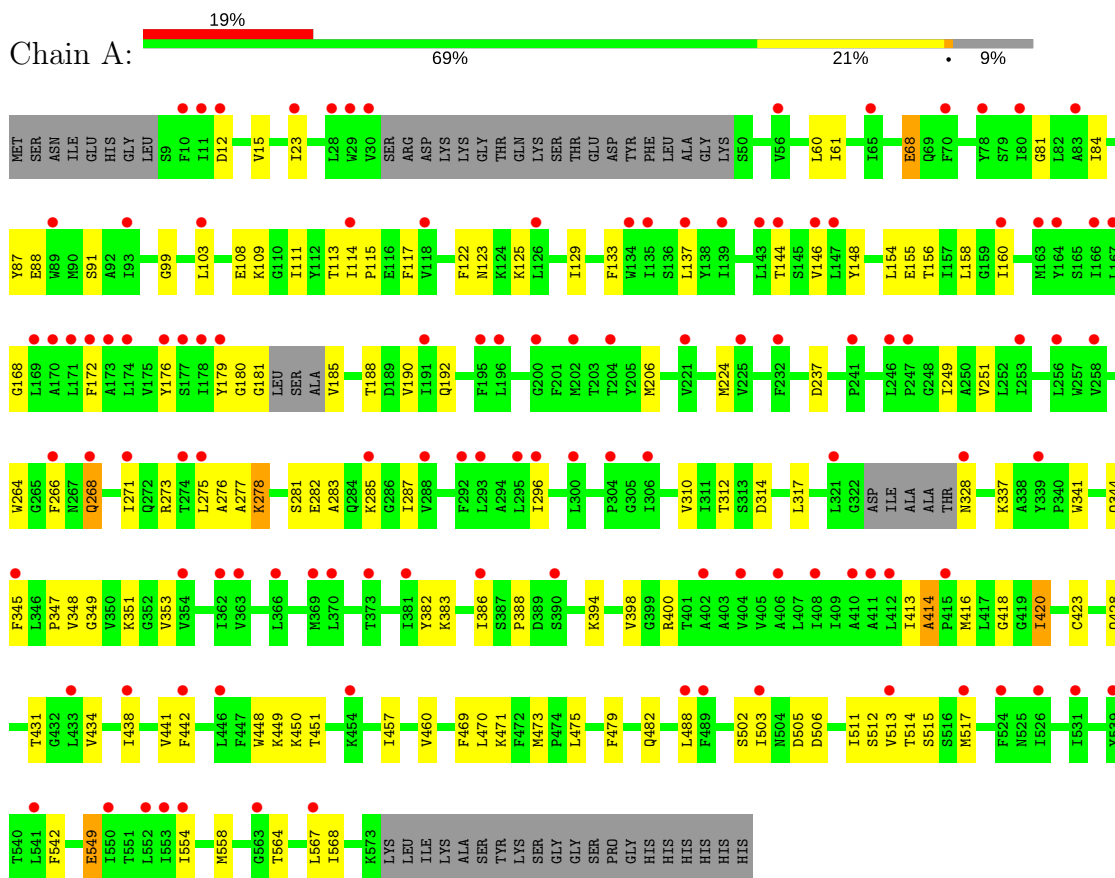
- Molecule 4 is water.

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

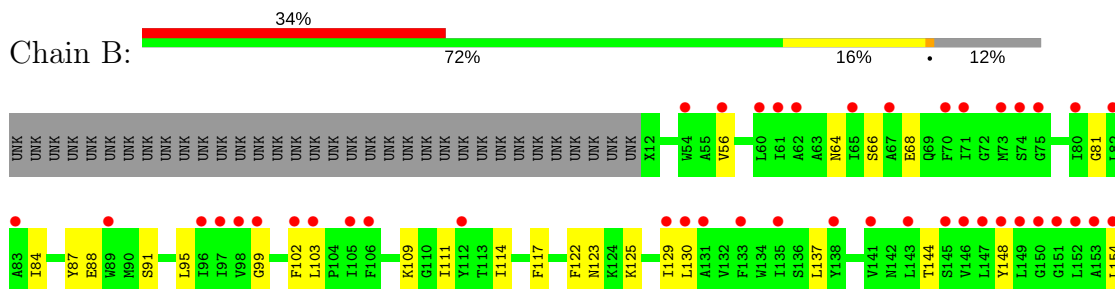
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

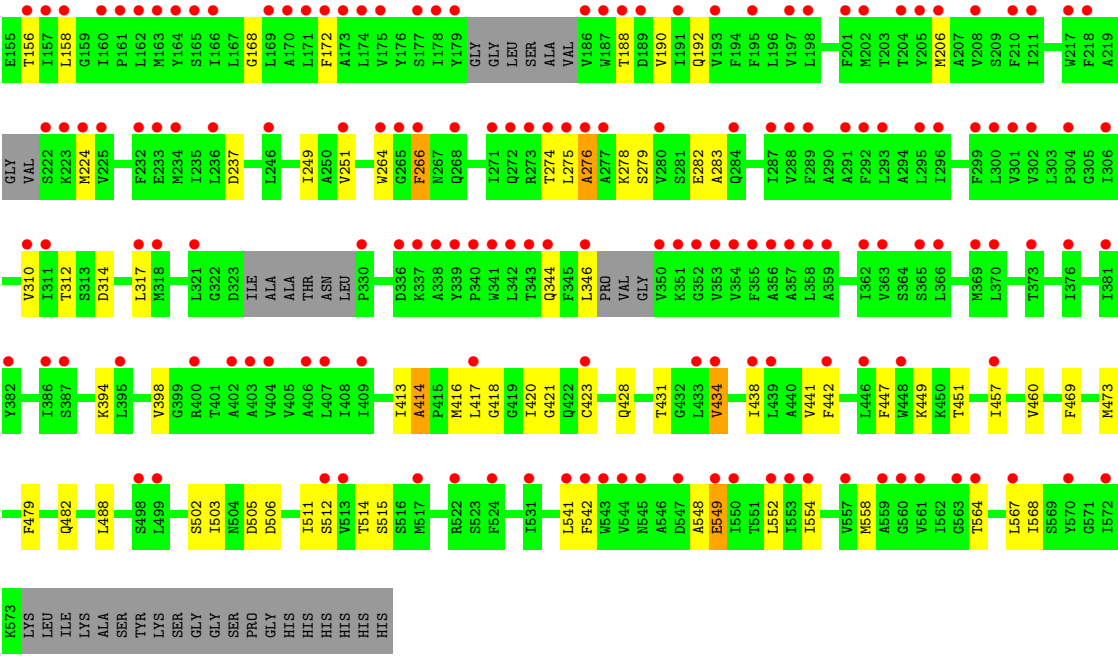
#### • Molecule 1: SODIUM/GLUCOSE COTRANSPORTER



#### • Molecule 2: SODIUM/GLUCOSE COTRANSPORTER







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.30Å 112.68Å 238.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.01 – 2.73 68.01 – 2.69	Depositor EDS
% Data completeness (in resolution range)	(Not available) (68.01-2.73) 96.5 (68.01-2.69)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.251 , 0.274 0.277 , 0.319	Depositor DCC
$R_{free}$ test set	3135 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.6	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	8090	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: PEG

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	0.51	0/4210	0.72	2/5741 (0.0%)
2	B	0.46	0/3973	0.70	2/5413 (0.0%)
All	All	0.48	0/8183	0.71	4/11154 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	276	ALA	CB-CA-C	7.57	121.45	110.10
2	B	266	PHE	N-CA-C	6.79	129.35	111.00
1	A	268	GLN	CB-CA-C	5.43	121.26	110.40
1	A	348	VAL	N-CA-C	5.06	124.67	111.00

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	4107	0	4252	122	0
2	B	3957	0	4022	89	0
3	A	21	0	30	0	0
4	A	5	0	0	0	0
All	All	8090	0	8304	201	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 12.

All (201) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:CG2	1:A:115:PRO:HD3	1.82	1.09
1:A:502:SER:O	2:B:515:SER:HB2	1.64	0.98
2:B:148:TYR:CD2	2:B:417:LEU:HD22	2.00	0.96
1:A:81:GLY:O	1:A:84:ILE:HG22	1.65	0.96
2:B:81:GLY:O	2:B:84:ILE:HG22	1.65	0.95
2:B:148:TYR:CE1	2:B:418:GLY:HA2	2.02	0.95
1:A:114:ILE:HG23	1:A:115:PRO:HD3	1.47	0.94
2:B:541:LEU:HD11	2:B:548:ALA:HB3	1.52	0.91
2:B:114:ILE:HG13	2:B:266:PHE:O	1.70	0.91
1:A:413:ILE:O	1:A:416:MET:HG2	1.71	0.90
1:A:114:ILE:HG22	1:A:115:PRO:HD3	1.50	0.90
2:B:413:ILE:O	2:B:416:MET:HG2	1.72	0.89
1:A:108:GLU:HB2	1:A:517:MET:HE1	1.52	0.89
1:A:114:ILE:HD11	1:A:442:PHE:CE2	2.09	0.86
1:A:264:TRP:HE3	1:A:268:GLN:OE1	1.59	0.86
2:B:417:LEU:O	2:B:417:LEU:HD23	1.75	0.85
1:A:122:PHE:HE1	1:A:451:THR:HG22	1.42	0.84
1:A:341:TRP:O	1:A:344:GLN:HG2	1.77	0.84
2:B:122:PHE:HE1	2:B:451:THR:HG22	1.42	0.84
2:B:541:LEU:HD23	2:B:552:LEU:HD22	1.62	0.82
2:B:541:LEU:HD11	2:B:548:ALA:CB	2.10	0.82
1:A:99:GLY:HA2	1:A:103:LEU:HD12	1.61	0.81
1:A:114:ILE:HD11	1:A:442:PHE:CZ	2.15	0.81
1:A:264:TRP:CE3	1:A:268:GLN:OE1	2.34	0.81
2:B:114:ILE:CD1	2:B:266:PHE:O	2.28	0.81
2:B:148:TYR:CD2	2:B:417:LEU:CD2	2.63	0.81
2:B:99:GLY:HA2	2:B:103:LEU:HD12	1.62	0.79
1:A:60:LEU:HD22	1:A:268:GLN:NE2	1.98	0.79
1:A:114:ILE:HG23	1:A:115:PRO:CD	2.11	0.79
1:A:428:GLN:NE2	1:A:428:GLN:HA	1.99	0.78
1:A:108:GLU:OE1	1:A:517:MET:SD	2.40	0.78
1:A:103:LEU:HD11	1:A:271:ILE:HD11	1.66	0.77
2:B:114:ILE:CG1	2:B:266:PHE:O	2.32	0.77
1:A:176:TYR:O	1:A:180:GLY:HA3	1.85	0.76
1:A:502:SER:O	2:B:515:SER:CB	2.33	0.76
1:A:114:ILE:CG2	1:A:115:PRO:CD	2.62	0.75
2:B:417:LEU:HD21	2:B:423:CYS:SG	2.28	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ILE:HA	2:B:515:SER:OG	1.89	0.73
1:A:148:TYR:CE1	1:A:418:GLY:HA2	2.24	0.73
2:B:428:GLN:NE2	2:B:428:GLN:HA	2.02	0.73
1:A:434:VAL:HG12	1:A:438:ILE:HD12	1.71	0.72
1:A:206:MET:SD	1:A:345:PHE:CD2	2.86	0.69
1:A:266:PHE:CE1	1:A:442:PHE:HB3	2.27	0.69
1:A:185:VAL:O	1:A:185:VAL:HG12	1.93	0.68
1:A:283:ALA:O	1:A:287:ILE:HG12	1.94	0.68
2:B:148:TYR:CG	2:B:417:LEU:HD22	2.28	0.68
1:A:60:LEU:HD22	1:A:268:GLN:HE21	1.58	0.67
1:A:515:SER:HB2	2:B:502:SER:O	1.96	0.66
1:A:148:TYR:HE1	1:A:418:GLY:HA2	1.59	0.66
2:B:469:PHE:O	2:B:473:MET:HB2	1.96	0.66
1:A:190:VAL:HG13	1:A:568:ILE:HD12	1.77	0.65
1:A:469:PHE:O	1:A:473:MET:HB2	1.97	0.64
1:A:108:GLU:HB2	1:A:517:MET:CE	2.27	0.63
2:B:417:LEU:O	2:B:420:ILE:HG23	1.99	0.62
1:A:275:LEU:HD23	1:A:275:LEU:C	2.19	0.62
2:B:190:VAL:HG13	2:B:568:ILE:HD12	1.80	0.62
1:A:68:GLU:HG2	1:A:146:VAL:HG22	1.82	0.62
2:B:148:TYR:HE1	2:B:418:GLY:HA2	1.59	0.62
2:B:420:ILE:HG13	2:B:421:GLY:N	2.14	0.62
1:A:275:LEU:C	1:A:277:ALA:H	2.03	0.61
1:A:206:MET:SD	1:A:345:PHE:HD2	2.24	0.61
1:A:266:PHE:CZ	1:A:442:PHE:HB3	2.35	0.61
1:A:449:LYS:HE2	1:A:506:ASP:CG	2.21	0.61
1:A:488:LEU:HD11	2:B:488:LEU:HD11	1.83	0.60
1:A:383:LYS:O	1:A:388:PRO:HA	2.02	0.60
2:B:114:ILE:HD11	2:B:266:PHE:O	2.02	0.59
1:A:137:LEU:HD21	1:A:431:THR:HA	1.85	0.59
1:A:275:LEU:HD23	1:A:275:LEU:O	2.04	0.58
2:B:449:LYS:HE2	2:B:506:ASP:CG	2.23	0.58
1:A:434:VAL:HG12	1:A:438:ILE:CD1	2.32	0.58
2:B:275:LEU:C	2:B:275:LEU:HD23	2.24	0.58
2:B:420:ILE:HD11	2:B:423:CYS:HA	1.86	0.58
2:B:102:PHE:HE1	2:B:266:PHE:CE2	2.23	0.57
1:A:413:ILE:HG23	1:A:416:MET:SD	2.44	0.57
1:A:15:VAL:CG1	1:A:353:VAL:HG22	2.35	0.56
1:A:449:LYS:HE2	1:A:506:ASP:OD2	2.05	0.56
2:B:122:PHE:HE1	2:B:451:THR:CG2	2.16	0.56
1:A:512:SER:HB2	2:B:505:ASP:OD1	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:514:THR:HG22	2:B:515:SER:N	2.20	0.56
1:A:382:TYR:HA	1:A:386:ILE:HG12	1.87	0.56
1:A:176:TYR:C	1:A:180:GLY:HA3	2.26	0.55
1:A:224:MET:HB2	1:A:310:VAL:HG21	1.88	0.55
2:B:224:MET:HB2	2:B:310:VAL:HG21	1.87	0.55
2:B:449:LYS:HE2	2:B:506:ASP:OD2	2.06	0.55
1:A:314:ASP:HB3	1:A:317:LEU:HB2	1.89	0.55
1:A:282:GLU:O	1:A:285:LYS:HB2	2.06	0.54
1:A:103:LEU:HD11	1:A:271:ILE:CD1	2.36	0.54
1:A:168:GLY:O	1:A:172:PHE:CG	2.60	0.54
1:A:268:GLN:HG2	1:A:271:ILE:H	1.71	0.54
2:B:168:GLY:O	2:B:172:PHE:CG	2.61	0.54
1:A:108:GLU:CB	1:A:517:MET:HE1	2.34	0.54
2:B:420:ILE:CD1	2:B:423:CYS:HA	2.38	0.54
2:B:314:ASP:HB3	2:B:317:LEU:HB2	1.90	0.53
1:A:281:SER:O	1:A:285:LYS:HG3	2.09	0.52
2:B:434:VAL:HG13	2:B:438:ILE:HD12	1.91	0.52
2:B:148:TYR:CZ	2:B:418:GLY:HA2	2.43	0.52
1:A:505:ASP:OD1	2:B:512:SER:HB2	2.09	0.52
1:A:87:TYR:OH	1:A:428:GLN:HG3	2.09	0.52
1:A:513:VAL:O	1:A:514:THR:OG1	2.26	0.52
1:A:122:PHE:CE1	1:A:451:THR:HG22	2.33	0.52
2:B:123:ASN:HD21	2:B:457:ILE:HD11	1.75	0.51
1:A:206:MET:CE	1:A:345:PHE:HD2	2.23	0.51
2:B:122:PHE:CE1	2:B:451:THR:HG22	2.33	0.51
2:B:87:TYR:OH	2:B:428:GLN:HG3	2.11	0.51
1:A:176:TYR:HA	1:A:180:GLY:HA3	1.93	0.51
2:B:137:LEU:HD21	2:B:431:THR:HA	1.92	0.51
2:B:111:ILE:HG21	2:B:117:PHE:HB2	1.92	0.51
2:B:541:LEU:CD1	2:B:548:ALA:HB3	2.33	0.51
1:A:479:PHE:O	1:A:482:GLN:HB2	2.12	0.51
1:A:113:THR:HG22	1:A:273:ARG:NH2	2.26	0.50
1:A:420:ILE:HD11	1:A:423:CYS:HA	1.93	0.50
1:A:449:LYS:NZ	1:A:506:ASP:OD2	2.44	0.50
1:A:564:THR:O	1:A:568:ILE:HG12	2.11	0.50
1:A:275:LEU:HG	1:A:283:ALA:CB	2.41	0.50
1:A:114:ILE:HG23	1:A:115:PRO:N	2.25	0.50
1:A:185:VAL:O	1:A:185:VAL:CG1	2.60	0.50
1:A:108:GLU:CB	1:A:517:MET:CE	2.90	0.49
1:A:113:THR:CG2	1:A:273:ARG:HH21	2.24	0.49
1:A:434:VAL:CG1	1:A:438:ILE:CD1	2.90	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:GLY:O	2:B:172:PHE:CD2	2.66	0.49
2:B:438:ILE:HG22	2:B:442:PHE:CE2	2.48	0.49
2:B:56:VAL:HG13	2:B:274:THR:HG22	1.95	0.49
2:B:154:LEU:HB3	2:B:158:LEU:HD12	1.95	0.49
1:A:449:LYS:CE	1:A:506:ASP:OD2	2.61	0.49
1:A:111:ILE:HG21	1:A:117:PHE:HB2	1.95	0.49
1:A:168:GLY:O	1:A:172:PHE:CD2	2.66	0.49
1:A:275:LEU:HG	1:A:283:ALA:HB3	1.94	0.48
1:A:154:LEU:HB3	1:A:158:LEU:HD12	1.95	0.48
2:B:564:THR:O	2:B:568:ILE:HG12	2.13	0.48
2:B:449:LYS:NZ	2:B:506:ASP:OD2	2.44	0.48
2:B:514:THR:CG2	2:B:515:SER:N	2.77	0.48
1:A:88:GLU:O	1:A:91:SER:HB2	2.14	0.47
2:B:542:PHE:HD2	2:B:549:GLU:HG3	1.79	0.47
2:B:420:ILE:HD11	2:B:423:CYS:CA	2.45	0.47
2:B:102:PHE:HE1	2:B:266:PHE:HE2	1.63	0.47
1:A:133:PHE:HB3	1:A:434:VAL:HG11	1.96	0.47
1:A:470:LEU:HB3	1:A:482:GLN:HG2	1.96	0.47
1:A:176:TYR:CA	1:A:180:GLY:HA3	2.44	0.47
2:B:88:GLU:O	2:B:91:SER:HB2	2.14	0.47
1:A:349:GLY:O	1:A:353:VAL:HG23	2.15	0.47
2:B:66:SER:HB3	2:B:68:GLU:OE1	2.15	0.47
2:B:275:LEU:HD23	2:B:275:LEU:O	2.14	0.47
2:B:102:PHE:CE1	2:B:266:PHE:CE2	3.03	0.47
1:A:394:LYS:O	1:A:398:VAL:HG23	2.14	0.47
1:A:268:GLN:HG2	1:A:271:ILE:N	2.30	0.46
2:B:449:LYS:CE	2:B:506:ASP:OD2	2.63	0.46
2:B:394:LYS:O	2:B:398:VAL:HG23	2.15	0.46
1:A:144:THR:HG23	1:A:414:ALA:HA	1.98	0.46
2:B:278:LYS:HG2	2:B:282:GLU:HG2	1.98	0.46
1:A:278:LYS:HG2	1:A:282:GLU:HG2	1.97	0.46
2:B:554:ILE:O	2:B:558:MET:HG2	2.16	0.46
2:B:123:ASN:HD21	2:B:457:ILE:CD1	2.28	0.46
2:B:148:TYR:CE2	2:B:417:LEU:CD2	2.99	0.45
1:A:156:THR:HG23	1:A:328:ASN:HB3	1.98	0.45
1:A:122:PHE:HE1	1:A:451:THR:CG2	2.19	0.45
1:A:515:SER:OG	2:B:503:ILE:HA	2.17	0.45
1:A:434:VAL:CG1	1:A:438:ILE:HD11	2.47	0.45
2:B:122:PHE:CE1	2:B:451:THR:CG2	2.98	0.45
2:B:417:LEU:HG	2:B:420:ILE:HG21	2.00	0.44
1:A:103:LEU:HD21	1:A:271:ILE:HG12	1.97	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:PRO:O	1:A:351:LYS:HB2	2.18	0.44
1:A:473:MET:HB3	1:A:475:LEU:HG	2.00	0.44
1:A:123:ASN:HD21	1:A:457:ILE:HD11	1.83	0.44
1:A:109:LYS:HD2	1:A:511:ILE:HG12	2.00	0.44
1:A:554:ILE:O	1:A:558:MET:HG2	2.18	0.44
1:A:188:THR:O	1:A:192:GLN:HB2	2.18	0.43
2:B:95:LEU:HD21	2:B:264:TRP:CE3	2.53	0.43
2:B:156:THR:O	2:B:344:GLN:OE1	2.36	0.43
1:A:514:THR:O	1:A:515:SER:HB3	2.19	0.43
1:A:122:PHE:CE1	1:A:451:THR:CG2	3.00	0.43
1:A:542:PHE:CD2	1:A:549:GLU:HG3	2.54	0.43
2:B:541:LEU:CD2	2:B:552:LEU:HD22	2.41	0.42
1:A:61:ILE:HA	1:A:61:ILE:HD12	1.95	0.42
1:A:155:GLU:OE1	1:A:337:LYS:NZ	2.52	0.42
2:B:188:THR:O	2:B:192:GLN:HB2	2.19	0.42
2:B:144:THR:HG23	2:B:414:ALA:HA	2.01	0.42
1:A:448:TRP:CZ3	2:B:447:PHE:O	2.73	0.42
1:A:160:ILE:HG13	1:A:160:ILE:H	1.71	0.42
1:A:420:ILE:CD1	1:A:423:CYS:HA	2.50	0.42
1:A:514:THR:HG22	1:A:515:SER:N	2.35	0.42
2:B:541:LEU:HD11	2:B:548:ALA:HB1	1.95	0.42
1:A:113:THR:CG2	1:A:273:ARG:NH2	2.82	0.41
2:B:64:ASN:HD21	2:B:264:TRP:HZ2	1.69	0.41
2:B:479:PHE:HA	2:B:482:GLN:NE2	2.35	0.41
1:A:87:TYR:CZ	1:A:428:GLN:HG3	2.55	0.41
1:A:471:LYS:HG2	1:A:482:GLN:OE1	2.20	0.41
1:A:450:LYS:HZ1	2:B:449:LYS:HG3	1.84	0.41
1:A:268:GLN:NE2	1:A:271:ILE:HB	2.36	0.41
1:A:181:GLY:HA2	1:A:400:ARG:HH12	1.86	0.41
2:B:109:LYS:HD2	2:B:511:ILE:HG12	2.03	0.41
2:B:148:TYR:CE2	2:B:417:LEU:HD23	2.56	0.41
1:A:179:TYR:CD2	1:A:179:TYR:N	2.89	0.41
1:A:113:THR:HG22	1:A:273:ARG:HH21	1.86	0.41
1:A:514:THR:CG2	1:A:515:SER:N	2.84	0.41
1:A:125:LYS:O	1:A:129:ILE:HG12	2.21	0.40
2:B:125:LYS:O	2:B:129:ILE:HG12	2.21	0.40
2:B:275:LEU:HG	2:B:283:ALA:CB	2.51	0.40
2:B:206:MET:HG3	2:B:346:LEU:HD23	2.02	0.40
1:A:275:LEU:CD2	1:A:275:LEU:C	2.89	0.40
2:B:417:LEU:CD2	2:B:417:LEU:O	2.59	0.40
2:B:130:LEU:HD22	2:B:438:ILE:HG12	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	530/593 (89%)	505 (95%)	22 (4%)	3 (1%)	28	54
2	B	496/593 (84%)	469 (95%)	25 (5%)	2 (0%)	38	65
All	All	1026/1186 (86%)	974 (95%)	47 (5%)	5 (0%)	32	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	LYS
2	B	276	ALA
1	A	276	ALA
1	A	414	ALA
2	B	414	ALA

### 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	434/478 (91%)	421 (97%)	13 (3%)	46	75
2	B	410/436 (94%)	400 (98%)	10 (2%)	54	81
All	All	844/914 (92%)	821 (97%)	23 (3%)	50	78

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	23	ILE
1	A	68	GLU
1	A	237	ASP
1	A	249	ILE
1	A	251	VAL
1	A	296	ILE
1	A	312	THR
1	A	420	ILE
1	A	441	VAL
1	A	460	VAL
1	A	549	GLU
1	A	567	LEU
2	B	237	ASP
2	B	249	ILE
2	B	251	VAL
2	B	279	SER
2	B	312	THR
2	B	434	VAL
2	B	441	VAL
2	B	460	VAL
2	B	549	GLU
2	B	567	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	A	268	GLN
1	A	422	GLN
1	A	428	GLN
1	A	525	ASN
2	B	245	ASN
2	B	422	GLN
2	B	428	GLN
2	B	525	ASN

### 5.3.3 RNA ⓘ

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](#)

3 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	PEG	A	1574	-	6,6,6	0.64	0	5,5,5	0.70	0
3	PEG	A	1575	-	6,6,6	0.56	0	5,5,5	0.73	0
3	PEG	A	1576	-	6,6,6	0.52	0	5,5,5	0.94	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	PEG	A	1574	-	-	0/4/4/4	0/0/0/0
3	PEG	A	1575	-	-	0/4/4/4	0/0/0/0
3	PEG	A	1576	-	-	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.

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	538/593 (90%)	1.26	114 (21%) <b>1</b> <b>1</b>	44, 88, 129, 164	0
2	B	506/593 (85%)	2.07	203 (40%) <b>0</b> <b>0</b>	67, 131, 188, 241	0
All	All	1044/1186 (88%)	1.65	317 (30%) <b>0</b> <b>0</b>	44, 104, 174, 241	0

All (317) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	353	VAL	13.8
2	B	354	VAL	10.1
2	B	218	PHE	10.0
2	B	179	TYR	9.4
2	B	154	LEU	8.9
2	B	175	VAL	8.6
2	B	217	TRP	8.6
2	B	339	TYR	8.6
2	B	395	LEU	8.3
2	B	276	ALA	8.1
2	B	195	PHE	7.9
2	B	189	ASP	7.6
2	B	160	ILE	7.5
2	B	340	PRO	7.4
2	B	161	PRO	7.2
2	B	233	GLU	7.2
2	B	60	LEU	7.1
2	B	222	SER	7.1
2	B	166	ILE	7.0
2	B	318	MET	7.0
2	B	158	LEU	7.0
2	B	187	TRP	7.0
2	B	198	LEU	7.0
2	B	274	THR	6.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	173	ALA	6.8
2	B	202	MET	6.8
2	B	404	VAL	6.7
2	B	169	LEU	6.7
2	B	358	LEU	6.7
2	B	317	LEU	6.6
2	B	177	SER	6.5
2	B	211	ILE	6.4
2	B	350	VAL	6.4
2	B	232	PHE	6.4
2	B	103	LEU	6.3
2	B	205	TYR	6.2
2	B	567	LEU	6.1
2	B	550	ILE	6.0
1	A	10	PHE	6.0
2	B	149	LEU	5.9
2	B	356	ALA	5.8
2	B	150	GLY	5.6
2	B	272	GLN	5.5
1	A	166	ILE	5.5
2	B	373	THR	5.4
2	B	352	GLY	5.4
2	B	162	LEU	5.4
2	B	547	ASP	5.3
2	B	311	ILE	5.3
2	B	225	VAL	5.3
2	B	133	PHE	5.1
1	A	147	LEU	5.1
2	B	82	LEU	5.1
2	B	201	PHE	5.1
2	B	549	GLU	5.1
2	B	554	ILE	5.1
2	B	359	ALA	5.1
2	B	174	LEU	5.0
2	B	355	PHE	5.0
2	B	343	THR	5.0
2	B	553	ILE	5.0
2	B	197	VAL	4.9
2	B	366	LEU	4.9
1	A	164	TYR	4.9
1	A	12	ASP	4.9
2	B	369	MET	4.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	552	LEU	4.8
2	B	56	VAL	4.8
2	B	266	PHE	4.7
2	B	300	LEU	4.7
2	B	351	LYS	4.6
1	A	176	TYR	4.6
2	B	376	ILE	4.5
2	B	102	PHE	4.5
2	B	400	ARG	4.4
2	B	560	GLY	4.4
1	A	345	PHE	4.4
2	B	210	PHE	4.3
2	B	273	ARG	4.3
2	B	363	VAL	4.3
1	A	366	LEU	4.2
2	B	156	THR	4.2
2	B	146	VAL	4.2
2	B	164	TYR	4.2
2	B	362	ILE	4.2
2	B	143	LEU	4.2
1	A	170	ALA	4.2
2	B	288	VAL	4.1
1	A	370	LEU	4.1
1	A	442	PHE	4.1
1	A	563	GLY	4.1
1	A	172	PHE	4.1
2	B	71	ILE	4.1
1	A	531	ILE	4.0
2	B	271	ILE	4.0
1	A	363	VAL	4.0
2	B	382	TYR	3.9
2	B	172	PHE	3.9
2	B	208	VAL	3.9
2	B	191	ILE	3.9
2	B	541	LEU	3.9
1	A	143	LEU	3.9
2	B	545	ASN	3.9
1	A	169	LEU	3.8
2	B	147	LEU	3.8
1	A	135	ILE	3.8
2	B	65	ILE	3.8
2	B	341	TRP	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	302	VAL	3.8
2	B	157	ILE	3.7
2	B	151	GLY	3.7
2	B	70	PHE	3.7
1	A	321	LEU	3.7
2	B	264	TRP	3.7
1	A	526	ILE	3.7
2	B	570	TYR	3.7
2	B	265	GLY	3.7
2	B	321	LEU	3.6
2	B	513	VAL	3.6
2	B	403	ALA	3.6
1	A	513	VAL	3.6
1	A	167	LEU	3.6
2	B	148	TYR	3.6
2	B	80	ILE	3.5
2	B	557	VAL	3.5
2	B	289	PHE	3.5
1	A	268	GLN	3.5
1	A	173	ALA	3.5
1	A	369	MET	3.5
1	A	103	LEU	3.5
2	B	386	ILE	3.5
2	B	346	LEU	3.4
2	B	406	ALA	3.4
2	B	564	THR	3.4
1	A	195	PHE	3.4
1	A	412	LEU	3.4
2	B	99	GLY	3.4
1	A	179	TYR	3.4
2	B	561	VAL	3.4
2	B	186	VAL	3.4
1	A	415	PRO	3.3
2	B	370	LEU	3.3
1	A	70	PHE	3.3
2	B	188	THR	3.3
2	B	54	TRP	3.2
2	B	89	TRP	3.2
2	B	442	PHE	3.2
2	B	105	ILE	3.2
1	A	288	VAL	3.2
1	A	296	ILE	3.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	30	VAL	3.1
2	B	544	VAL	3.1
1	A	410	ALA	3.1
2	B	330	PRO	3.1
1	A	386	ILE	3.1
2	B	295	LEU	3.1
2	B	129	ILE	3.1
2	B	145	SER	3.1
1	A	139	ILE	3.0
1	A	292	PHE	3.0
2	B	152	LEU	3.0
1	A	550	ILE	3.0
1	A	554	ILE	3.0
2	B	563	GLY	3.0
2	B	275	LEU	3.0
2	B	310	VAL	3.0
2	B	409	ILE	3.0
1	A	567	LEU	3.0
2	B	417	LEU	3.0
2	B	171	LEU	3.0
1	A	178	ILE	3.0
2	B	67	ALA	3.0
2	B	338	ALA	3.0
1	A	160	ILE	2.9
1	A	408	ILE	2.9
2	B	304	PRO	2.9
1	A	438	ILE	2.9
1	A	552	LEU	2.9
2	B	336	ASP	2.9
1	A	274	THR	2.9
1	A	553	ILE	2.9
1	A	29	TRP	2.9
2	B	306	ILE	2.9
2	B	234	MET	2.8
2	B	284	GLN	2.8
2	B	423	CYS	2.8
1	A	433	LEU	2.8
2	B	165	SER	2.8
1	A	114	ILE	2.8
1	A	362	ILE	2.8
2	B	287	ILE	2.8
2	B	292	PHE	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	542	PHE	2.8
1	A	390	SER	2.8
2	B	381	ILE	2.8
2	B	365	SER	2.8
2	B	178	ILE	2.8
2	B	402	ALA	2.7
1	A	402	ALA	2.7
1	A	411	ALA	2.7
2	B	251	VAL	2.7
1	A	163	MET	2.7
1	A	293	LEU	2.7
2	B	224	MET	2.7
1	A	78	TYR	2.7
1	A	295	LEU	2.7
2	B	543	TRP	2.7
2	B	291	ALA	2.7
1	A	65	ILE	2.7
1	A	381	ILE	2.7
2	B	299	PHE	2.7
1	A	221	VAL	2.7
1	A	503	ILE	2.7
2	B	153	ALA	2.7
1	A	454	LYS	2.7
1	A	300	LEU	2.6
1	A	80	ILE	2.6
1	A	258	VAL	2.6
2	B	387	SER	2.6
2	B	135	ILE	2.6
2	B	277	ALA	2.6
2	B	163	MET	2.6
1	A	541	LEU	2.6
1	A	89	TRP	2.6
1	A	328	ASN	2.6
1	A	200	GLY	2.6
2	B	357	ALA	2.5
2	B	141	VAL	2.5
1	A	517	MET	2.5
2	B	512	SER	2.5
2	B	223	LYS	2.5
2	B	438	ILE	2.5
2	B	268	GLN	2.5
2	B	524	PHE	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	83	ALA	2.5
2	B	559	ALA	2.5
2	B	204	THR	2.5
1	A	171	LEU	2.5
2	B	246	LEU	2.5
2	B	98	VAL	2.4
1	A	225	VAL	2.4
2	B	301	VAL	2.4
1	A	196	LEU	2.4
1	A	118	VAL	2.4
2	B	193	VAL	2.4
2	B	130	LEU	2.4
1	A	354	VAL	2.4
2	B	106	PHE	2.4
2	B	448	TRP	2.4
1	A	93	ILE	2.4
1	A	144	THR	2.4
1	A	191	ILE	2.4
1	A	285	LYS	2.3
1	A	56	VAL	2.3
2	B	206	MET	2.3
1	A	275	LEU	2.3
2	B	498	SER	2.3
1	A	232	PHE	2.3
2	B	61	ILE	2.3
2	B	572	ILE	2.3
1	A	256	LEU	2.3
2	B	457	ILE	2.3
2	B	446	LEU	2.3
2	B	112	TYR	2.2
1	A	241	PRO	2.2
1	A	488	LEU	2.2
2	B	236	LEU	2.2
1	A	126	LEU	2.2
1	A	134	TRP	2.2
1	A	246	LEU	2.2
1	A	247	PRO	2.2
1	A	539	TYR	2.2
1	A	306	ILE	2.2
2	B	170	ALA	2.2
1	A	524	PHE	2.2
2	B	97	ILE	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	296	ILE	2.2
2	B	434	VAL	2.2
2	B	439	LEU	2.2
1	A	406	ALA	2.2
1	A	373	THR	2.2
1	A	404	VAL	2.2
2	B	280	VAL	2.2
1	A	28	LEU	2.2
1	A	304	PRO	2.2
1	A	23	ILE	2.2
2	B	531	ILE	2.1
1	A	446	LEU	2.1
2	B	344	GLN	2.1
1	A	202	MET	2.1
1	A	11	ILE	2.1
2	B	433	LEU	2.1
2	B	138	TYR	2.1
2	B	342	LEU	2.1
2	B	62	ALA	2.1
2	B	73	MET	2.1
1	A	489	PHE	2.1
1	A	339	TYR	2.1
2	B	96	ILE	2.1
2	B	522	ARG	2.1
1	A	174	LEU	2.1
1	A	271	ILE	2.1
2	B	337	LYS	2.1
1	A	204	THR	2.1
2	B	499	LEU	2.1
2	B	131	ALA	2.1
1	A	177	SER	2.1
1	A	137	LEU	2.0
1	A	83	ALA	2.0
2	B	407	LEU	2.0
1	A	146	VAL	2.0
2	B	74	SER	2.0
2	B	75	GLY	2.0
1	A	266	PHE	2.0
1	A	253	ILE	2.0
2	B	517	MET	2.0
2	B	293	LEU	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	PEG	A	1576	7/7	0.65	0.60	5.98	45,63,205,221	0
3	PEG	A	1575	7/7	0.41	0.46	4.82	55,128,205,249	0
3	PEG	A	1574	7/7	0.29	0.51	3.29	121,207,245,253	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.